ASSOCIATION POUR LE DÉVELOPPEMENT DE L'ENSEIGNEMENT
ET DE LA RECHERCHE EN SYSTÉMATIQUE APPLIQUÉE

MELISSA

Gas - Liquid equilibrium in global simulator
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1. INTRODUCTION

The aim of this study is to add the gas-liquid equilibria to the global simulator (fig. 1). The model was built by L. Poughon of LGCB (TN 17.1 and 23.1) upon the theory of ideal behaviour of gases and solutions.

A partition coefficient is defined for water, acetic acid, butyric acid, O_2, N_2, CO_2 and NH_3. The dissociation effect is taken into account for the weak electrolytes.

The system of non linear equations is solved by means of an iterative algorithm whose results are quite similar to those of Prosim (ProSim S.A., France).

An example of simulation is given, with the assumptions of the TN 28.3 (N. Fulget, ADERSA) :

- the flow rates of food, oxygen and water at the input of the compartment 5 (crew) fit the need of energy of 3000 kcal/day/person for a crew of 3 persons ;
- the key elements are completely transformed.

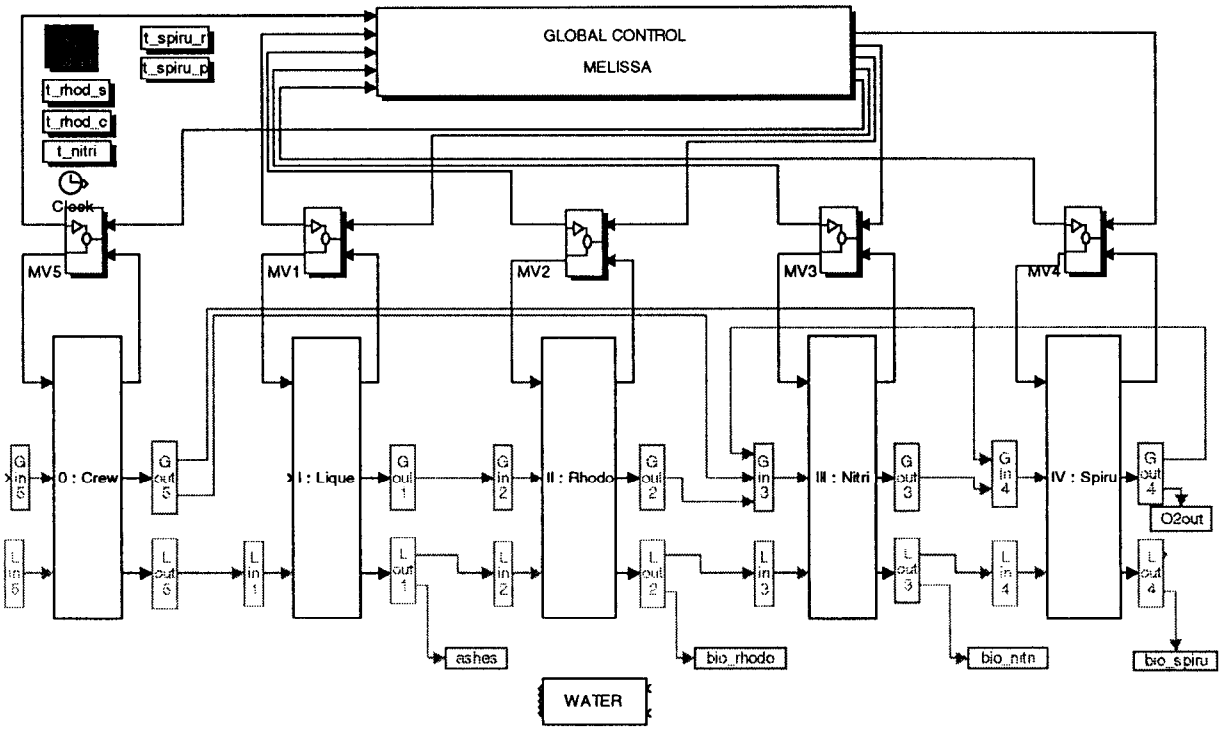

Figure 1 : Global simulator

2. GAS-LIQUID EQUILIBRIUM

2.1. Recall of the equations

The model is extracted from the technical notes 17.1 and 23.1 (L. Poughon, LGCB).

