Chapter 3

Square Matrices Associated to Mixing Problems ODE Systems

Victor Martinez-Luaces

Additional information is available at the end of the chapter

http://dx.doi.org/10.5772/intechopen.74437

Abstract

In this chapter, mixing problems are considered since they always lead to linear ordinary differential equation (ODE) systems, and the corresponding associated matrices have different structures that deserve to be studied deeply. This structure depends on whether or not there is recirculation of fluids and if the system is open or closed, among other characteristics such as the number of tanks and their internal connections. Several statements about the matrix eigenvalues are analyzed for different structures, and also some questions and conjectures are posed. Finally, qualitative remarks about the differential equation system solutions and their stability or asymptotical stability are included.

Keywords: eigenvalues, Gershgorin circle theorem, mixing problems, linear ODE systems, associated matrices

1. Introduction

Mixing problems (MPs), also known as "compartment analysis" [1], in chemistry involve creating a mixture of two or more substances and then determining some quantity (usually concentration) of the resulting mixture. For instance, a typical mixing problem deals with the amount of salt in a mixing tank. Salt and water enter to the tank at a certain rate, they are mixed with what is already in the tank, and the mixture leaves at a certain rate. This process is modeled by an ordinary differential equation (ODE), as Groestch affirms: "The direct problem for one-compartment mixing models is treated in almost all elementary differential equations texts" [2].

Instead of only one tank, there is a group, as it was stated by Groestch: "The multicompartment model is more challenging and requires the use of techniques of linear algebra" [2].

IntechOpen

© 2018 The Author(s). Licensee IntechOpen. This chapter is distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/3.0), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

In particular, the ODE system-associated matrix deserves to be studied since it determines the qualitative behavior of the solutions.

In several previous papers and book chapters [3–6], MPs were studied from different points of view. In the first paper [3], a particular MP with three compartments was proposed, and after applying Laplace transform, this example was connected with important concepts in reactor design, like the transference function. 2 years later, another work [4] analyzed more general MPs in order to obtain characterization results independent of the internal geometry of the tank system. In the third paper [5], the educative potential of MPs was studied, focusing on inverse modeling problems. Finally, in a recent book chapter [6], results for MPs with and without recirculation of fluids were analyzed, and other general results were obtained.

In all these works, a given MP is modeled through an ODE linear system, in which qualitative properties (like stability and asymptotic stability) depend on the eigenvalues and eigenvectors of the associated matrices, so-called MP-matrix.

Taking into account previous results about MP-matrices, and the new ones presented here, two main conjectures can be proposed:

- All the solutions of a given MP are stable.
- If the MP corresponds to an open system, then the solutions are asymptotically stable.

In order to investigate if these conjectures—among others, introduced in the following sections—are true or not, MP-matrices (i.e., square matrices associated to the ODE linear system that models a given MP) should be deeply analyzed.

2. Nomenclature

In this section we introduce a specific terminology useful to allow understanding of the terms properly.

In order to analyze MPs and MP-matrices, we begin by studying a problem already considered in a previous book chapter [6], which involves a tank with five compartments, shown in **Figure 1**.

In this scheme, C_0 is the initial concentration (e.g., salt concentration in water at the entrance of the tank system), C_i is the concentration in the ith compartment (i = 1,…,5), and $\Phi_0 \neq 0$ is the incoming and also outgoing flux.

For instance, if Φ_{1k} is the flux that goes from the left (first) to the kth compartment (being k = 2, 3, 4) and V_1 is the volume of the first container, then a mass balance gives the following ODE:

$$V_1 \frac{dC_1}{dt} = \Phi_0 C_0 - \Phi_{12} C_1 - \Phi_{13} C_1 - \Phi_{14} C_1 = \Phi_0 C_0 - (\Phi_{12} + \Phi_{13} + \Phi_{14}) C_1 \tag{1}$$

The ODEs associated with the central compartments (i = 2, 3, 4) are simpler, since in each case, there is only one incoming flux Φ_{1k} (being k = 2, 3, 4) and a unique outgoing flux Φ_{k5} (being

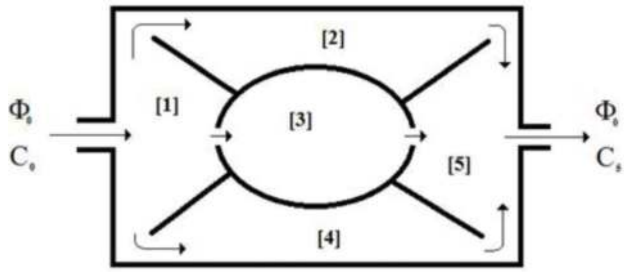

Figure 1. A tank with five internal compartments.

