Chapter 4

Compartments systems

The notion of compartments system is used to specify a wide set of systems for which the dynamic can be described by balanced equations. It is used in many engineering fields (such as chemistry engineering, biomedical engineering or ecology), in economy and social sciences as well.

4.1. Definitions and notations

A compartment is a conceptual tank or box for which the content (matter, energy, money, population...) can be quantified. The symbolic notation used is depicted at figure 4.1 where q_{in} and q_{out} are respectively the filling and emptying flows of the compartment expressed in quantity of content by time unit. These flows are always *positive*, by convention.

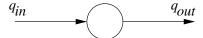


Figure 4.1: Symbolic representation of a compartment.

A compartments system is made of one *network* of compartments interconnected and labelled 1 through n. To be clear, an example of system made of 3 compartments is shown at figure 4.2. The arrows specify the flows of content exchanged by the the compartments in the network and with outside of the system.

In general, a compartments system is represented by an *oriented graph* whose nodes correspond to compartments and arcs to flows. The following notations are introduced:

 x_i is the quantity of content in the compartment of indices i, (i = 1, ..., n). This

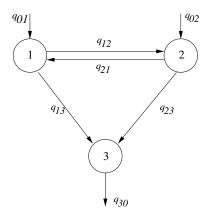


Figure 4.2: An example of a compartments system graph.

quantity is always *positive*. Using a slight abuse of terms, x_i is used to depict the *level* of matter in the compartment i.

 q_{ij} specify the flow flowing from compartment i towards the compartment j, (i=1,...,n;j=1,...,n). As mentioned above, it is a variable which is always *positive* by convention.

Definition 4.1. Open or close system

A system is **open** when there exists a possibility to exchange matter with outside of the system. In this case :

 q_{io} specify the flow from compartment i towards the outside

 q_{oi} specify the flow from the outside towards the compartment i

Otherwise, the system is said to be close : $q_{io} = q_{oi} = 0$ for all i.

Definition 4.2. System connected to entrances and exits

A compartment i is connected to an exit if there is a path $i \to j \to k \to \cdots \to \ell$ from this compartment ending in a compartment ℓ from which there is an outgoing flow $q_{\ell o}$. The system is completely connected to the exits (CCO) if each compartment is connected to an exit.

A compartment ℓ is connected to an entry if there is a path $i \to j \to k \to \cdots \to \ell$ ending in this compartment and coming from a compartment i in which there is an entering flow q_{oi} . The system is completely connected to the entries (CCI) if each compartment is connected to an entry.

4.2. State model 3

4.2. State model

The balanced equation of each compartment (also called continuity equation)

$$\dot{x}_i = \sum_{j=0}^n q_{ji}(t) - \sum_{j=0}^n q_{ij}(t)$$
 $i = 1, ..., n$

is the basic statement to establish the state model of a compartments system. This equation tells us that the variation, per unit of time, of the quantity contained in a compartment is the difference between the sum of the entering flows (or debits) and the sum of the outgoing flows (or debits). In practice, of course, the flows which are structurally null are not explicitly in the equation ((4.1)).

Computing the equations of the sate model of a compartments system required two fundamental aspects.

First of all, the structure of the graph related to the system determines the number and the structure of the balanced equations ((4.1)); the variables x_i are the state variables whereas the order of the model is the number n of compartments.

To complete the state model, the flows should be specified in terms of the state variables and input variables :

$$q_{ij}(x,u)$$

where x and u are, as usual, the vector of states and entries. This modelling is the point of the next section.

The general form of the state equations of a compartments system is the following :

$$\dot{x}_i = \sum_{j=0}^n q_{ji}(x, u) - \sum_{j=0}^n q_{ij}(x, u)$$
 $i = 1, ..., n$

In this model, the physical meaning of the state variables x_i is obvious: these are the quantities contained in each compartment. But, the input variables u can be of different natures, depending on the applications, as the next examples will show.

