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On modelling and control of mass balance systems

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ON MODELLING AND CONTROL OF MASS BALANCE SYSTEMS

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1 Introduction

The aim of this chapter is to give a self content presentation of the modelling of engineering systems that are governed by a law of mass conservation and to briefly discuss some control problems regarding these systems.

A general state-space model of mass balance systems is presented. The equations of the model are shown to satisfy physical constraints of positivity and mass conservation. These conditions have strong structural implications that lead to particular Hamiltonian, Compartmental and Stoichiometric representations. The modelling of mass balance systems is illustrated with two simple industrial examples : a biochemical process and a grinding process.

In general, mass balance systems have multiple equilibria, one of them being the operating point of interest which is locally asymptotically stable. However if big enough disturbances occur, the process may be lead by accident to a behaviour which may be undesirable or even catastrophic. The control challenge is then to design a feedback controller which is able to prevent the process from such undesirable behaviours. Two solutions of this problem are briefly described for inflow controlled systems : (i) robust state feedback stabilisation of the total mass, (ii) output regulation for a class of minimum phase systems.

Some interesting stability properties of open loop mass balance systems are reviewed in Appendix.

2 Mass balance systems

In mass balance systems, each state variable x_i $(i = 1, \ldots, n)$ represents an amount of some material (or some matter) inside the system, while each state equation describes a balance of flows as illustrated in Fig. 1 :

$$\dot{x}_i = r_i - q_i + p_i \tag{1}$$

where p_i represents the inflow rate, q_i the outflow rate and r_i an internal transformation rate. The flows p_i, q_i and r_i can be function of the state variables $x_1, \dots x_n$ and possibly of control inputs $u_1, \dots, u_m$. The state space model which is the natural behavioural representation of the system is therefore written in vector form :

$$\dot{x} = r(x,u) - q(x,u) + p(x,u) \tag{2}$$

As a matter of illustration, some concrete examples of the phenomena that can be represented by the (p,q,r) flow rates in engineering applications are given in Table 1.

Transformations	
	Physical : grinding, evaporation, condensation
	Chemical : reaction, catalysis, inhibition
	Biological : infection, predation, parasitism
Outflows	
	Withdrawals, extraction
	Excretion, decanting, adsorption
	Emigration, mortality
Inflows	
	Supply of raw material
	Feeding of nutrients
	Birth, immigration
	etc...etc...

Table 1.

In this paper, we shall assume that the functions $p(x,u), q(x,u), r(x,u)$ are differentiable with respect to their arguments. The physical meaning of the model (2) implies that these functions must satisfy two kinds of conditions : positivity conditions and mass conservation conditions which are explicited hereafter.

3 Positivity

Since there cannot be negative masses, the model (2) makes sense only if the state variables $x_i(t)$ remain *non-negative* for all t :

$$x_i(t) \in R_+$$

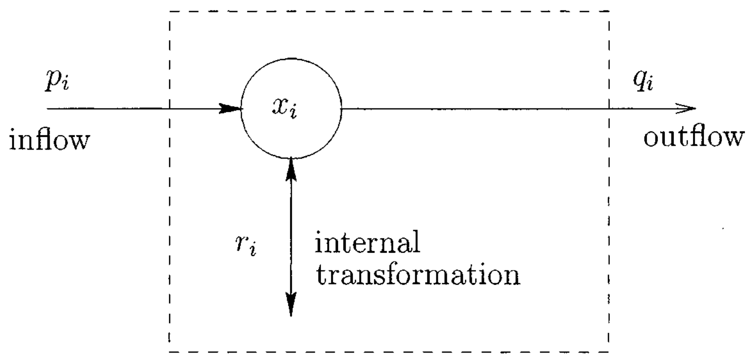

Figure 1: Balance of flows

where R_+ denotes the set of real non-negative numbers. It follows that :

$$x_i = 0 \implies \dot{x}_i \geq 0 \tag{3}$$

whatever the values of $x_j \in R_+$, $j \neq i$ and u_k. This requirement is satisfied if the functions $p(x,u), q(x,u), r(x,u)$ have the following properties :

1. The inflow and outflow functions are defined to be non-negative :

$$\left.\begin{array}{l} p(x,u) \\ q(x,u) \end{array}\right\} : R_+^n \times R^m \to R_+^n$$

2. There cannot be an outflow if there is no material inside the system :

$$x_i = 0 \Longrightarrow q_i(x,u) = 0 \tag{4}$$

3. The transformation rate $r_i(x,u) : R_+^n \times R^m \to R$ may be positive or negative but it must be defined to be positive when x_i is zero :

$$x_i = 0 \Longrightarrow r_i(x,u) \geq 0 \tag{5}$$

4 Conservation of mass

Provided the quantities x_i are expressed in appropriate normalized units, the total mass contained in the system may be expressed as[1] :

$$M = \sum_i x_i$$

[1]To simplify the notations, it will be assumed throughout the paper that the summation $\sum_i$ is taken over all possible values of i (here $i = 1, \ldots, n$) and $\sum_{i \neq j}$ over all possible values of i except j.

When the system is *closed* (neither inflows nor outflows), the dynamics of M are written :

$$\dot{M} = \sum_i r_i(x, u)$$

It is obvious that the total mass inside a closed system must be conserved ($\dot{M} = 0$), which implies that the transformation functions $r_i(x, u)$ satisfy the condition :

$$\sum_i r_i(x, u) = 0 \tag{6}$$

The positivity conditions (4)- (5) and the mass conservation condition (6) have strong structural implications that are now presented.

