MELISSA

TN 4

TN4 - MODELLING

The first part of the present technical note describes the methodology and mathematical tools foreseen to perform a complete modelling of the MELISSA system. In the second part, mass balances informations on each compartment are given. If they do not exist, the lacking data are identified (i.e. liquefying and phototrophic compartment).

I- THEORETICAL CONSIDERATIONS

1.1. Preliminary balances studies on the MELISSA system

The preliminary study of the semi-closed MELISSA system requires the knowledge of the flow rates between the compartments, of their composition and of the descrition of any additional inputs and outputs. A collection of bibliographic data is therefore necessary to analyse the degrees of freedom of the entire MELISSA system. Moreover, these data (some of them are already available from literature or from experimentation) should allow to calculate the elemental mass balances on C, H, O, N, S and eventually P or other elements and to define the theoretical conversion yields of substrates into biomass and products in the process.

1.2. Modular approach

Mathematical modelling of MELISSA loop will be performed by the modular approach. This means that each compartment will be modellized apart with its own inputs and outputs and that the composition of an outlet state vector will be determined from the inlet one. In a second step, the different compartments will be related for a study of the convergence and stability of MELISSA and for a simulation of the whole system.

1.3. Compartment modelling

At every step of the work, special emphasis will be paid on the robustness of the mathematical model, i.e. its ability to predict the behaviour of each compartment in a large range of operating conditions including extreme environmental conditions.

The goal of this part is to obtain models including a minimal number of unknown parameters to be identified from experimental data. Different operations involved in and tending to a mathematical model are summarized in figure 1. Two levels of modelling will be considered.

1.3.1. *Unstructured model*

This approach includes several steps:

- A limited number of variables (E for example) describing the system behaviour have to be chosen. These variables concern the main gas or liquid substrates and products. Moreover, other parameters involved in the process such as gas-liquid transfer, mixing or heat transfer have to be taken into account.

- Hypotheses on the kinetics of biomass production, particularly in limiting conditions must be defined.

- Let us apply to the variable E defined above the macroscopic theory for open systems: E stands for the total amount of substrates or products present in the system. In general, two mechanisms may be distinguished by which the total amount of E present in the system may vary. E may be exchanged with the environment by transport over the system boundary, and/or E may be produced or consumed in processes taking place inside the system. The amount of E present in the system then can be given by the following formulation of a balance equation:

Accumulation = Conversion + Transport

This statement can be translated into the following mathematical expression :

$$\dot{E} = \Pi_E + \Phi_E$$

where:

Π_E represents the total net rate of production of E in the process taking place in the system, Φ_E represents the total rate of exchange of E with the environment. For each variable, conversion yields of substrates into biomass or products may be obtained by theoretical mass balance on the system.

- Special emphasis will be paid to the maintenance of the microorganism which is of great importance in biochemical engineering. The maintenance energy represents the part of the total available energy which does not lead to synthesis of biomass because derived for concentration gradients, membrane potentials, osmotic pressure, turn over of molecules, second law of thermodynamics.... As a consequence, conversion yields cannot be considered to be constant: they depend on environmental conditions (especially when tey are extreme) and they were shown to be a function of the specific growth rate of the biomass. This point must not be disregarded in modelling microorganisms although different conceptions exist on the way to define coefficients of maintenance (1).

- Finally, the following phenomena are important to consider in MELISSA compartments :
. Gas-liquid transfer in gravitational or micro-gravitational conditions (gas permeable membranes) especially in non-newtonian fluids (polysaccharides).
. light supply in the two photosynthetic compartments and possible light limitation of the kinetics. In modelling, the equation of radiative transfer (2) is considered to take this fact into account.

1.3.2. *Biochemically structured model*

Further informations on the bioenergetics of the main metabolism are required to establish a biochemically structured model. These informations allow the following studies :
- The derivation of microbial metabolism biochemically structured balances, including energy balances (ATP, hydrogen carriers such as NADPH2) to get free enthalpy balances and entropy balances on each compartment (linear thermodynamics of irreversible processes).
- The enhancement of coupling between ATP production by metabolism and energy inputs (light or substrates). This analysis will lead to the theoretical determination of conversion yields of substrates into biomass and products under limiting or non limiting conditions.