The gas-liquid equilibrium of each compound i is characterized by the partition coefficient, k_i, function of temperature :

$$k_i = \frac{y_i}{x_i}$$

where y_i = molar fraction of compound i in the gaseous phase
x_i = molar fraction of compound i in the liquid phase

If the compound i is a weak electrolyte, it is judicious, for the simplification of calculation, to count the dissociated form and the non dissociated one together, and to modify consequently the definition of k_i.

Given a weak electrolyte AH. It dissociates in water according to the reaction :

$$AH \rightleftarrows A^- + H^+$$

whose equilibrium constant, K_a, is expressed by :

$$Ka = \frac{[A^-].[H^+]}{[AH]}$$

Given k and k^{ap} : partition coefficient of AH and AH + A^-, respectively
x and x^{ap} : molar fraction of AH and AH + A^- in liquid phase
y : molar fraction of AH in gaseous phase

By definition $k = \frac{y}{x}$ and $k^{ap} = \frac{y}{x^{ap}}$.

With the assumption that the dissociation and the pH control (which is done by addition of strong acid or base) do not modify the total number of mols, the expression of x^{ap} is directly :

$$x^{ap} = x(1 + \xi) \qquad \text{with} \quad \xi = \frac{[A^-]}{[AH]}$$

For each weak electrolyte i, the new expression of k_i, k_i^{ap}, which takes into account the pH and the dissociation constant K_{ai} is then expressed by :

$$k_i^{ap} = k_i \frac{1}{1 + \xi_i} \qquad \text{with} \quad \xi_i = \frac{K_{ai}}{10^{-pH}} \left(\text{deduced from : } \frac{[A^-]}{[AH]} = \frac{K_{ai}}{10^{-pH}} \right)$$

Remark : *If the compound i exists only under the non-dissociated form,* $k_i^{ap} = k_i$.

- System of equations :

As in TN 17.1, each compartment (from 1 to 4) is extended with a flash where the gas-liquid equilibria take place under 1 atmosphere.

Given, for each compound i :

- e_i : molar flow rate at the input of the flash
- a_i : molar flow rate at the output of the flash in the liquid phase
- b_i : molar flow rate at the output of the flash in the gaseous phase

For the N compounds of a compartment, the system of equations is composed of 2N relations with 2N unknowns :

$$\left| \begin{array}{ll} a_i + b_i = e_i & \\ \dfrac{b_i}{a_i} \cdot \dfrac{\sum a_i}{\sum b_i} = k_i & 1 \le i \le N \end{array} \right.$$

where k_i means k_i^{ap} defined in the previous paragraph, in order to simplify the writing.

2.2. Solution of the system of equations

The algorithm is iterative, and its programme, written in Matlab ® code, is detailed in annex 1.

Given $\qquad z_j = \dfrac{\sum e_i}{\sum a_{ij}}$

where a_{ij} is the value of a_i at the calculation step j. At the step j, the value of a_i depends on its value at j-1 :

$$a_{ij} = \frac{e_i}{1 + k_i (z_{j-1} - 1)}$$

The computation is stopped when $\dfrac{a_{ij} - a_{ij-1}}{a_{ij-1}} \le \varepsilon$ $\left(\text{here, } \varepsilon = 10^{-2}\right)$.

The initialization of a_i, a_{io}, is done according 2 different ways :

1. At the first instant of a simulation, the value of a_{io} is :

   - $a_{io} = 0$ for each gazeous compound i (0_2, $C0_2$, H_2 and N_2)
   - $a_{io} = e_i$ for any other compound i

2. In the run of a simulation, a_{io} at instant n is equal to the solution of a_i at previous instant n-1.

The solution depends on a convergence condition (whose detail is given in annex 2) :

$$v_1 \cdot v_2 > 0$$

with :

$$v_1 = \Sigma e_i(1 - k_i) \qquad 1 \leq i \leq N$$

$$v_2 = \Sigma e_i \left(1 - \frac{1}{k_i}\right)$$

3. SIMULATION RESULTS

3.1. Example of values of the partition coefficient for extreme pH values

In the case of a weak electrolyte, such as CO_2, the value of the partition coefficient k_{CO_2} is highly bound to the pH.