If the *flows vector* q(x,u) is defined as containing, in an arbitrary order, all the flows $q_{ij}(x,u)$ which are not structurally null, then the sate model ((4.1)) can also be written in a more compact matrix form :

$$\dot{x} = Lq(x, u) \tag{4.1}$$

where L is the incident matrix of the oriented graph, whose coefficients all belong to (-1,0,1).

Example 4.3. For the system depicted at figure 4.2, the state model is written as :

$$\dot{x_1} = q_{01}(x, u) - q_{12}(x, u) - q_{13}(x, u) + q_{21}(x, u)
\dot{x_2} = q_{02}(x, u) + q_{12}(x, u) - q_{21}(x, u) - q_{23}(x, u)
\dot{x_3} = q_{13}(x, u) + q_{23}(x, u) - q_{30}(x, u)$$

If the flows vector is defined as:

$$q(x,u) \triangleq \begin{pmatrix} q_{01}(x,u) \\ q_{02}(x,u) \\ q_{12}(x,u) \\ q_{13}(x,u) \\ q_{21}(x,u) \\ q_{23}(x,u) \\ q_{30}(x,u) \end{pmatrix}$$

the state model is written in a matrix format ((4.1)) with the matrix L:

$$L \triangleq \left(\begin{array}{ccccccc} 1 & 0 & -1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & -1 \end{array}\right).$$

4.3. Modelling of the flows

Depending on the applications, the functions $q_{ij}(x,u)$ depicting the flows can take different types of forms. However, they must be defined in a way which guarantees the compartment system to be a *positive system*, that is a system for which each state variable remains positive along the trajectories. It is a likelihood guarantee of the model, because the state variables represent measures which do not have a physical meaning if they are negative.

Definition 4.4. Positive vector and positive orthant

A vector $x=(x_1,\ldots,x_n)^T$ is positive (notation $x\geq 0$) if each of its component is a positive real number : $x_i\geq 0$ for all i.

The positive orthant of dimension n (written \mathbb{R}^n_+) is the set of all positive vectors of dimension n.

Definition 4.5. Positive system

A dynamical system $\dot{x}=f(x,u)$ is a positive system if, for every admissible input u(t), its state is confined in the positive orthant when the initial state is positive :

$$x(t_0) \in \mathbb{R}^n_+$$
 et $u(t) \in \mathcal{U} \Longrightarrow x(t) \in \mathbb{R}^n_+ \ \forall t \geq t_0$. \square

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The following theorem gives a sufficient condition which can be easily used to check that a system is positive.

Theorem 4.6. A dynamical system $\dot{x} = f(x, u)$ is a positive system if f(x, u) is differentiable and if

$$x \in \mathbb{R}^n_+$$
 et $x_i = 0 \implies \dot{x}_i \ge 0 \quad \forall i.$

To ensure that a compartments system is a positive system, let's impose the following conditions on the flows functions $q_{ij}(x,u)$:

C1. The functions $q_{ij}(x,u)$ are positive functions of their arguments on their definition domain :

$$q_{ij}(x,u): \mathbb{R}^n_+ \times \mathbb{R}^m \to \mathbb{R}_+$$

- C2. The functions $q_{ij}(x, u)$ are continuous and differentiable functions of their arguments on their definition domain.
- C3. As there cannot be an outgoing flow from an empty compartment, the functions $q_{ij}(x,u)$ verify the condition :

$$x_i = 0 \Rightarrow q_{ij}(x, u) = 0$$

Theorem 4.7. Under conditions C1, C2, C3, a dynamical compartment system $\dot{x} = Lq(x,u)$ is a positive system.

Example 4.8. Hydraulic system

Let's consider an hydraulic system made of a set of tanks located at different elevations and whose the liquid content flows "as waterfalls" from the highest tanks to the lowest tanks, thanks to gravity action. An example is illustrated at figure 4.3.