The main advantages of such biochemically stuctured models are that contrary to unstructured models, they allow :
- to predict the theoretical evolution of conversion yields under limiting conditions.
- to strongly decrease the number of empirical parameters to be identified.
- to define the energy maintenance as an hydrolysis of ATP.

1.3.3. *Experimental*

The main experimental part consists in batch cultures which are used to :
- identify the parameters of the model,
- quantify specific rates of biomass and products formation,
- calculate optimal steady state cultures conditions.

Finally, the above requirements for modelization will allow to improve productivity , automation and scale up of the process under steady state conditions (see Fig. 1).

1.4. <u>The entire MELISSA system. Flow sheeting</u>

From the work defined in the above discussion and which concerned separate compartments, a complete study of the MELISSA system will have to be considered. We suggest for this purpose to use existing simulation software for steady state processes. Such simulators would permit the simulation

of MELISSA including unit operations (operations on the gas and liquid fluxes in the MELISSA system, additional to those of the five compartments are necessary) and the study of convergence and stability of the system.

The whole of these investigations should lead to a flow sheet of a stable MELISSA in steady state conditions.

II- PRELIMINARY RESULTS ON THE MASS BALANCES OF MELISSA

2.1. Consumer compartment

Assuming that the human food consists of 65 % sugars, 25 % pròteins and 10 % lipids and taking the following global formula (3) :

Sugar : CH_2O
Protein : $CH_{1.25}O_{0.25}N_{0.25}$
Lipid : $CH_2O_{0.125}$
Urine solids : CH_3ON
Feces solids : $CH_{2.15}ON_{0.15}$ (50 % protein, 25 % fat, 25 % carbohydrate)

One can write the stoechiometric equation of human metabolism without including other waste solids :

$$3.4\ CH_{1.25}O_{0.25}N_{0.25} + 6.1\ CH_2O + 1.8\ CH_2O_{0.125} + 10.8\ O_2 \longrightarrow 0.7\ CH_3ON + CH_{2.15}ON_{0.15} + 9.6\ CO_2 + 7.9\ H_2O$$

This equation is in good agreement with the waste composition given in WP 1200 :
24 % H_2O, 68 % CO_2, 4 % urine solids, 4 % feces solids (in weight).

Further investigations will demonstrate if the MELISSA system is able to eliminate the other human wastes (WP 1200).

2.2. Liquefying and photoheterotrophic compartment

It seems that global formulae for axenic strains of *Rhodobacter* or *Clostridia* species do not exist in the literature. They thus will have to be experimentally determined. Moreover, a study of the metabolism of these strains should allow to solve the problems concerning:

- the nitrogen transformation in the liquefying compartment and the equilibration of the elemental N balance.

- the CO_2-evolved/biomass ratio in the phototrophic compartment (equilibration of the elemental C balance) and the transformation of H_2 in SCP.

- the volatile fatty acids, H_2, H_2S produced in the liquefying compartment.

However, waiting for experimental determinations and in a first approximation, we can take the formula given by Radmer (4) for *Rhodobacter* species, and the average formula given by Roels (5) for *Clostridia* species :

Rhodobacter : $CH_{1.73}O_{0.36}N_{0.16}$

Clostridia : $CH_{1.79}O_{0.5}N_{0.2}$

2.3. Nitrifying compartment

The following stoechiometric equation already given in WP 1100 is available :

$$9.72\ NH_4^+ + CO_2 + 18.03\ O_2 \longrightarrow$$

$$CH_{1.4}O_{0.4}N_{0.2} + 9.52\ NO_3^- + 9.12\ H_2O + 19.23\ H^+$$

This compartment might also transform H_2S evolved by the liquefying compartment into SO_4^{2-} used by the photosynthetic compartment.