$k = 2, 3, 4$). Once again, if V_k is the volume of the kth container, these equations can be written as.

$$V_2\frac{dC_2}{dt} = \Phi_{12}C_1 - \Phi_{25}C_2, V_3\frac{dC_3}{dt} = \Phi_{13}C_1 - \Phi_{35}C_3, V_4\frac{dC_4}{dt} = \Phi_{14}C_1 - \Phi_{45}C_4 \tag{2}$$

Finally, for the right (fifth) container, we have:

$$V_5\frac{dC_5}{dt} = \Phi_{25}C_2 + \Phi_{35}C_3 + \Phi_{45}C_4 - \Phi_0C_5 \tag{3}$$

If all these equations are put together, the following ODE system is obtained:

$$\begin{cases} V_1\frac{dC_1}{dt} = \Phi_0C_0 - (\Phi_{12} + \Phi_{13} + \Phi_{14})C_1 \\ V_2\frac{dC_2}{dt} = \Phi_{12}C_1 - \Phi_{25}C_2 \\ V_3\frac{dC_3}{dt} = \Phi_{13}C_1 - \Phi_{35}C_3 \\ V_4\frac{dC_4}{dt} = \Phi_{14}C_1 - \Phi_{45}C_4 \\ V_5\frac{dC_5}{dt} = \Phi_{25}C_2 + \Phi_{35}C_3 + \Phi_{45}C_4 - \Phi_0C_5 \end{cases} \tag{4}$$

After some algebraic manipulations, the corresponding mathematical model can be written as $\frac{d}{dt}\mathbf{C} = \mathbf{AC} + C_0\mathbf{B}$, where.

$$\mathbf{C} = \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \\ C_5 \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} \Phi_0/V_1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{5}$$

The system-associated matrix (MP-matrix) is

$$\mathbf{A} = \begin{pmatrix} -(\Phi_{12}+\Phi_{13}+\Phi_{14})/V_1 & 0 & 0 & 0 & 0 \\ \Phi_{12}/V_2 & -\Phi_{25}/V_2 & 0 & 0 & 0 \\ \Phi_{13}/V_3 & 0 & -\Phi_{35}/V_3 & 0 & 0 \\ \Phi_{14}/V_4 & 0 & 0 & -\Phi_{45}/V_4 & 0 \\ 0 & \Phi_{25}/V_5 & \Phi_{35}/V_5 & \Phi_{45}/V_5 & -\Phi_0/V_5 \end{pmatrix} \quad (6)$$

Hereafter, we will call MP-matrix to any ODE system-associated matrix related to a given MP, like matrix **A** of Eq. (6).

In the previous example, the MP-matrix obviously depends on the numbers given to the different containers. In that example it was possible to enumerate the compartments such that the flux always goes from the ith compartment to the jth one, where $i < j$. For instance, a possible enumeration for this purpose is the one illustrated in **Figure 1**.

In general, if in a given MP it is possible to enumerate the containers such that the flux always goes from the ith compartment to the jth one, with $i < j$, then the MP will be considered as a mixing problem without recirculation (MP-WR).

Now, let us analyze a different problem, where a couple of tanks are linked by all possible connections between them, including recirculation from the second tank back to the first one, as in **Figure 2**. This problem represents an interesting variation of an MP analyzed by Zill [7] in his textbook, where the main difference is that this new MP has no incoming and/or outgoing flux, i.e., it is a closed system.

If in a given MP we have that $\sum \Phi_i = 0$, being Φ_i all the system incoming fluxes, and $\sum \Phi_k = 0$, being Φ_k all the system outgoing fluxes, then it will be named MP closed system (MP-CS). Otherwise, it will be an open system (MP-OS).

Taking into account the abovementioned nomenclature, the example considered in **Figure 2** corresponds to an MP-CS, while the MP analyzed in Zill's textbook [7] is an MP-OS, and both are systems with recirculation.

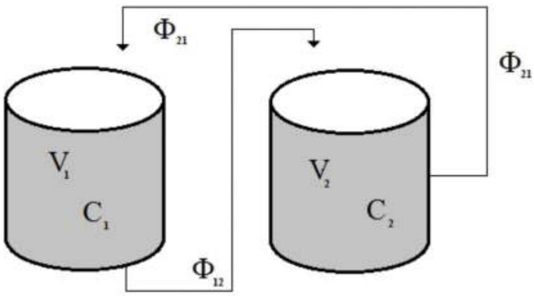

Figure 2. Two tanks with recirculation and no incoming or outgoing fluxes.