5 Hamiltonian representation

A necessary consequence of the mass conservation condition (6) is that $n(n-1)$ functions $r_{ij}(x, u)$ $(i = 1, \ldots, n \; ; \; j = 1, \ldots, n \; ; \; i \neq j)$ may be selected such that :

$$r_i(x, u) = \sum_{j \neq i} r_{ji}(x, u) - \sum_{j \neq i} r_{ij}(x, u) \tag{7}$$

(note the indices !). Indeed, the summation over i of the right hand sides of (7) equals zero. It follows that any mass balance system (2) can be written under the form of a so-called *port-controlled Hamiltonian representation* (see [10], [11]) :

$$\dot{x} = [F(x, u) - D(x, u)] \left(\frac{\partial M}{\partial x} \right)^T + p(x, u) \tag{8}$$

where the storage function is the total mass $M(x) = \sum_i x_i$. The matrix $F(x, u)$ is skew-symmetric :

$$F(x, u) = -F^T(x, u)$$

with off-diagonal entries $f_{ij}(x, u) = r_{ji}(x, u) - r_{ij}(x, u)$. The matrix $D(x, u)$ represents the natural damping or dissipation provided by the outflows. It is diagonal and positive :

$$D(x, u) = \text{diag}\,(q_i(x, u)) \geq 0$$

The last term $p(x, u)$ in (8) obviously represents a supply of mass to the system from the outside.

6 Compartmental representation

There is obviously an infinity of ways of defining the r_{ij} functions in (7). We assume that they are selected to be non-negative :

$$r_{ij}(x, u) : R_+^n \times R^m \to R_+$$

and differentiable since $r_i(x,u)$ is required to be differentiable.

Then condition (5) is satisfied if :

$$x_i = 0 \Rightarrow r_{ij}(x,u) = 0 \tag{9}$$

Now, it is a well known fact (see e.g. [7], page 67) that if $r_{ij}(x,u)$ is differentiable and if condition (9) holds, then $r_{ij}(x,u)$ may be written as :

$$r_{ij} = x_i \bar{r}_{ij}(x,u)$$

for some appropriate function $\bar{r}_{ij}(x,u)$ which is defined on $R^n_+ \times R^m$, non-negative and at least continuous. Obviously, the same is true for $q_i(x,u)$ due to condition (4) :

$$q_i(x,u) = x_i \bar{q}_i(x,u)$$

The functions $\bar{r}_{ij}$ and $\bar{q}_i$ are called fractional rates. It follows that the mass balance system (2) is then written under the following alternative representation :

$$\dot{x} = G(x,u)x + p(x,u) \tag{10}$$

where $G(x,u)$ is a so-called *compartmental matrix* with the following properties :

1. $G(x,u)$ is a Metzler matrix with non-negative off-diagonal entries :

   $$g_{ij}(x,u) = \bar{r}_{ji}(x,u) \geq 0 \quad i \neq j$$

   (note the inversion of indices !)

2. The diagonal entries of $G(x,u)$ are non-positive :

   $$g_{ii}(x,u) = -\bar{q}_i(x,u) - \sum_{j \neq i} \bar{r}_{ij}(x,u) \leq 0$$

3. The matrix $G(x,u)$ is diagonally dominant :

   $$|g_{ii}(x,u)| \geq \sum_{j \neq i} g_{ji}(x,u)$$

The term *compartmental* is motivated by the fact that a mass balance system may be represented by a network of conceptual reservoirs called compartments. Each quantity (state variable) x_i is supposed to be contained in a compartment which is represented by a box in the network (see Fig. 2). The internal transformation rates are represented by directed arcs : there is an arc from compartment i to compartment j when there is a non-zero entry $g_{ji} = \bar{r}_{ij}$ in the compartmental matrix G. These arcs are labeled with the fractional rates $\bar{r}_{ij}$. Additional arcs, labeled respectively with fractional outflow rates $\bar{q}_i$ and inflow rates p_i are used to represent inflows and outflows. Concrete examples of compartmental networks will be given in Fig.4 and Fig.6.

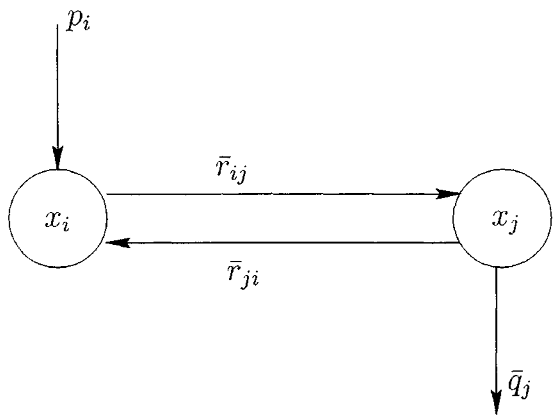

Figure 2: Network of compartments

A compartment is said to be *outflow connected* if there is a path from that compartment to a compartment from which there is an outflow arc. The system is said to be *fully outflow connected* if all compartments are outflow connected. As stated in the following property, the non singularity of a compartmental matrix can be checked directly on the network.

Property 1. For a given value of $(x, u) \in R^n_+ \times R^m$, the compartmental matrix $G(x, u)$ of a mass balance system (10) is non singular if and only if the system is fully outflow connected. ■

A proof of this property can be found e.g. in [7].

7 Stoichiometric representation

In many cases the transformation rates $r_i(x, u), i = 1, n$ can be expressed as linear combinations of a smaller set of non-negative and differentiable basis functions $\rho_1(x, u), \rho_2(x, u), ..., \rho_k(x, u)$ $(k < n)$:

$$r_i(x, u) = \sum_j c_{ij} \rho_j(x, u)$$

This situation typically arises in chemical systems where the non-zero coefficients c_{ij} are the stoichiometric coefficients of the underlying reaction network and the functions $\rho_j(x, u)$ are the reaction rates. The matrix $C = [c_{ij}]$ is therefore called *stoichiometric* and by defining the vector $\rho(x, u) = (\rho_1(x, u), \rho_2(x, u), ..., \rho_k(x, u))^T$ we have :

$$r(x, u) = C\rho(x, u)$$

As we will see in the examples, this stoichiometric representation is also relevant in many other physical and biological systems, As stated in the following

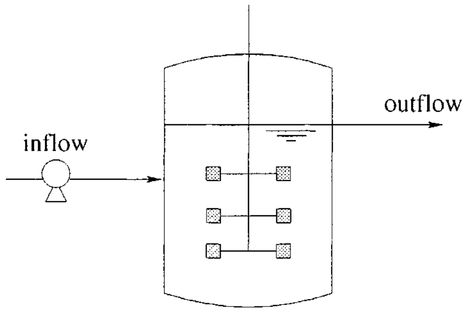

Figure 3: Stirred tank reactor

property, the mass conservation condition (6) can easily be checked from the stoichiometric matrix C independently of the rate functions $\rho_j(x, u)$.