Here are the values of k_{CO_2} for extreme pH values at 293k :

$$pH = 4 \qquad k_{CO_2} = 1.411\ 10^{3}$$
$$pH = 10 \qquad k_{CO_2} = 2.458\ 10^{-1}$$

This is in complete agreement with the fact that CO_2 is dissolved (under the $CO_3^{=}$ form) in a basic solution and is turned into gas as a strong acid is added to the solution.

3.2. Simulation on the global simulator

This simulation is done with the assumptions of the TN 28.3 (N. Fulget, ADERSA) :

- the flow rates of food, oxygen and water at the input of the compartment 0 (crew) fit the need of energy of 3000 kcal/day/person for a crew of 3 persons (table 0) ;

- the key elements (see annex 3) are completely transformed ;
- the conditions of temperature and pH in each compartment are recalled in table 1.

	mol/h	g/h	g/day
food	3.1142	72.61	1742
0_2	3.48555	111.54	2677
H_20	10.4167	187.50	4500

Table 0 : Input flow of the crew compartment

Compartment	1	2	3	4
temperature (K)	330	303	303	309
pH	5	7	8	9.5

Table 1 : Temperature and pH in each compartment

For each compartment, the following tables give the output flow rates of each compound, expressed in 3 different units :

- total flow rate (part 1 of each table) ;
- flow rate in the liquid phase (part 2) ;
- flow rate in the gaseous phase (part 3).

The part 1 of the table gives also the value of k_i in the conditions of temperature and pH, for the compartments 1 to 4.

1_ total flow rate

	mole/h	g/h	g/day
2: faeces	9.5000e-02	1.6650e+00	3.9959e+01
3: urea	1.0358e-01	6.2148e+00	1.4916e+02
13: H2O	1.3082e+01	2.3548e+02	5.6515e+03
15: CO2	2.9157e+00	1.2829e+02	3.0790e+03

2_ flow rate in the liquid phase

	mole/h	g/h	g/day
2: faeces	9.5000e-02	1.6650e+00	3.9959e+01
3: urea	1.0358e-01	6.2148e+00	1.4916e+02
13: H2O	1.3082e+01	2.3548e+02	5.6515e+03

3_ flow rate in the gas phase

	mole/h	g/h	g/day
15: CO2	2.9157e+00	1.2829e+02	3.0790e+03

Table 2 :Output flow of compartment 0

1_ total flow rate

		mole/h	g/h	g/day	ki
4:	acetic acid	2.3750e-02	1.4250e+00	3.4200e+01	9.9507e-02
5:	butyric acid	5.9375e-03	5.2250e-01	1.2540e+01	3.9439e-03
13:	H2O	1.2886e+01	2.3195e+02	5.5667e+03	1.6965e-01
15:	CO2	1.2733e-01	5.6025e+00	1.3446e+02	3.0232e+03
16:	NH3	2.1718e-01	3.6921e+00	8.8610e+01	1.0832e-02
17:	H2	8.4669e-02	1.6934e-01	4.0641e+00	7.6398e+04

2_ flow rate in the liquid phase

		mole/h	g/h	g/day
4:	acetic acid	2.3705e-02	1.4223e+00	3.4135e+01
5:	butyric acid	5.9370e-03	5.2246e-01	1.2539e+01
13:	H2O	1.2844e+01	2.3119e+02	5.5486e+03
15:	CO2	2.1532e-03	9.4739e-02	2.2737e+00
16:	NH3	2.1714e-01	3.6913e+00	8.8592e+01
17:	H2	5.7592e-05	1.1518e-04	2.7644e-03