2.4. Photosynthetic compartment

Preliminary experimental results permit to establish the following equation for Spirulina (see WP 1100) :

$$CO_2 + 0.76\ H_2O + 0.174\ NO_3^- + 0.174\ H^+$$

$$\longrightarrow CH_{1.69}O_{0.47}N_{0.17} + 1.41\ O_2$$

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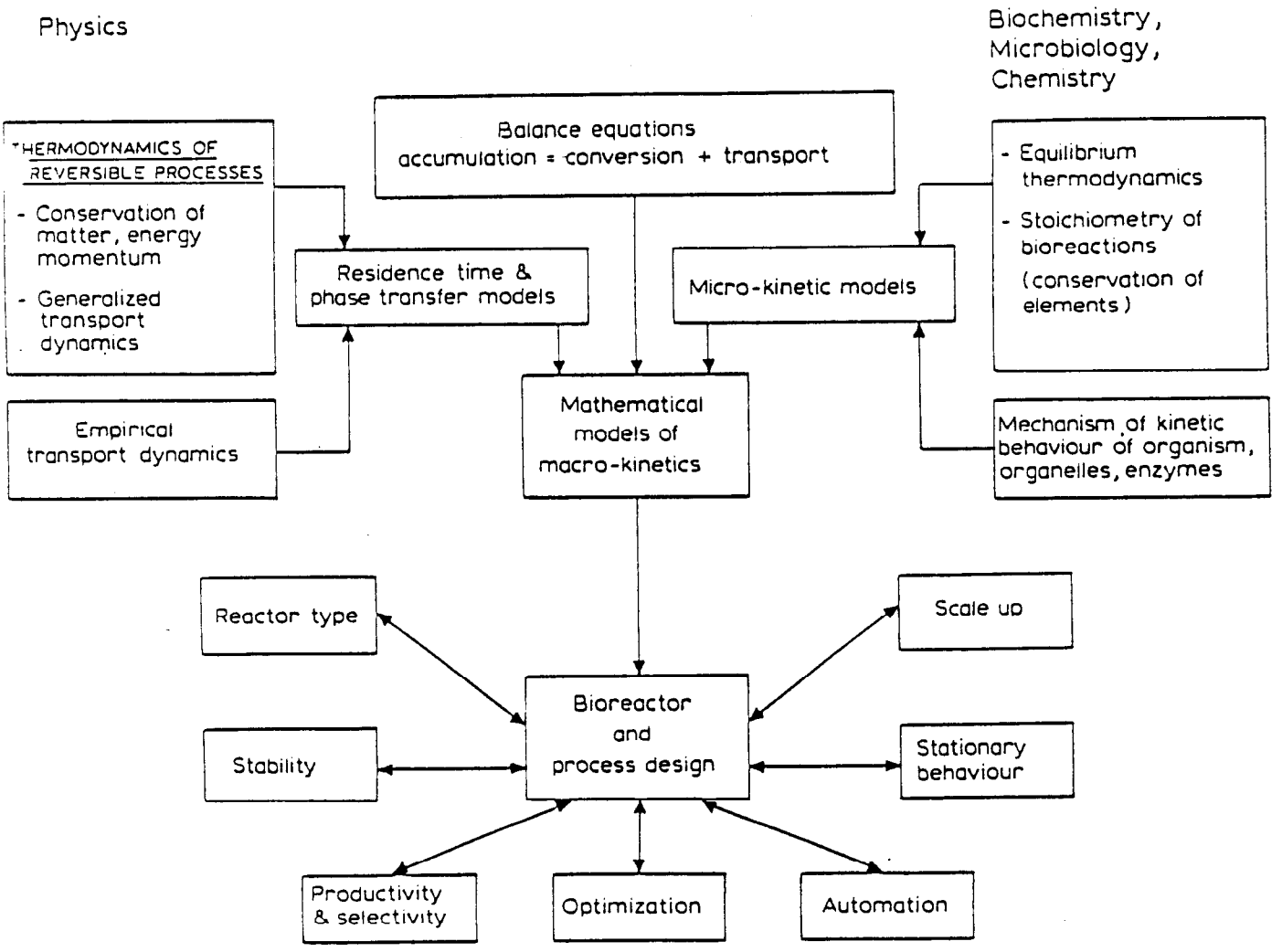

Fig. 1 The structure of (bio)chemical reaction engineering. (From Roels, J.A. (1982) J. Appl. Chem. Biotechnol. 32, 59.)