Property 2. The mass conservation condition $\sum_i r_i(x, u) = 0$ is satisfied if the sum of the entries of each column of C is zero :

$$\sum_i c_{ij} = 0 \quad \forall j$$

or equivalently if the vector $\varepsilon = (1, 1, \ldots, 1)^T$ belongs to the kernel of the transpose of the stoichiometric matrix : $\varepsilon^T C = 0$. ■

8 Examples of mass-balance systems

8.1 A biochemical process

A continuous stirred tank reactor is represented in Fig.3. The following biochemical reactions take place in the reactor :

$$\begin{array}{c} A \underset{X}{\longrightarrow} B \\ B \underset{X}{\longrightarrow} X \end{array}$$

where X represents a microbial population and A, B organic matters. The first reaction represents the hydrolysis of species A into species B, catalysed by cellular enzymes. The second reaction represents the growth of microorganisms on substrate B. It is obviously an auto-catalytic reaction. Assuming mass action kinetics, the dynamics of the reactor may be described by the model :

$$\begin{aligned} \dot{x}_1 &= +k_1 x_1 x_2 - u x_1 \\ \dot{x}_2 &= -k_1 x_1 x_2 + k_2 x_1 x_3 - u x_2 \\ \dot{x}_3 &= -k_2 x_1 x_3 - u x_3 + u x_3^{in} \end{aligned}$$

with the following notations and definitions :

x_1 = concentration of species X in the reactor
x_2 = concentration of species B in the reactor
x_3 = concentration of species A in the reactor
x_3^{in} = concentration of species A in the influent
u = dilution rate (control input)
k_1, k_2 = rate constants.

This could be for instance the model of a biological depollution process where ux_3^{in} is the pollutant inflow while $u(x_2 + x_3)$ is the residual pollution outflow. It is readily seen to be a mass-balance model with the following definitions :

$$r(x,u) = \begin{pmatrix} +k_1x_1x_2 \\ -k_1x_1x_2 + k_2x_1x_3 \\ -k_2x_1x_3 \end{pmatrix} \quad q(x,u) = \begin{pmatrix} ux_1 \\ ux_2 \\ ux_3 \end{pmatrix} \quad p(x,u) = \begin{pmatrix} 0 \\ 0 \\ ux_3^{in} \end{pmatrix}$$

The Hamiltonian representation is :

$$F(x,u) = \begin{pmatrix} 0 & k_1x_1x_2 & 0 \\ -k_1x_1x_2 & 0 & k_2x_1x_3 \\ 0 & -k_2x_1x_3 & 0 \end{pmatrix} \quad D(x,u) = \begin{pmatrix} ux_1 & 0 & 0 \\ & ux_2 & 0 \\ 0 & 0 & ux_3 \end{pmatrix}$$

The compartmental matrix is :

$$G(x,u) = \begin{pmatrix} -u & k_1x_1 & 0 \\ 0 & -u - k_1x_1 & k_2x_1 \\ 0 & 0 & -u - k_2x_1 \end{pmatrix}$$

The compartmental network of the process is shown in Fig.4 where it can be seen that the system is fully outflow connected. The stoichiometric representation

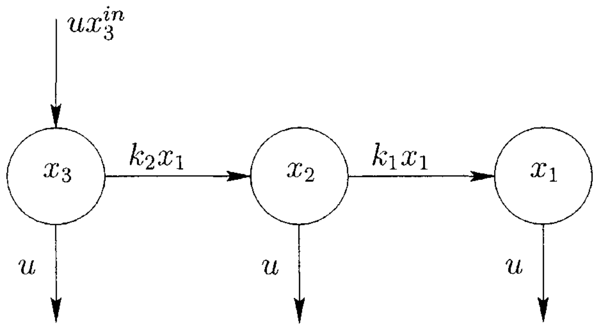

Figure 4: Compartmental network of the biochemical process model

is :

$$C = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{pmatrix} \quad \rho(x) = \begin{pmatrix} k_1x_1x_2 \\ k_2x_1x_3 \end{pmatrix}$$

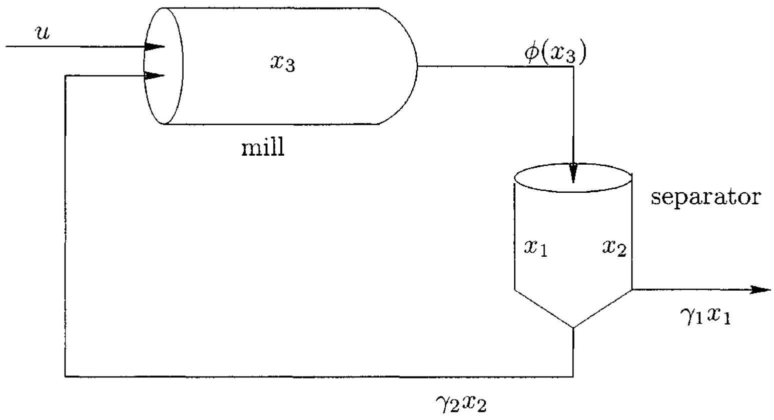

Figure 5: Grinding circuit

8.2 A grinding process

An industrial grinding circuit, as represented in Fig.5 is made up of the interconnection of a mill and a separator. The mill is fed with raw material. After grinding, the material is introduced in a separator where it is separated in two classes : fine particles which are given off and oversize particles which are recycled to the mill. A simple dynamical model has been proposed for this system in [6]:

$$\begin{aligned}
\dot{x}_1 &= -\gamma_1 x_1 + (1-\alpha)\phi(x_3) \\
\dot{x}_2 &= -\gamma_2 x_2 + \alpha\phi(x_3) \\
\dot{x}_3 &= \gamma_2 x_2 - \phi(x_3) + u \\
\phi(x_3) &= k_1 x_3 e^{-k_2 x_3}
\end{aligned}$$

with the following notations and definitions :

x_1 = hold-up of fine particles in the separator
x_2 = hold-up of oversize particles in the separator
x_3 = hold-up of material in the mill
u = inflow rate
$\gamma_1 x_1$ = outflow rate of fine particles
$\gamma_2 x_2$ = flowrate of recycled particles
$\phi(x_3)$ = outflowrate from the mill = grinding function
α = separation constant $(0 < \alpha < 1)$
$\gamma_1, \gamma_2, k_1, k_2$ = characteristic positive constant parameters