It is clearly a compartments system whose the associated graph is depicted at figure 4.4 and whose the continuity equations are written as :

$$\dot{x}_1 = q_{01} - q_{12} - q_{13}
\dot{x}_2 = q_{12} - q_{23}
\dot{x}_3 = q_{13} + q_{23} - q_{30}$$

In these equations, the sate variables x_1, x_2 et x_3 specify, obviously, the volumes of water contained in the tanks; and the flows q_{ij} depict the debits flowing from the upper tanks toward the lower tanks. In order to complete the model, the flows should be expressed in terms of the sate variables and the input signals, correctly chosen. The flow provided by the supply pomp of the upper tank can obviously

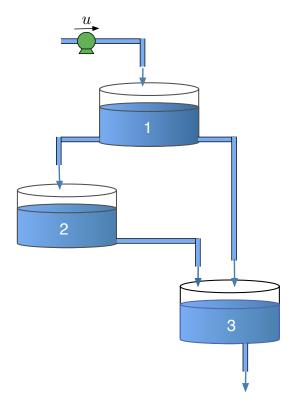


Figure 4.3: Waterfall of tanks.

be chosen as an input variable. The outgoing flow q_{ij} of each tank is a positive function of the volume x_i of the tank. The form of this function depends on the shape of the tanks and the configuration of the holes through which the water flows. Let's consider the case where the tanks have a constant horizontal section and where the flow goes through a rectangular hole located at the bottom of the tanks. The water elevation in a tank is expressed as :

$$h_i = \frac{x_i}{S_i}$$

where S_i specifies the section of the tank. According to the hydraulic laws, we know that when the elevation of the water h_i is big toward the elevation of the hole, the link between the debit and the elevation of the water is proportional to $\sqrt{h_i}$ (Torricelli's law ¹). However, when the elevation of the water is lower than the elevation of the hole, the flows becomes proportional to $h_i\sqrt{h_i}$ (law of flows

¹This law written by Torricelli in 1643 states that the speed v of the outgoing water of a tank of elevation h verifies $v^2 = 2gh$. It can be proven intuitively by analogy with a body in free fall: a elementary volume of water at the surface of the tank has a potential energy ρgh

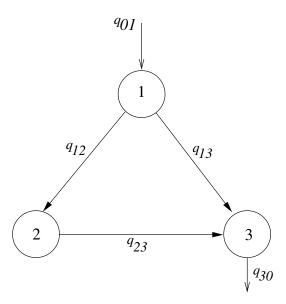


Figure 4.4: Graph of the waterfall of tanks.

for a rectangular tank). A model of the following form can be given :

$$q_{ij} = \frac{\alpha_{ij} h_i \sqrt{h_i}}{\beta_{ij} + h_i}$$

where α_{ij} et β_{ij} are positive constants. Indeed, this model verifies the property telling that, for low water elevations $(h_i \ll \beta_{ij})$, the flow q_{ij} is proportional to $h_i \sqrt{h_i}$ whereas for high water elevations $(h_i \gg \beta_{ij})$, the flow q_{ij} is proportional to $\sqrt{h_i}$. The flows q_{ij} can be expressed in terms of x_i :

$$q_{ij}(x_i) = \frac{k_{ij}x_i\sqrt{x_i}}{S_i\beta_{ij} + x_i}$$
 avec $k_{ij} \triangleq \frac{\alpha_{ij}}{\sqrt{S_i}}$

Finally, the state model can be written as:

$$\dot{x}_{1} = -\frac{k_{12}x_{1}\sqrt{x_{1}}}{S_{1}\beta_{12} + x_{1}} - \frac{k_{13}x_{1}\sqrt{x_{1}}}{S_{1}\beta_{13} + x_{1}} + u,$$

$$\dot{x}_{2} = \frac{k_{12}x_{1}\sqrt{x_{1}}}{S_{1}\beta_{12} + x_{1}} - \frac{k_{23}x_{2}\sqrt{x_{2}}}{S_{2}\beta_{23} + x_{2}},$$

$$\dot{x}_{3} = \frac{k_{13}x_{1}\sqrt{x_{1}}}{S_{1}\beta_{13} + x_{1}} + \frac{k_{23}x_{2}\sqrt{x_{2}}}{S_{2}\beta_{23} + x_{2}} - \frac{k_{30}x_{3}\sqrt{x_{3}}}{S_{3}\beta_{30} + x_{3}}.$$
(4.2)

and a kinetic energy $\rho v^2/2$ when it reaches the exit of the tank, where ρ depicts the density. More rigorously, this can be deduced from Bernoulli's theorem without pressure loss or pump $p + \rho gz + \rho v^2/2 = {\rm constante}$, where p depicts the pressure and z the elevation.