3_ flow rate in the gas phase

		mole/h	g/h	g/day
4:	acetic acid	4.5360e-05	2.7216e-03	6.5318e-02
5:	butyric acid	4.5028e-07	3.9625e-05	9.5100e-04
13:	H2O	4.1902e-02	7.5423e-01	1.8101e+01
15:	CO2	1.2518e-01	5.5078e+00	1.3219e+02
16:	NH3	4.5230e-05	7.6891e-04	1.8454e-02
17:	H2	8.4611e-02	1.6922e-01	4.0613e+00

Table 3 :Output flow of compartment 1

1_ total flow rate

	mole/h	g/h	g/day	ki
6: biomass rhodo	1.1058e-01	2.4018e+00	5.7643e+01	0.0000e+00
13: H2O	1.2988e+01	2.3379e+02	5.6110e+03	4.1288e-02
15: CO2	8.7996e-02	3.8718e+00	9.2923e+01	3.2918e+02
16: NH3	1.9402e-01	3.2984e+00	7.9162e+01	9.5637e-02

2_ flow rate in the liquid phase

	mole/h	g/h	g/day
6: biomass rhodo	1.1058e-01	2.4018e+00	5.7643e+01
13: H2O	1.2986e+01	2.3375e+02	5.6101e+03
15: CO2	3.8808e-02	1.7075e+00	4.0981e+01
16: NH3	1.9395e-01	3.2972e+00	7.9132e+01

3_ flow rate in the gas phase

	mole/h	g/h	g/day
6: biomass rhodo	0.0000e+00	0.0000e+00	0.0000e+00
13: H2O	2.0645e-03	3.7161e-02	8.9187e-01
15: CO2	4.9188e-02	2.1643e+00	5.1942e+01
16: NH3	7.1422e-05	1.2142e-03	2.9140e-02

Table 4 :Output flow of compartment 2

1_ total flow rate

	mole/h	g/h	g/day	ki
7: biomass nitri	1.2996e-02	2.8905e-01	6.9373e+00	0.0000e+00
13: H2O	1.2417e+01	2.2351e+02	5.3641e+03	4.1288e-02
14: O2	1.3111e-01	4.1955e+00	1.0069e+02	4.5990e+04
15: CO2	2.9907e+00	1.3159e+02	3.1582e+03	3.9006e+01
19: HNO3	1.9143e-01	1.2060e+01	2.8945e+02	0.0000e+00

2_ flow rate in the liquid phase

	mole/h	g/h	g/day
7: biomass nitri	1.2996e-02	2.8905e-01	6.9373e+00
13: H2O	1.2300e+01	2.2141e+02	5.3138e+03
14: O2	1.2426e-05	3.9762e-04	9.5429e-03
15: CO2	3.0063e-01	1.3228e+01	3.1746e+02
19: HNO3	1.9143e-01	1.2060e+01	2.8945e+02

3_ flow rate in the gas phase

	mole/h	g/h	g/day
7: biomass nitri	0.0000e+00	0.0000e+00	0.0000e+00
13: H2O	1.1651e-01	2.0971e+00	5.0330e+01
14: O2	1.3110e-01	4.1951e+00	1.0068e+02
15: CO2	2.6901e+00	1.1836e+02	2.8407e+03
19: HNO3	0.0000e+00	0.0000e+00	0.0000e+00

Table 5 :Output flow of compartment 3

1_ total flow rate

	mole/h	g/h	g/day	ki
8: carbohydrate	3.5606e-01	8.9180e+00	2.1403e+02	0.0000e+00
9: fat	3.8462e-01	6.5300e+00	1.5672e+02	0.0000e+00
10: proteins	6.8685e-01	1.5284e+01	3.6682e+02	0.0000e+00
11: nucleic acid	4.2492e-02	1.2805e+00	3.0732e+01	0.0000e+00
12: EPS	1.2481e+00	3.6007e+01	8.6417e+02	0.0000e+00
13: H2O	2.2472e+03	4.0450e+04	9.7079e+05	5.7956e-02
14: O2	3.3025e+00	1.0568e+02	2.5363e+03	4.9856e+04
15: CO2	2.7264e-01	1.1996e+01	2.8790e+02	1.1726e+00
19: HNO3	3.2984e-03	2.0780e-01	4.9872e+00	0.0000e+00