This model is readily seen to be a mass-balance system with the following definitions :

$$r(x,u) = \begin{pmatrix} (1-\alpha)\phi(x_3) \\ -\gamma_2 x_2 + \alpha\phi(x_3) \\ \gamma_2 x_2 - \phi(x_3) \end{pmatrix} \quad q(x,u) = \begin{pmatrix} -\gamma_1 x_1 \\ 0 \\ 0 \end{pmatrix} \quad p(x,u) = \begin{pmatrix} 0 \\ 0 \\ u \end{pmatrix}$$

The Hamiltonian representation is :

$$F(x,u) = \begin{pmatrix} 0 & 0 & (1-\alpha)\phi(x_3) \\ 0 & 0 & -\gamma_2 x_2 + \alpha\phi(x_3) \\ -(1-\alpha)\phi(x_3) & \gamma_2 x_2 - \alpha\phi(x_3) & 0 \end{pmatrix}$$

$$D(x,u) = \begin{pmatrix} \gamma_1 x_1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The compartmental matrix is :

$$G(x,u) = \begin{pmatrix} -\gamma_1 & 0 & (1-\alpha)k_1 e^{-k_2 x_3} \\ 0 & -\gamma_2 & \alpha k_1 e^{-k_2 x_3} \\ 0 & +\gamma_2 & -k_1 e^{-k_2 x_3} \end{pmatrix}$$

The compartmental network of the process is shown in Fig.6 where it can be seen that the system is fully outflow connected.

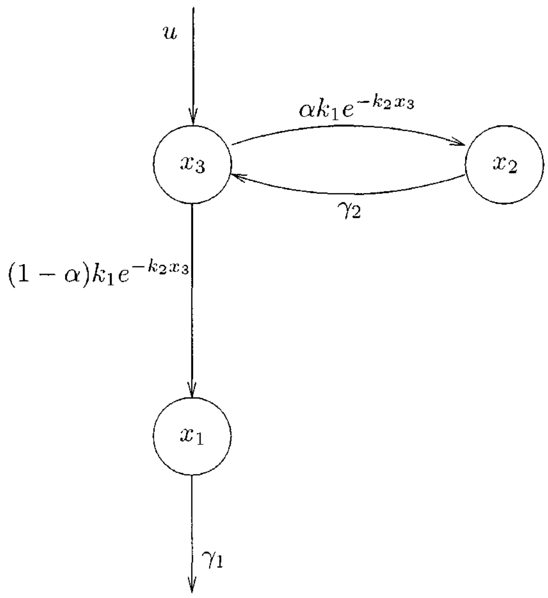

Figure 6: Compartmental network of the grinding process model

The stoichiometric representation is :

$$C = \begin{pmatrix} 1-\alpha & 0 \\ \alpha & -1 \\ -1 & 1 \end{pmatrix} \quad \rho(x) = \begin{pmatrix} \phi(x_3) \\ \gamma_2 x_2 \end{pmatrix}$$

9 A fundamental control problem

Let us consider a mass-balance system with constant inputs denoted $\bar{u}$:

$$\dot{x} = r(x,\bar{u}) - q(x,\bar{u}) + p(x,\bar{u}) \tag{11}$$

An equilibrium of this system is a state vector $\bar{x}$ which satisfies the equilibrium equation :

$$r(\bar{x},\bar{u}) - q(\bar{x},\bar{u}) + p(\bar{x},\bar{u}) = 0$$

In general, mass balance systems (11) have multiple equilibria. One of these equilibria is the operating point of interest. It is generally locally asymptotically stable. This means that an open loop operation may be acceptable in practice. But if big enough disturbances occur, it may arise that the system is driven too far from the operating point towards a region of the state space which is outside of its basin of attraction. From time to time, the process may therefore be lead by accident to a behaviour which may be undesirable or even catastrophic. We illustrate the point with our two examples.

Example 1 : The biochemical process

For a constant inflow rate $\bar{u} < k_1 x_3^{in}$, the biochemical process has three equilibria (see Fig.7). Two of these equilibria (E_1, E_2) are solutions of the following equations :

$$\bar{x}_2 = \frac{\bar{u}}{k_1} \quad \bar{x}_1 + \bar{x}_3 = x_3^{in} - \frac{\bar{u}}{k_1} \quad \bar{x}_3(\bar{u} + k_2\bar{x}_1) = \bar{u}x_3^{in}$$

The third equilibrium $(E3)$ is

$$\bar{x}_1 = 0 \quad \bar{x}_2 = 0 \quad \bar{x}_3 = x_3^{in}$$

As we shall see later on, this system is globally stable in the sense that all trajectories are bounded independently of $\bar{u}$. Furthermore, by computing the Jacobian matrix, it can be easily checked that $E1$ and $E3$ are asymptotically stable while $E2$ is unstable.

$E1$ is the normal operating point corresponding to a high conversion of substrate x_3 into product x_1. It is stable and the process can be normally operated at this point. But there is another stable equilibrium $E3$ called "wash-out steady state" which is highly undesirable because it corresponds to a complete loss of productivity : $\bar{x}_1 = 0$. The pollutant just goes through the tank without any degradation.