Let's notice that the functions $q_{ij}(x_i)$ verify the positivity conditions C1, C2 and C3.

4.4. Linear models driven by controlled external supplies

This is the most represented class of compartmental models within the literature. It is characterized by the following flow definitions:

1. Flows between compartments and system output flows are linear in function of the providing compartment level:

$$q_{ij} = k_{ij}x_i$$
 $k_{ij} > 0$ $(i = 1, ..., n; j = 0, ..., n)$

2. The system inputs u_{ℓ} are proportional to the supply flow:

$$q_{0\ell} = k_{0\ell} u_{\ell}$$

In that case, the required information used to write the state model is entirely unclosed within the system graph. The state model can be represented as a linear system (see chapter 1):

$$\dot{x} = Ax + Bu$$

with the following structural features:

- 1. Matrix A is a Metzler matrix i.e. such that $a_{ij} \geq 0$ for all $i \neq j$
- 2. Matrix A is diagonally dominant i.e.

$$|a_{ii}| \ge \sum_{j \ne i} a_{ji}$$

3. Matrix B is a full rank *elementary matrix*, i.e. a matrix containing at most one non null element per line and per column.

Example 4.9. The compartmental system linear state model corresponds to the graph shown on 4.2 and can be written as:

$$\begin{pmatrix} \dot{x}_{1} \\ \dot{x}_{2} \\ \dot{x}_{3} \end{pmatrix} = \begin{pmatrix} -(k_{12} + k_{13}) & k_{21} & 0 \\ k_{12} & -(k_{21} + k_{23}) & 0 \\ k_{13} & k_{23} & -k_{30} \end{pmatrix} \begin{pmatrix} x_{1} \\ x_{2} \\ x_{3} \end{pmatrix} + \begin{pmatrix} k_{01} & 0 \\ 0 & k_{02} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} u_{1} \\ u_{2} \end{pmatrix}$$

$$(4.3)$$

We observe that A is a diagonally dominant Metzler matrix and that B is a full rank elementary matrix (rank = 2).

Example 4.10. *Physiological modelling* Physiologists are often interested in describing and analyzing biological or chemical substance propagation within mammal body. Those substances can stand for medicinal substances (Pharmacokinetic studies) or toxic substances voluntary or accidentally absorbed. They can also be natural substances such as hormones or proteins. Compartmental models are frequently used to process such studies: the mammal body is therefore represented as a more or less diversified group of interconnected vessels.

Let us consider the example on figure 4.5.

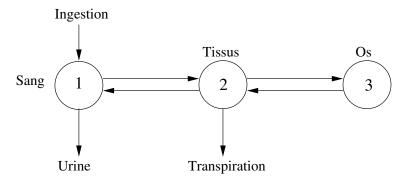


Figure 4.5: Pharmacokinetic compartmental graph model

A toxic substance (lead for example) is absorbed by an animal and permeated in its blood. This substance progressively propagates within the body, from the blood to tissues at first, towards bones afterwards. It is secreted by sweating from one part and by urinating from the other part. The linear compartmental model corresponding to the graph on figure 4.5 is the following model:

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{pmatrix} -(k_{10} + k_{12}) & k_{21} & 0 \\ k_{12} & -(k_{20} + k_{21} + k_{23}) & k_{32} \\ 0 & k_{23} & -k_{32} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} k_{01} \\ 0 \\ 0 \end{pmatrix} u.$$

In this model, the state variables are: x_1 , x_2 et x_3 , which stands for toxial substance quantities within the three compartments (blood, tissues and bones). The input variable u stands for the body ingestion flow.