Finally, it is important to observe that in both examples (**Figures 1** and **2**), we have $\sum \Phi_i = \sum \Phi_k$, being Φ_i all the system incoming fluxes and Φ_k the corresponding outgoing fluxes. This equation must be satisfied, since the compartments are neither filled up nor emptied with time, at least for the typical MPs' real-life most interesting situations.

In that case all the compartment volumes remain constant, and so if in an MP the following equation $\sum \Phi_i = \sum \Phi_k$ (being Φ_i all the system incoming fluxes and Φ_k the corresponding outgoing fluxes) is satisfied, it will refer to a mixing problem with constant volumes (MP-CV).

Taking into account all these terms, several previous results can be reformulated, as shown in the next section.

3. Previous results revisited

In order to give some general results, it is convenient to consider two different situations: MP without recirculation and MP with recirculation.

Considering again the example in **Figure 1**, it is possible to enumerate the compartments, such that the flux always goes from the ith container to the jth one, being $i < j$, shown in brackets.

Analyzing the system (Eq. (4)), it is easy to observe that for the jth container, the ODE right hand side is a linear combination of a subset of $\{C_0, C_1, \ldots, C'_{j-1}, C_j\}$, and this result can be extended straightforward. In fact, in a previous book chapter [6], it was proved that if in a given MP the compartments can be enumerated such that there is no recirculation (i.e., if $i < j$ there is no flux from compartment j to compartment i), then the ODE corresponding to the jth compartment will be of the form:

$$V_j \frac{dC_j}{dt} = \alpha_{i1} C_{i1} + \alpha_{i2} C_{i2} + \ldots + \alpha_{ik} C_{ik} \tag{7}$$

being $\{i1, i2, \ldots, ik\} \subset \{1, 2, \ldots, j\}$ and $\alpha_{i1}, \alpha_{i2}, \ldots, \alpha_{ik} \in R$.

As a consequence, under the previous conditions, the corresponding ODE system has an associated upper matrix.

Revisiting the ODE system (Eq. (4)), corresponding to **Figure 1**, it can be rewritten as

$$\begin{cases} \dfrac{dC_1}{dt} = \dfrac{\Phi_0}{V_1} C_0 - \dfrac{(\Phi_{12} + \Phi_{13} + \Phi_{14})}{V_1} C_1 \\ \dfrac{dC_2}{dt} = \dfrac{\Phi_{12}}{V_2} C_1 - \dfrac{\Phi_{25}}{V_2} C_2 \\ \dfrac{dC_3}{dt} = \dfrac{\Phi_{13}}{V_3} C_1 - \dfrac{\Phi_{35}}{V_3} C_3 \\ \dfrac{dC_4}{dt} = \dfrac{\Phi_{14}}{V_4} C_1 - \dfrac{\Phi_{45}}{V_4} C_4 \\ \dfrac{dC_5}{dt} = \dfrac{\Phi_{25}}{V_5} C_2 + \dfrac{\Phi_{35}}{V_5} C_3 + \dfrac{\Phi_{45}}{V_5} C_4 - \dfrac{\Phi_0}{V_5} C_5 \end{cases} \tag{8}$$

It follows that for the jth compartment, the coefficient corresponding to C_j can be written as $\frac{-\sum_k \Phi_{jk}}{V_j}$, where $\sum_k \Phi_{jk}$ represents the sum of outgoing fluxes. This situation can be easily generalized, since concentration C_j only appears in the right hand side of the corresponding ODE when a certain flux is leaving the tank. Combining this result with the previous one—about the upper matrix—it is easy to observe that the ODE system has only negative eigenvalues of the form $\lambda_j = \frac{-\sum_k \Phi_{jk}}{V_j} < 0$, for all $j = 1, 2, \ldots, n$.

However, not all of these results can be extended to MPs with recirculation as will be analyzed in the following subsection.

In previous works [4, 5], a "black box" system was analyzed (see **Figure 3**), in order to obtain a necessary condition to be satisfied by any MP-matrix with any number of compartments and unknown internal geometry. In **Figure 3** Φ_0 and C_0 represent flux and concentration at the input, and Φ_0 is also the output flux (since tanks neither fill up nor empty with time), and C_n is the final concentration. In this system there are *n* compartments inside the black box with volumes V_i and concentrations C_i, and recirculation fluxes may exist or not.