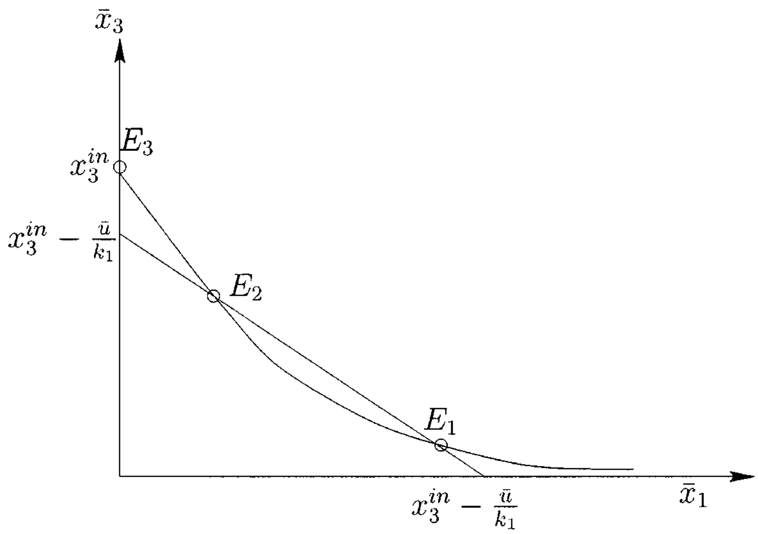

Figure 7: Equilibria of the biochemical process

The problem is that an intermittent disturbance (like for instance a pulse of toxic matter) may irreversibly drive the process to this wash-out steady-state, making the process totally unproductive.

Example 2 : The grinding process

The equilibria of the grinding process $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$ are parametrized by a constant input flowrate $\bar{u}$ as follows :

$$\bar{x}_1 = \frac{\gamma_1}{\bar{u}} \qquad \bar{x}_2 = \frac{\alpha\bar{u}}{\gamma_2(1-\alpha)} \qquad \phi(\bar{x}_3) = \frac{\bar{u}}{(1-\alpha)}$$

In view of the shape of $\phi(x_3)$ as illustrated in Fig.8, there are two distinct equilibria if :

$$\bar{u} < (1-\alpha)\phi_{max}$$

The equilibrium $E1$ on the left of the maximum is stable and the other one $E2$ is unstable. Furthermore, for any value of $\bar{u}$, the trajectories become unstable as soon as the state enters the set D defined by :

$$D \left\{ \begin{array}{c} (1-\alpha)\phi(x_3) < \gamma_1 x_1 < \bar{u} \\ \alpha\phi(x_3) < \gamma_2 x_2 \\ \partial\phi/\partial x_3 < 0 \end{array} \right.$$

Indeed, it can be shown that this set D is forward invariant and if $x(0) \in D$ then $x_1 \to 0 \quad x_2 \to 0 \quad x_3 \to \infty$. In some sense, the system is *Bounded Input - Unbounded State (BIUS)*. This means that there can be an irreversible

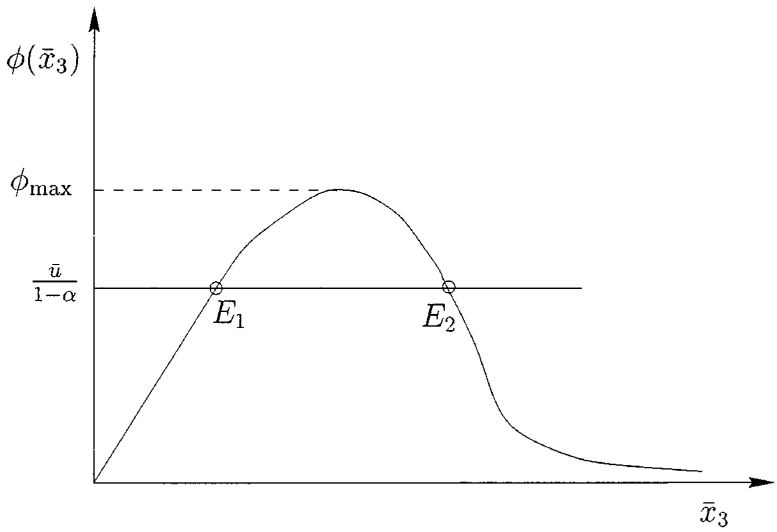

Figure 8: Equilibria of the grinding process

accumulation of material in the mill with a decrease of the production to zero. In the industrial jargon, this is called *mill plugging*. In practice, the state may be lead to the set D by intermittent disturbances like variations of hardness of the raw material. ∎

In both examples we thus have a stable open loop operating point with a potential process destabilisation which can take two forms :

- drift of the state x towards another (unproductive) equilibrium
- unbounded increase of the total mass $M(x)$

The control challenge is then to design a feedback controller which is able to prevent the process from such undesirable behaviours.

Ideally a good control law should meet the following specifications :

S1. The feedback control action is bounded;

S2. The closed loop system has a single equilibrium in the positive orthant which is globally asymptotically stable;

S3. The single closed-loop equilibrium may be assigned by an appropriate set point.

Moreover, it could be desirable that the feedback stabilisation be robust against modelling uncertainties regarding $r(x)$ which is the most uncertain term of the model in many applications.

This is indeed a vast problem which is far to be completely explored. Hereafter, we limit ourselves to the presentation of two specific solutions of this problem namely (i) the state feedback stabilisation of the total mass in inflow controlled systems; (ii) the output regulation with state boundedness in stirred tank systems.

10 Inflow controlled systems

In this section, we will focus on the special case of *inflow-controlled* mass-balance systems where the inflow rates $p_i(x,u)$ do not depend on the state x and are linear with respect to the control inputs u_k :

$$p_i(x,u) = \sum_k b_{ik}u_k \qquad b_{ik} \geq 0 \qquad u_k \geq 0$$

while the transformation rates $r_i(x,u)$ and the outflow rates $q_i(x,u)$ are independent of u. The model (2) is thus written as :

$$\dot{x} = r(x) - q(x) + Bu \tag{12}$$

with B the $n \times m$ matrix with entries b_{ik}.