4.5. Non linear model with controlled flows

We will now consider non linear compartmental systems which flows q_{ij} can be non linear functions whose arguments respect the C1 - C3 conditions. We already approached a non linear model in the vessels cascade example. However, flows between compartments were not depending on input variables u_ℓ in that example. We will here consider a case where flows between compartments are explicit functions of input variables u_ℓ allowing to monitor the debit between compartments. The symbolic representation presented on figure 4.6 shows the presence of such a monitoring variable.

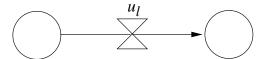


Figure 4.6: Symbolic representation of a monitored flow

Example 4.11. Vessels network Let us consider the hydraulic system represented on figure 4.7. This vessels network corresponds to the vessel cascade example (4.8 with a small modification: the flow between vessel 2 and vessel 3 is now monitored by a pump. As this pump is controllable, we can consider the pumped debit F as an input variable.

The state model (4.2) we obtained for the vessels cascade is therefore simply modified as follows:

$$\dot{x}_1 = -q_{12}(x_1) - q_{13}(x_1) + u_1
\dot{x}_2 = q_{12}(x_1) - u_2
\dot{x}_3 = q_{13}(x_1) - q_{30}(x_3) + u_2$$
(4.4)

where the state variables x_i stand for water volumes contained in vessels, input variable u_1 corresponds to the first vessel supply debit, input variable $u_2 = F$ corresponds to the pumped flow from the second vessel towards the third vessel and functions $q_{ij}(x_i)$ are defined as follows:

$$q_{ij}(x_i) = \frac{k_{ij}x_i\sqrt{x_i}}{S_i\beta_{ij} + x_i}$$

We observe that this state model *cannot* represents a compartmental system respecting C1-C3 conditions. The flow $q_{23}=u_2$ does indeed not respect the C3 condition and the system is not positive: simulations of this model can lead to negative vessels levels (even if the pumped debits remain positive) which is obviously conflicting with physical reality.

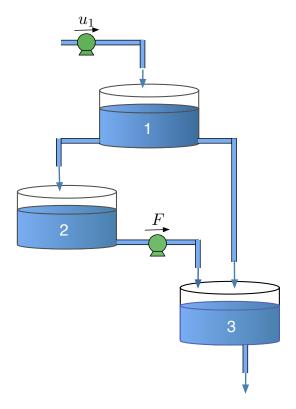


Figure 4.7: Vessels networks

The model as stated indeed allows to pump water in the second vessel even when it is empty!

This problem can be easily avoided if the flow q_{23} (where the pumped debit is F) is modeled such as it respects the physical reality and the C3 condition as:

$$q_{23}(x_2, u_2) = \phi(x_2)u_2$$

where $\phi(x_2)$ is a positive function satisfying $\phi(0) = 0$ and u_2 represents the pump activation.

We therefore obtain a compartment system which graph is presented on figure 4.8 and the state model can be written as:

$$\dot{x}_1 = -q_{12}(x_1) - q_{13}(x_1) + u_1
\dot{x}_2 = q_{12}(x_1) - \phi(x_2)u_2
\dot{x}_3 = q_{13}(x_1) - q_{30}(x_3) + \phi(x_2)u_2$$

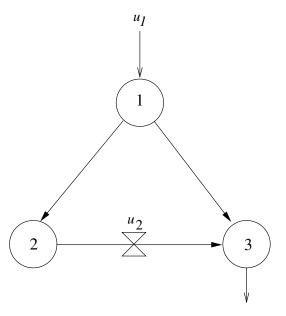


Figure 4.8: Vessels network associated graph

The fundamental structural property of compartments linear systems can be generalized to non linear system with the following theorem.