If all volumes V_i remain constant, by performing a mass balance, it can be proved that.

$$\sum_{i=1}^{n} V_i \frac{dC_i}{dt} = \Phi_0 (C_0 - C_n) \tag{9}$$

Then, Eq. (9) is obtained without any consideration of the internal geometry of the tank system and can be easily verified in the previous example (see **Figure 1**). In fact, by adding the equations of the ODE system (Eq. (4)), it follows straightforward that the condition given in Eq. (9) is satisfied. The same conclusion can be drawn from other possible examples, corresponding to open or closed MPs, with or without recirculation. For instance, in the case schematized in **Figure 2**, the ODE system can be written as follows:

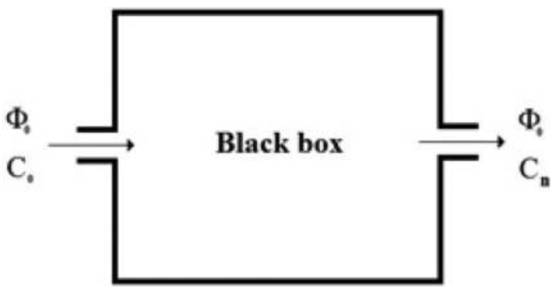

Figure 3. A "black box" tank system.

$$\begin{cases} \frac{dC_1}{dt} = -\frac{\Phi_{12}}{V_1}C_1 + \frac{\Phi_{21}}{V_1}C_2 \\ \frac{dC_2}{dt} = \frac{\Phi_{12}}{V_2}C_1 - \frac{\Phi_{21}}{V_2}C_2 \end{cases} \tag{10}$$

Operating with these equations, it can be proved that $V_1\frac{dC_1}{dt} + V_2\frac{dC_2}{dt} = 0$, which satisfies condition Eq. (9) since Φ_0 is zero.

The previous result can be generalized as follows: in a given MP—with or without recirculation—with input and output concentrations C_0 and C_n, respectively, and being Φ_0 the incoming and outgoing flux, then, independently of the internal geometry, the condition given by Eq. (9) $\sum_{i=1}^{n} V_i \frac{dC_i}{dt} = \Phi_0(C_0 - C_n)$ is satisfied.

An analogous condition may be used to know if a given matrix may or may not be an MP-matrix. For this purpose, let us consider the MP-matrix $\mathbf{A}$, associated to the ODE system given by Eq. (10):

$$\mathbf{A} = \begin{pmatrix} -\frac{\Phi_{12}}{V_1} & \frac{\Phi_{21}}{V_1} \\ \frac{\Phi_{12}}{V_2} & -\frac{\Phi_{21}}{V_2} \end{pmatrix} \tag{11}$$

It is easy to observe that

$$(V_1 \ \ V_2) \begin{pmatrix} -\frac{\Phi_{12}}{V_1} & \frac{\Phi_{21}}{V_1} \\ \frac{\Phi_{12}}{V_2} & -\frac{\Phi_{21}}{V_2} \end{pmatrix} = (0 \quad 0) \tag{12}$$

This equation can be written as $\mathbf{V}^{\mathbf{T}}\mathbf{A} = \mathbf{0}$, being $\mathbf{V}$ the volumes' vector.

If there exists an incoming (and outgoing) flux $\Phi_0 \neq 0$, the last result will change. For instance, if we compute $\mathbf{V}^{\mathbf{T}}\mathbf{A}$, being $\mathbf{V} = (V_1 \quad V_2 \quad V_3 \quad V_4 \quad V_5)$ the volumes' vector and $\mathbf{A}$ the MP-matrix corresponding to **Figure 1**, the result will be

$$\mathbf{V}^{\mathbf{T}}\mathbf{A} = (0 \quad 0 \quad 0 \quad 0 \quad -\Phi_0) \tag{13}$$

It can be noted that Eq. (12) and Eq. (13) are particular cases of the following result: in a given MP—with or without recirculation—with an incoming and outgoing flux $\Phi_0 \neq 0$, the condition $\mathbf{V}^{\mathbf{T}}\mathbf{A} = (0 \quad \cdots \quad 0 \quad -\Phi_0)$ is satisfied, being $\mathbf{V} = (V_1 \quad V_2 \quad \cdots \quad V_n)$ the volumes' vector and $\mathbf{A}$ the MP-matrix.