The Hamiltonian representation specializes as :

$$\dot{x} = [F(x) - D(x)]\left(\frac{\partial M}{\partial x}\right)^T + Bu \tag{13}$$

and the compartmental representation as :

$$\dot{x} = G(x)x + Bu \tag{14}$$

with appropriate definitions of the matrices $F(x), D(x)$ and $G(x)$.

The grinding process model presented in the previous section is an example of an inflow-controlled mass balance system.

10.1 Bounded input - (un)bounded state

Obviously, the state x of any mass-balance system is bounded if and only if the total mass $M(x) = \sum_i x_i$ is itself bounded. In an inflow-controlled system, the dynamics of the total mass are written as :

$$\dot{M} = -\sum_i q_i(x) + \sum_{i,k} b_{ik}u_k \tag{15}$$

From this expression, a natural condition for state boundedness is clearly that the total outflow $\sum_i q_i(x)$ should exceed the total inflow $\sum_{i,k} b_{ik}u_k$ when the total mass $M(x)$ is big enough (in order to make the right hand side of (15) negative). This intuitive condition is made technically precise as follows.

Property 3. Assume that :

(A1) the input $u(t)$ is bounded :

$$0 \leq u_k(t) \leq u_k^{\max} \quad \forall t \;\; \forall k = 1, \ldots, m$$

(A2) There exists a constant M_0 such that

$$\sum_i q_i(x) \geq \sum_{i,k} b_{ik} u_k^{\max}$$

when $M(x) \geq M_0$

Then, the state of the system (12) is bounded and the simplex

$$\Delta = \{x \in R_+^n : M(x) \leq M_0\}$$

is forward invariant.

The system is BIBS if condition (A2) holds for any $u^{\max}$, for example if each $q_i(x) \to \infty$ as $x_i \to \infty$. ■

As a matter of illustration, it is readily checked that inflow-controlled systems with linear outflows in all compartments i.e. $q_i(x) = a_i x_i, a_i > 0, \forall i$ are necessarily BIBS. Indeed in this case we have

$$\sum_i q_i(x) = \sum_i a_i x_i \geq \min_i(a_i) M(x)$$

and therefore $M_0 = \frac{\sum_k b_{ik} u_k^{max}}{\min_i(a_i)}$

In contrast, as we have seen in the previous section, the grinding process of Example 2 is *not* BIBS. Even worse, the state variable x_3 may be unbounded for any value of $u^{\max} > 0$. This means that the process is *globally unstable* for any bounded input.

10.2 Systems without inflows

Consider the case of systems *without inflows* $u = 0$ which are written in compartmental form

$$\dot{x} = G(x)x \tag{16}$$

Obviously, the origin $x = 0$ is an equilibrium of the system.

Property 4. If the compartmental matrix $G(x)$ is full rank for all $x \in R_+^n$ (equivalently if the system is fully outflow connected), then the origin $x = 0$ is a globally asymptotically stable (GAS) equilibrium of the unforced system $\dot{x} = G(x)x$ in the non negative orthant, with the total mass $M(x) = \sum_i x_i$ as Lyapunov function. ■

Indeed, for such systems, the total mass can only decrease along the system trajectories since there are outflows but no inflows :

$$\dot{M} = -\sum_i q_i(x)$$

Property 4 says that the total mass $M(x)$ and the state x will decrease until the system is empty if there are no inflows and the compartmental matrix is nonsingular for all x. A proof of this property and other related results can be found in [2].

10.3 Robust state feedback stabilisation of the total mass

We now consider a single-input inflow-controlled mass-balance system of the form :

$$\dot{x}_i = r_i(x) - q_i(x) + b_i u \quad i = 1, \ldots, n \tag{17}$$

with $b_i \geq 0 \ \forall i, \sum_i b_i > 0$

This system may be globally unstable (bounded input/unbounded state). The symptom of this instability is an unbounded accumulation of mass inside the system like for instance in the case of the grinding process of Example 2.

One way of approaching the problem is to consider that the control objective is to globally stabilise the total mass $M(x)$ at a given set point $M^* > 0$ in order to prevent the unbounded mass accumulation.

In order to achieve this control objective, the following *positive* control law is proposed in [1] :

$$u(x) = \max(0, \tilde{u}(x)) \tag{18}$$

$$\tilde{u}(x) = \left(\sum_i b_i\right)^{-1} \left[\sum_i q_i(x) + \lambda(M^* - M(x))\right] \tag{19}$$

where $\lambda > 0$ is an arbitrary design parameter. The stabilising properties of this control law are as follows.

Property 5. If the system (17) is fully outflow connected, then the closed loop system (17)-(18)-(19) has the following properties for any initial condition $x(0) \in R^n_+$:

1. the set $\Omega = \{x \in R^n_+ : M(x) = M^*\}$ is forward invariant
2. the state $x(t)$ is bounded for all $t \geq 0$ and $\lim_{t\to\infty} M(x) = M^*$.

■

The proof of this property can be found in [1]. It is worth noting that the control law (18)-(19) is independent from the internal transformation term $r(x)$. This means that the feedback stabilisation is robust against a full modelling uncertainty regarding $r(x)$ provided it satisfies the conditions of positivity and mass conservativity.

The application of this control law to the example of the grinding process is studied in [1] where it shown that the closed loop system has indeed a single globally stable equilibrium (although the open loop may have 0, 1, or 2 equlibria).

10.4 Output regulation for a class of BIBS systems

In order to avoid undesirable equilibria, a possible solution is to regulate some output variable at a set point y^* which uniquely assigns the equilibrium of interest. Here is an example of such a solution. We consider the class of single-input BIBS mass-balance systems of the form :

$$\begin{aligned} \dot{x}_i &= r_i(x) - a_i x_i \quad i = 1, \ldots, n-1 \\ \dot{x}_n &= r_n(x) - a_n x_n + u \end{aligned}$$

with $a_i > 0 \ \forall i$. We assume that the measured output $y = x_n$ is the state of an *initial* compartment. The species x_n can only be consumed inside the system but not produced. In other terms, in the compartmental graph of the system, there are several arcs going from compartment n to other compartments but absolutely *no* arcs coming from other compartments. Then, with the notations :

$$\xi = (x_1, \ldots, x_{n-1})^T \qquad y = x_n$$

and appropriate definitions of φ and ψ, the system is rewritten as :

$$\begin{aligned} \dot{\xi} &= \varphi(\xi, y) & (20) \\ \dot{y} &= -(\psi(\xi, y) + a_n)y + u & (21) \end{aligned}$$

and the function $\psi(\xi, y)$ is non-negative.