Theorem 4.12. Given a compartments non linear system which flows q_{ij} satisfy C1-C3 conditions. Therefore, the flows can be written as follows:

$$q_{ij}(x,u) = a_{ij}(x,u)x_i \quad (i = 1, ..., n; j = 1, ..., n)$$

$$q_{i0}(x,u) = a_{i0}(x,u)x_i \quad (i = 1, ..., n)$$

$$q_{0i} = k_{0i}u_i$$

where functions $a_{ij}(x,u)$ et $a_{i0}(x,u)$, defined on the positive orthant, are continuous.

Therefore, the system state model can be written as:

$$\dot{x} = A(x, u)x + Bu$$

where the matrix A(x,u) is a diagonally dominant Metzler matrix for all (x,u) in the positive orthant and B an elementary matrix.

We will end this chapter with another industrial classical compartmental system example.

Example 4.13. Binary distillation process

A binary distillation process is a process used to split a liquid load composed of two liquid chemical components. A *depropanizer* used to split propane from butane is a typical example of binary distillation process within the petrochemical industry.

The split is made by evaporation in an enclosed vessel called *round-bottom* flask (see figure 4.9). The *distillate* containing mainly the lightest component with

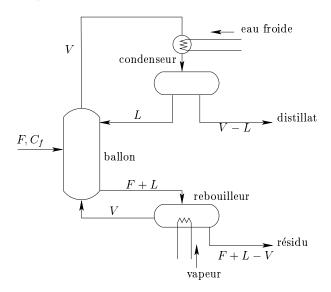


Figure 4.9: Distillation process

a bit of the heaviest one exits from the top of the flask.

The *residue* containing mainly the heaviest component with a bit of the lightest one exits from the bottom of the flask.

The flask is filled by the liquid load with a molar debit F (mol/min). The steam flow spreading out the flask is cooled down and entirely condensed. The outgoing liquid is partially recycled toward the flask with a molar debit L.

The remaining part, called *distillate*, is extracted from the system.

At the bottom of the flask, the outgoing liquid is warmed up a boiler and the produced steam is recycled within the flask. The remaining part, called *residue*, is extracted from the system.

The distillation process dynamic is simplified by the following modeling assumptions and represented below:

- 1. the load is liquid and has the flask temperature;
- 2. the liquid and steam state in the flask and the boiler are homogeneous and at equilibrium;

- 3. the flask pressure is constant and there is no steam accumulation; this assumption allows to omit pressure dependencies in the equations and implies that the steam debit V exiting the flask is equivalent to the input debit;
- 4. the liquid extraction debits are adjusted such as the total molar masses of the components in liquid state remain constant : the distillate is therefore extracted with a molar debit V-L, the liquid at the bottom of the flask is extracted with a molar debit F+L and the residue is extracted with a molar debit F+L-V. Obviously, this implies that the inequality 0 < L < V < F+L has to be verified.

Given this definition, the distillation process can be interpreted as a compartments system which dynamic model is based on balance equations of one of the two components in the flask, in the condenser and in the boiler. This compartments system graph is presented on figure 4.10 and the state equations are:

$$\dot{x}_1 = u_2 k(x_2) - u_1 \frac{x_1}{m_1} - (u_2 - u_1) \frac{x_1}{m_1}$$

$$\dot{x}_2 = u_1 \frac{x_1}{m_1} - (u_1 + u_3) \frac{x_2}{m_2} + u_2 (k(x_3) - k(x_2)) + u_3 c_f$$

$$\dot{x}_3 = (u_1 + u_3) (\frac{x_2}{m_2} - \frac{x_3}{m_3}) + u_2 (\frac{x_3}{m_3} - k(x_3))$$

State variables x_i stand for the molar mass of the lightest component in the liquid state within the condenser (index 1), the flask (index 2) and the boiler(index 3);

Parameters m_i represent those total (and constant) molar masses : the ratio x_i/m_i corresponds to the *molar fraction*; parameter c_f molar fraction of the lightest component within the load;

Input variables $u_1=L$, $u_2=V$ and $u_3=F$ are, respectively, molar debit of the reflux, the steam production and the supply. Finally, the function k(x) is a liquid-steam equilibrium relationship allowing to link the molar fraction of the lightest component leaving the liquid by vaporization to the molar fraction of the component in liquid state.