2_ flow rate in the liquid phase

	mole/h	g/h	g/day
8: carbohydrate	3.5606e-01	8.9180e+00	2.1403e+02
9: fat	3.8462e-01	6.5300e+00	1.5672e+02
10: proteins	6.8685e-01	1.5284e+01	3.6682e+02
11: nucleic acid	4.2492e-02	1.2805e+00	3.0732e+01
12: EPS	1.2481e+00	3.6007e+01	8.6417e+02
13: H2O	2.2470e+03	4.0446e+04	9.7071e+05
14: O2	4.2527e-02	1.3609e+00	3.2661e+01
15: CO2	2.7215e-01	1.1974e+01	2.8739e+02
19: HNO3	3.2984e-03	2.0780e-01	4.9872e+00

3_ flow rate in the gas phase

	mole/h	g/h	g/day
8: carbohydrate	0.0000e+00	0.0000e+00	0.0000e+00
9: fat	0.0000e+00	0.0000e+00	0.0000e+00
10: proteins	0.0000e+00	0.0000e+00	0.0000e+00
11: nucleic acid	0.0000e+00	0.0000e+00	0.0000e+00
12: EPS	0.0000e+00	0.0000e+00	0.0000e+00
13: H2O	2.0023e-01	3.6042e+00	8.6500e+01
14: O2	3.2600e+00	1.0432e+02	2.5037e+03
15: CO2	4.9066e-04	2.1589e-02	5.1814e-01
19: HNO3	0.0000e+00	0.0000e+00	0.0000e+00

Table 6 :Output flow of compartment 4

4. CONCLUSION

The gas-liquid equilibria are modelled for the compartments 1 to 4 and for each of the 20 compounds choosen in TN 28.3 (N. Fulget, ADERSA).

The solution of the system of non linear equations is computed by means of an iterative algorithm which must comply with a convergence condition.

The results obtained from this way were compared with those of the software ProSim used by LGCB : the distances are generally lower than 1 ‰ (annex 4). If the convergence condition is not satisfied, the simulator gives a message. The algorithm is optimised to reduce the computation time.

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POUGHON L. "MELISSA SIMULATION AND MODELLING. Gas Streams". ESTEC/CONTRACT 8125/88/NL/FG, February 1994, TN17.1.

POUGHON L. "Modelling of the MELISSA artificial ecosystem. Gas liquid equilibrium modelling for VFA and ammonia". ESTEC/CONTRACT 8125/88/NL/FG, January 1995, TN 23.1.

ANNEXE 1

gl_equi.m

```
function y=gl_equi(u, ncom, kpart, compart)

% gas liquid equilibrium        (details in TN35.1)
%
%       y       vector of molar flow for gaseous and liquid phases (size 2*ncom)
%       u(1:ncom)       vector of molar flow for the input components
%       u(ncom+1:2*ncom)=u(1:ncom) at previous step
%       ncom    number of components
%       kpart   matrix of partition coefficients
%       compart number of the compartment

global name molmas

some = sum(u(1:ncom));

%> Convergence condition
%-----------------------
v1 = some - sum((u(1:ncom)) .* (kpart(:,compart)));
if compart ==1  % convergence condition for compartment 1 (Liquefying)
        ind = [4 5 13 15 16 17];
        v2 = sum(u(ind)) - sum((u(ind)) ./ (kpart(ind,compart)));
        if (v1*v2 <= 0)
                sprintf('No convergence condition compartment %g \n', compart)
        end
else            % partial convergence condition for the other compartments
        if (v1 >= 0)
                sprintf('No convergence condition compartment %g \n', compart)
        end
end

%> Initialization
%----------------
compteur = 0; compteurmax = 100;
epsilon = 1e-2;

aa0 = u(ncom+1:2*ncom);
zz = some / sum(aa0);
sc = zeros(ncom,1);     % stopping criterium


%> Calculation of the molar flow for the liquid phase
%----------------------------------------------------
while ~all(sc) & compteur < compteurmax
        compteur = compteur + 1;

        aa = u(1:ncom) ./ (1 + (zz - 1) * kpart(:,compart));
        zz = some / sum(aa);
        sc = (abs(aa-aa0) - epsilon * abs(aa)) <= zeros(ncom,1);
        aa0 = aa;
end

%> Results
%---------
if compteur >= compteurmax
        sprintf('No convergence in compartment %g \n', compart)
else
        %sprintf('Compart %g   Number of steps : %g \n',compart, compteur)
        yg = u(1:ncom)-aa;
        y=[yg;aa];
end
```

ANNEXE 2

Gas-liquid equilibrium
Condition of convergence

The notations are those of paragraph 2.