The goal is to regulate the measured output y at a given set point $y^* > 0$. In order to achieve this objective, the following control law is considered :

$$u = (\psi(\xi, y) + a_n)[(1 - \lambda)y + \lambda y^*] \qquad (22)$$

where λ is a design parameter such that :

$$0 < \lambda < 1$$

With this control law, the closed loop system is written as :

$$\begin{aligned} \dot{\xi} &= \varphi(\xi, y) & (23) \\ \dot{y} &= -(\psi(\xi, y) + a_n)\lambda(y^* - y) & (24) \end{aligned}$$

The stabilisation properties of this control law are analysed under the following assumptions :

A1. The state is initialised in the non negative orthant with $0 \leq y(0) \leq y^{max}$ for some arbitrary $y^{max} > y^*$.

A2. The function $\psi(\xi, y)$ is bounded :

$$0 \leq \psi(\xi, y) \leq \psi^{max} \quad \forall (\xi, y) \in R^n_+$$

A3. The zero dynamics $\dot{\xi} = \varphi(\xi, y^*)$ have a single equilibrium $\bar{\xi} \in R^{n-1}_+$ which is GAS in the non negative orthant.

Assumption A3 is a standard global minimum phase assumption.

Property 6 Under Assumptions A1, A2 and A3, the closed loop system (23)-(24) has the following properties :

1. The control input is positive and bounded :

$$0 \leq u(t) \leq (\psi^{max} + a_n)[(1 - \lambda)y^{max} + \lambda y^*]$$

2. The state is bounded

3. The regulation error converges to zero : $(y^* - y) \to 0$ as $t \to \infty$.

4. The closed loop system has a single equilibrium $(\bar{\xi}, y^*)$ which is GAS in the non negative orthant.

■

Again the important point is that the closed loop system is guaranteed to have a single GAS equilibrium although the open loop system may have several equilibria as we have seen above.

11 Mass balance systems in stirred tanks

In many engineering applications, the system under consideration takes place in liquid phase in a stirred tank with a constant volume as represented in Fig.3. The state variables x_i represent the concentrations of various species in the tank. We consider the very common case of stirred tank mass balance systems with the volumetric flow rate as single control input. In such systems, both the mass inflow rates $p_i(x, u)$ and the mass outflow rates $q_i(x, u)$ linearly depend on the input u :

$$p_i(x, u) = ux_i^{in} \qquad q_i(x, u) = ux_i \tag{25}$$

while the transformation rates $r_i(x, u)$ are independent of u. $x_i^{in} \geq 0$ denotes the constant concentration of the i-th species in the influent stream. Obviously, $x_i^{in} = 0$ for those species which are not fed to the tank but are only produced inside the system. The consistency of the model also requires that the control input be non negative : $u(t) \geq 0 \quad \forall t$. The general mass-balance (2) is thus written as :

$$\dot{x} = r(x) + u(x^{in} - x)$$

with x^{in} the $n \times 1$ vector with entries x_i^{in}. The stoichiometric representation specializes as :

$$\dot{x} = C\rho(x) + u(x^{in} - x) \tag{26}$$

The biochemical process model presented above is an example of a stirred tank mass balance system.

State boudedness

For a stirred tank system, the dynamics of the total mass $M(x) = \sum_i x_i$ are written as :

$$\dot{M} = u(\sum_i x_i^{in} - M) \tag{27}$$

which implies that $M(x)$ and therefore x are bounded *independently of the control input* u. Furthermore, the simplex

$$\Delta = \{x_i \geq 0 : \sum_i (x_i^{in} - x_i) \geq 0\}$$

is forward invariant. A weaker but more explicit consequence is that if x is initialised in Δ, then each state variable is bounded as :

$$0 \leq x_i(t) \leq \sum_i x_i^{in} \quad \forall t$$

Stoichiometric invariants

From equation (27) we see also that the set $\Omega = \{x \in R_+^n : \sum_i (x_i - x_i^{in}) = 0\}$ is forward invariant. This is a typical special case of *stoichiometric invariants* which are classically considered in the Chemical Engineering literature (see e.g. [3]). For any non-zero vector $\lambda^T = (\lambda_1, \ldots, \lambda_n)$ such that $\lambda^T C = 0$ (the vector λ is in the kernel of the transpose of the stoichiometric matrix C), a stoichiometric invariant is defined as the set

$$\Omega = \{x \in R_+^n : \lambda^T (x - x^{in}) = 0\}$$

It is indeed easy to check that this set is forward invariant along the trajectories of the stirred tank system (26).

The nonlinear control of mass balance systems in stirred tank reactors is discussed e.g. in [8] (see also [9] for related results).

12 Summary

In this chapter a general state-space model of mass balance systems has been presented and illustrated with two simple industrial examples : a biochemical process and a grinding process. In general, mass balance systems have multiple equilibria, one of them being the operating point of interest which is locally asymptotically stable. However if big enough disturbances occur, the process may be lead by accident to a behaviour which may be undesirable or even catastrophic. The control challenge is then to design a feedback controller which is able to prevent the process from such undesirable behaviours. We have presented two very specific solutions for single input systems. But it is obvious that the fundamental control problem formulated in this chapter is far from being solved and deserves deeper investigations. In particular a special interest should be devoted to control design methodologies which explicitely account for the structural specificities (Hamiltonian, Compartmental, Stoichiometric) of mass balance systems and rely on the construction of physically based control laws.

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Appendix : stability conditions

In this appendix some interesting stability results for mass balance systems with constant inputs are collected. These results can be useful for Lyapunov control design or for the stability analysis of zero-dynamics.