This relationship is classically expressed as follows:

$$k(x_i) \triangleq \frac{\alpha x_i}{m_i + (\alpha - 1)x_i}$$

where the constant parameter $\alpha > 1$ is called separation factor. This function, defined on the interval $[0, m_i]$, checks k(0) = 0 and $k(m_i) = 1$ (see figure 4.11).

4.6. Exercises

Exercise 4.1. A compartments system

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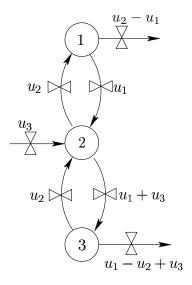


Figure 4.10: Distillation process associated graph

Given the following dynamical system:

$$\dot{x}_1 = x_3 - \log(1 + x_1)$$
$$\dot{x}_2 = x_3 - x_2^2$$
$$\dot{x}_3 = x_2^2 - 2x_3 + u$$

Demonstrate that it is a compartments system. Draw the associated graph. Compute the flows q_{ij} , the matrix L and the matrix A(x,u).

Exercise 4.2. A hydraulic system

A hydraulic system containing three vessels and two pumps is presented on figure 4.12.

- 1. Establish a state model for the system, where the volumetric debits $u_1=F_1$ and $u_2=F_2$ are input variables. Show that the obtained system is *not* a positive system.
- 2. Suggest an alternative definition for the input variable u_2 which ensure a postive system.
- 3. Draw the obtained compartments graph model. □

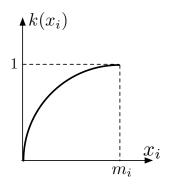


Figure 4.11: Liquid-steam equilibrium relationship

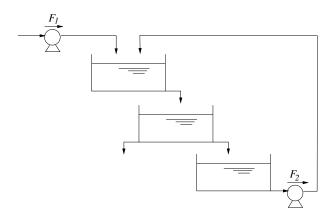


Figure 4.12: Hydraulic system

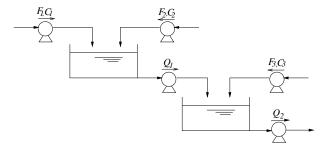


Figure 4.13: Mixing vessels network

Exercise 4.3. A mixing vessels network

The system represented on figure 4.13 is designed for mixing three substances X_1, X_2, X_3 whose supply concentrations are denoted C_1, C_2, C_3 respectively.

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The contained volumes in the two vessels are denoted V_1 and V_2 . The pump volumetric debits are denoted as Q_1, Q_2, F_1, F_2, F_3 .

1. Establish a state model of the system with the following input variables: $u_1=Q_1/V_1, u_2=Q_2/V_2, u_3=C_1, u_4=C_2, u_5=C_3$. The debits F_i , $i=1,\ldots,3$, are supposed constants.

2. Justify the input variables u_1 and u_2 form.

Exercise 4.4. Compartments linear model

Characterize the graph structure of a compartments linear model whose associated matrix \boldsymbol{A} is:

- 1. bidiagonal
- 2. tridiagonal
- 3. lower triangular □

Exercise 4.5. Distillation process model

Determine the matrix A(x, u) of the distillation process model.

Exercise 4.6. Communicating vessels

A system with two communicating vessels is represented on figure 4.14. The liquid flows freely between the two vessels and towards the outside under the hydrostatic pressure action.

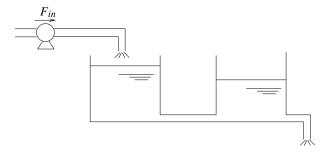


Figure 4.14: Communicating vessels

- 1. Establish a state model of the system. The provided debit (by the supply pump) is the only input variable.
- 2. Show that it is a compartments system. Draw the associated graph. Explain the flow between the compartments. \Box