At the calculation step j,

$$z_j = \frac{\Sigma e_i}{\Sigma a_{ij}} \quad \text{and} \quad a_{ij} = \frac{e_i}{1 + k_i \left(z_{j-1} - 1\right)}$$

So :

$$z_j = \frac{\Sigma e_i}{\Sigma \dfrac{e_i}{1 + k_i \left(z_{j-1} - 1\right)}} \tag{1}$$

With the change of variable $u = z - 1$, (1) becomes :

$$\Sigma \frac{e_i}{1 + k_i \, u_{j-1}} = \frac{\Sigma e_i}{u_j + 1} \tag{2}$$

It is obvious that $a_i \leq e_i \quad \forall_i$

So : $z \geq 1$ and $u \geq 0$

There is convergence if $u_j = u_{j-1} = \alpha$

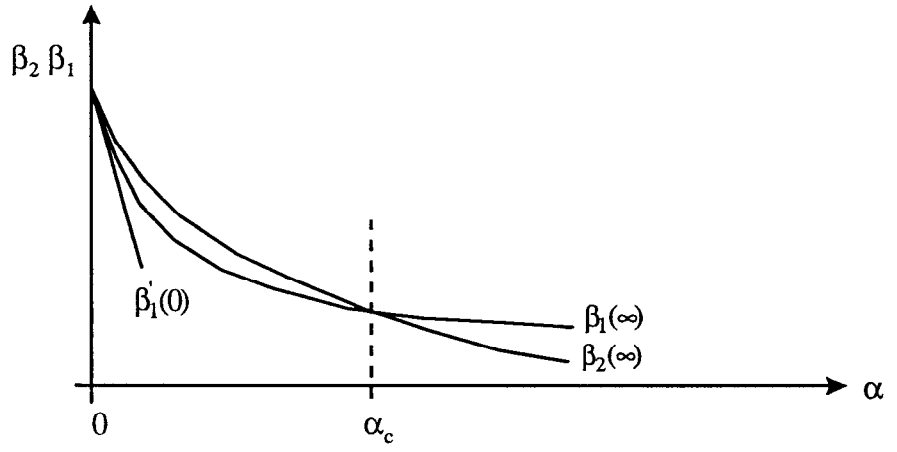
$$(2) \rightarrow \quad \Sigma \frac{e_i}{1 + k_i \, \alpha} = \frac{\Sigma e_i}{\alpha + 1} \tag{3}$$

It is equivalent to check that the curves β_1 and β_2, function of α,

$$\beta_1 = \Sigma \frac{e_i}{1 + k_i \alpha} \qquad \beta_2 = \frac{\Sigma e_i}{\alpha + 1}$$

have one and only one common point.

As all the e_i and k_i have the same sign (positive), the functions β_1 and β_2 are monotonous and decreasing.



The derivatives β_1' and β_2' are :

$$\beta_1' = -\Sigma \frac{e_i k_i}{(1 + k_i \alpha)^2} \qquad \beta_2' = -\frac{\Sigma e_i}{(\alpha + 1)^2}$$

$$\beta_1'(0) = -\Sigma e_i k_i \quad (4) \qquad \beta_2'(0) = -\Sigma e_i \quad (5)$$

Given $v_1 = \beta_1'(0) - \beta_2'(0) \rightarrow v_1 = \Sigma e_i - \Sigma e_i k_i$ (6)

When $\alpha \rightarrow \infty$, the distance $\beta_2 - \beta_1$ is :

$$v_2 = \frac{1}{\alpha} \left(\Sigma e_i - \Sigma \frac{e_i}{k_i} \right) \qquad (7)$$

Then the condition of convergence is :

$v_1 < 0$ and $v_2 < 0$

or

$v_1 > 0$ and $v_2 > 0$

That is equivalent to $v_1 \cdot v_2 > 0$ (8)

Remark : *At the output of the compartment 2, 3 and 4, the biomass concentration, whose* $k_i = 0$*, is never null.*

Then $v_2 < 0$

and the partial condition is $v_1 < 0$.