Compartmental Jacobian matrix

We consider the general case of inflow controlled mass balance systems with constant inflows :

$$\dot{x} = r(x) - q(x) + p(\bar{u})$$

The Jacobian matrix of the system is defined as :

$$J(x) = \frac{\partial}{\partial x}[r(x) - q(x)]$$

When this matrix has a compartmental structure, we have the following stability result.

Property A1

a) If $J(x)$ is a compartmental matrix $\forall\, x \in R^n_+$, then all bounded orbits tend to an equilibrium in R^n_+.

b) If there is a *bounded* closed convex set $D \subseteq R^n_+$ which is *forward invariant* and if $J(x)$ is a *non singular* compartmental matrix $\forall x \in D$, then there is a *unique* equilibrium $\bar{x} \in D$ which is GAS in D with Lyapunov function $V(x) = \sum_i |r_i(x) - q_i(x) + p_i(\bar{u})|$.

■

A proof of part a) can be found in [7] Appendix 4 while part b) is a concise reformulation of a theorem by Rosenbrock [12].

The assumption that $J(x)$ is compartmental $\forall x \in R^n_+$ is fairly restrictive. For instance, this assumption is *not* satisfied neither for the grinding process nor for the biochemical processes that we have used as examples in this paper. A simple sufficient condition to have $J(x)$ compartmental for all x is as follows.

Property A2 The Jacobian matrix $J(x) = \frac{\partial}{\partial x}[r(x) - q(x)]$ is compartmental $\forall x \in R^n_+$ if the functions $r(x)$ and $q(x)$ satisfy the following *monotonicity* conditions :

$$
\begin{array}{ll}
1) & \dfrac{\partial q_i}{\partial x_i} \geq 0 \quad \dfrac{\partial q_i}{\partial x_k} = 0 \quad k \neq i \\
2) & \dfrac{\partial r_{ij}}{\partial x_i} \geq 0 \quad \dfrac{\partial r_{ij}}{\partial x_j} \leq 0 \quad \dfrac{\partial r_{ij}}{\partial x_k} = 0 \quad k \neq i \neq j
\end{array}
$$

■

In the next two sections, we describe two examples of systems that have a single GAS equilibrium in the nonnegative orthant although their Jacobian matrix is not compartmental.

The Gouzé 's condition

We consider a class of stirred tank mass-balance systems of the form :

$$\dot{x}_i = \sum_{j \neq i} [r_{ji}(x_j) - r_{ij}(x_i)] + \bar{u}(x_i^{in} - x_i) \tag{28}$$

where the transformation rates $r_{ij}(x_i)$ depend on x_i only.

For example this can be the model of a stirred tank chemical reactor with monomolecular reactions as explained in [5] (see also [13]).

The set $\Omega = \{x \in R^n_+ : M(x) = \sum_i x_i^{in}\}$ is bounded, convex, compact and invariant. By the Brouwer fixed point theorem, it contains at least an equilibrium point $\bar{x} = (\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)$ which satisfies the set of algebraic equations :

$$\sum_{j \neq i} [r_{ji}(\bar{x}_j) - r_{ij}(\bar{x}_i)] + \bar{u}(x_i^{in} - \bar{x}_i) = 0$$

The following property then gives a condition for this equilibrium to be unique and GAS in the non negative orthant.

Property A3 If $(r_{ij}(x_i) - r_{ij}(\bar{x}_i))(x_i - \bar{x}_i) \geq \quad \forall x_i \geq 0$, then the equilibrium $(\bar{x}_1, \ldots, \bar{x}_n)$ of the system (28) is GAS in the non negative orthant with Lyapunov function.

$$V(x) = \sum_i |x_i - \bar{x}_i|$$

■

The proof of this property is given in [5]. The interesting feature is that the rate functions $r_{ij}(x_i)$ can be *non-monotonic* (which makes the Jacobian matrix non-compartmental) in contrast with the assumptions of Property A2.

Conservative Lotka-Volterra systems

We consider now a class of Lotka-Volterra ecologies of the form :

$$\dot{x}_i = x_i \left(\sum_{j \neq i} a_{ij} x_j - a_{i0} \right) + \bar{u}_i \quad i = 1, \ldots, n \tag{29}$$

with $a_{i0} > 0$ the natural mortality rates;
$a_{ij} = -a_{ij} \; \forall i \neq j$ the predation coefficients (i.e. $A = [a_{ij}]$ is skew symmetric);
$\bar{u}_i \geq 0$ the feeding rate of species x_i with $\sum_i \bar{u}_i > 0$.

This is a mass balance system with a bilinear Hamiltonian representation :

$$F(x) = [a_{ij} x_i x_j] \qquad D(x) = (\text{diag } a_{i0} x_i)$$

Assume that the system has an equilibrium in the positive orthant $\text{int}\{R^n_+\}$ i.e. there is a strictly positive solution $(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)$ to the set of algebraic equations :

$$a_{i0} = \sum_{j \neq i} a_{ij} \bar{x}_j + \frac{\bar{u}_i}{\bar{x}_i} \quad i = 1, \ldots, n$$

Assume that this equilibrium $(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)$ is the only trajectory in the set :

$$D = \{x \in \text{ int}\{R^n_+\} : \bar{u}_i(x_i - \bar{x}_i) = 0 \forall i\}$$

Then we have the following stability property.
Property A4 The equilibrium $(\bar{x}_1, \bar{x}_2, \ldots, \bar{x}_n)$ of the Lotka-Volterra system (29) is unique and GAS in the positive orthant with Lyapunov function

$$V(x) = \sum_i (x_i - \bar{x}_i ln x_i)$$

■

The proof is established, as usual, by using the time derivative of V:

$$\dot{V}(x) = -\sum_i \left[\frac{\bar{u}_i \bar{x}_i}{x_i} \left(1 - \frac{x_i}{\bar{x}_i} \right)^2 \right]$$

and the La Salle's invariance principle (see also [4] for related results).

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