ANNEXE 3

Stoïchiometric equations in the different compartments

The key elements are underlined.

Compartment 0 : Crew

Degradation of food : stoichio 1 :

$$3.1142\ [\underline{food}] + 3.48555\ O_2 \downarrow$$
$$2.9157\ CO_2 + 0.10358\ CH_4ON_2 + 0.0950\ [faeces] + 2.6654\ H_2O$$

Compartment I : Liquefying

Degradation of faeces : stoichio 2 :

$$1\ [\underline{faeces}] + 0.975\ H_2O \downarrow$$
$$0.25\ CO_2 + 0.89125\ H_2 + 0.25\ C_2H_4O_2 + 0.0625\ C_4H_8O_2 + 0.1055\ NH_3$$

Degradation of urea : stoichio 3 :

$$CH_4ON_2 + H_2O \rightarrow CO_2 + 2\ NH_3$$

Compartment II : Photoheterotroph (Rhodobacter)

Degradation of acetic acid and butyric acid :

- *Stoichio 4 :*

$$C_2H_4O_2 + 0.9281\ NH_3 + 2.4314\ CO_2 + 5.5790\ \underline{H_2} \downarrow$$
$$4.4314\ [biomass\ Rhodo] + 5.4254\ H_2O$$

- *Stoichio 5 :*

$\underline{C_2H_4O_2} + 0.3873\ NH_3$

$\downarrow$

1.8505 [biomass Rhodo] $+ 0.1495\ CO_2 + 1.1007\ H_2O$

- *Stoichio 6 :*

$\underline{C_4H_8O_2} + 0.9689\ NH_3 + 0.6261\ CO_2$

$\downarrow$

4.6261 [biomass Rhodo] $+ 1.7518\ H_2O$

Compartment III : Nitrifying

- *Stoichio 7 : Nitrosomonas*

$CO_2 + 26.0166\ O_2 + 18.2606\ \underline{NH_3}$

$\downarrow$

[biomass nitri] $+ 18.0612\ HNO_2 + 17.5469\ H_2O$

- *Stoichio 8 : Nitrobacter*

$CO_2 + 38.8496\ O_2 + 79.8494\ \underline{HNO_2} + 0.1994\ NH_3 + 0.5143\ H_2O$

$\downarrow$

[biomass nitri] $+ 79.8494\ HNO_3$

Compartment IV : Photoautotroph (Spirulina)

- *Stoichio 9 : Carbohydrate*

$CO_2 + 0.8355\ H_2O \rightarrow$ [carbohydrate] $+ 1.06225\ O_2$

- *Stoichio 10 : Fat*

$CO_2 + 0.8570\ H_2O \rightarrow$ [fat] $+ 1.3265\ O_2$

- *Stoichio 11 : Proteins*

$CO_2 + 0.6383\ H_2O + 0.2496\ \underline{HNO_3}$

$\downarrow$

[proteins] $+ 1.5302\ O_2$

- *Stoichio 12 : Nucleic acid*

$$CO_2 + 0.440\ H_2O + 0.393\ \underline{HNO_3} \downarrow [\text{nucleic acid}] + 1.4545\ O_2$$

- *Stoichio 13 : Exopolysaccharide*

$$CO_2 + 0.825\ H_2O \rightarrow [EPS] + 0.9375\ O_2$$

ANNEXE 4

This annex allows to compare the results obtained with the ADERSA algorithm and with the software ProSim. The comparison is done on the main compounds of 2 compartments : liquifying and photoautotroph (Spirulina). The values of the input flow rate of each compound were chosen by LGCB.

Meaning of the labels used in the following tables :

input : flow rate at the input of the flash

liq_P : flow rate at the output of the flash in the liquid phase, computed by the software ProSim

liq_A : liquid output flow rate, computed by ADERSA algorithm

gas_P : gas output flow rate, computed by software ProSim

gas_A : gas output flow rate, computed by ADERSA algorithm

$$dist\_liq = \frac{liq\_P - liq\_A}{liq\_A}$$

$$dist\_gas = \frac{gas\_P - gas\_A}{gas\_A}$$

ki_theo : value of the partition coefficient given by the formula, function of temperature and pH

$$ki\_check = \frac{gas\_A}{\Sigma gas\_A} \cdot \frac{\Sigma liq\_A}{liq\_A}$$

$$disk\_ki = \frac{ki\_check - ki\_theo}{ki\_theo}$$

Liquefying compartment ; temperature : 330 K | pH : 5

total input of the flash : 22.736 mol/h
total output of liquid : 21.136 mol/h
total output of gas : 1.5999 mol/h

compound	CO2	H2O	NH3	Ar
input (mol/h)	7.1136e-02	2.1262e+01	1.3713e-01	1.2516e+00
liq_P (mol/h)	3.0962e-04	2.0993e+01	1.3713e-01	0 (1)
liq_A (mol/h)	3.0925e-04	2.0993e+01	1.3702e-01	1.4802e-04
gas_P (mol/h)	7.0830e-02	2.6952e-01	0 (2)	1.2516e+00
gas_A (mol/h)	7.0827e-02	2.6980e-01	1.1244e-04	1.2515e+00
dist_liq	1.2009e-03	1.4123e-05	8.2061e-04	-1. (1)
dist_gaz	4.1773e-05	-1.0137e-03	-1. (2)	1.1827e-04
ki_theo	3.0232e+03	1.6965e-01	1.0832e-02	1.1161e+05
ki_check	3.0257e+03	1.6979e-01	1.0841e-02	1.1170e+05
dist_ki	8.4906e-04	8.4906e-04	8.4906e-04	8.4906e-04

Photoautotroph (Spiru) compartment ; temperature : 303 K | pH : 9.5

total input of the flash : 41.866 mol/h
total output of liquid_A : 12.572 mol/h
total output of gas_A : 29.294 mol/h

compound	O2	CO2	H2O	N2
input (mol/h)	6.0479e+00	8.6766e-01*	1.3346e+01	2.1452e+01
liq_P (mol/h)	5.6415e-05	2.4176e-01*	1.2175e+01	1.0215e-04
liq_A (mol/h)	5.6413e-05	2.4514e-01	1.2174e+01	1.0215e-04
gas_P (mol/h)	6.0478e+00	6.2304e-01*	1.1717e+00	2.1453e+01
gas_A (mol/h)	6.0479e+00	6.2252e-01	1.1717e+00	2.1452e+01
dist_liq	3.9477e-05	-1.3761e-02*	2.4922e-05	2.9881e-05
dist_gas	-8.8605e-06	8.3575e-04	-1.1437e-05	3.2731e-05
ki_theo	4.5990e+04	1.0894e+00	4.1288e-02	9.0091e+04
ki_check	4.6010e+04	1.0899e+00	4.1305e-02	9.0128e+04
dist_ki	4.1508e-04	4.1508e-04	4.1508e-04	4.1508e-04

Table 7 : Comparison ADERSA/ProSim softwares

The comparison of ADERSA algorithm with ProSim Software is establish from the values of dist_liq and dist_gas which are generally lower than 10^{-3}, except the following cases :

(1) : the partition coefficient of Ar is infinite in LGCB simulation

(2) : the partition coefficient of NH_3 is equal to 0 in LGCB simulation

(*) : the sum of liquid and gas output flow rates of CO_2 (0,24176 + 0,62304 mol/h) is different from the input flow rate of CO_2 (0,86766 mol/h) with the ProSim software (there is no explanation to this problem).

Remark : *As Ar is not a compound of the global simulator, the partition coefficient of this compound was replaced by the partition coefficient of N_2.*