Then, independently of the internal geometry of the system, the following condition is satisfied:

$$\mathbf{V}^{\mathbf{T}}\mathbf{A} = (0 \quad \cdots \quad 0 \quad -\Phi_0) \tag{14}$$

Now, let us consider again the MP-matrix $\mathbf{A}$, corresponding to the system of **Figure 2**:

$$\mathbf{A} = \begin{pmatrix} -\dfrac{\Phi_{12}}{V_1} & \dfrac{\Phi_{21}}{V_1} \\ \dfrac{\Phi_{12}}{V_2} & -\dfrac{\Phi_{21}}{V_2} \end{pmatrix} \tag{15}$$

If $\mathbf{A}$ is slightly changed only in its first entry, we have the following matrix:

$$\mathbf{A}_\varepsilon = \begin{pmatrix} -\dfrac{\Phi_{12}}{V_1} + \varepsilon & \dfrac{\Phi_{21}}{V_1} \\ \dfrac{\Phi_{12}}{V_2} & -\dfrac{\Phi_{21}}{V_2} \end{pmatrix} \tag{16}$$

It is easy to observe that this new matrix will not satisfy the condition given by Eq. (14). Moreover, there is no MP associated to this matrix $\mathbf{A}_\varepsilon$, since this condition must be satisfied independently of the internal geometry of the system.

As a first consequence, not every square matrix is an MP-matrix. A second observation is that if a given MP-matrix is slightly changed, the result is not necessarily a new MP-matrix.

Furthermore, if volumes V_i and fluxes Φ_i are multiplied by a scale factor, then the MP-matrix $\mathbf{A}$ Eq. (11) remains unchanged, and so, a scale factor in geometry, not in concentrations, produces exactly the same mathematical model.

After interpreting the previous results, we note that when working with MP-matrices, existence, uniqueness, and stability questions for the inverse-modeling problem have negative answers.

The same situation can be observed in many other inverse problems [2], and it is not an exclusive property of compartment analysis.

4. Some considerations about terminology

We start this section explaining three simple and intuitive terms.

Firstly, we will consider that an input tank is a tank with one or more incoming fluxes. Secondly, a tank with one or more outgoing fluxes will be called output tank. Finally, we will say that an internal tank is a tank without incoming and/or outgoing fluxes to or from outside the system.

Taking into account the previous nomenclature, if $\Phi_{ki}\ \ \forall k = 1, 2, \cdots, m$ represent all the ith tank incoming fluxes, then $\sum \Phi_{ki} \neq 0$ for an input tank, and in the same way, if $\Phi_{jk}\ \ \forall k = 1, 2, \cdots, m$ represent all the jth tank outgoing fluxes, then $\sum \Phi_{jk} \neq 0$ for an output tank.

Input and output tanks are not mutually exclusive. For instance, in **Figure 4**, the first tank is an input tank, and at same time, it is an output tank, since it has an incoming flux Φ_0 from outside

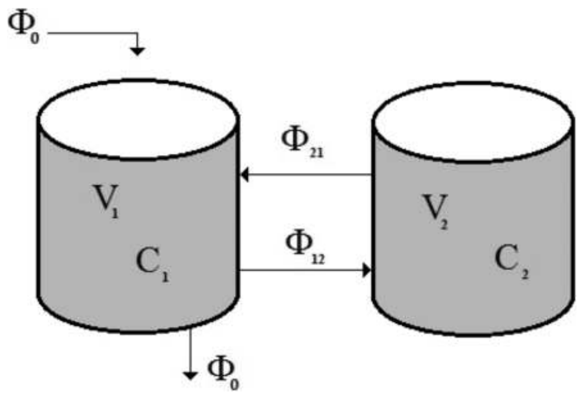

Figure 4. A tank system with recirculation and with incoming and outgoing fluxes.

the system and it also has an outgoing flux Φ_0 that leaves the tank system. It should be noted that in **Figure 4**, the second tank is an internal one.

Another interesting example was proposed by Boelkins et al. [8]. The authors considered a three-tank system connected such that each tank contains an independent inflow that drops salt solution to it, each individual tank has a separated outflow, and each one is connected to the rest of them with inflow and outflow pipes. In this case, all tanks are input and output ones, and there is no internal tank.

It is important to mention that those types of tanks or compartments play different roles in the ODE-associated system and also—as a consequence—in the corresponding MP-matrix. In order to show this fact, let us examine a three-tank system with all the possible connections among them, as in **Figure 5**.

As a first remark, **Figure 5** system has recirculation—unless $\Phi_{21} = \Phi_{32} = \Phi_{31} = 0$, which represents a trivial case—and consequently, an associated upper MP-matrix will not be expected for this problem.

In the mass balance for the first tank—which is an input one—a term $\Phi_0 C_0$ must be considered. In the same way, in the mass balance of the third tank—which is an output one—a term $\Phi_0 C_3$ will appear. These two terms will not be part of the second equation of the ODE system, which can be formulated as follows:

$$\begin{cases} V_1 \dfrac{dC_1}{dt} = \Phi_0 C_0 + \Phi_{21} C_2 + \Phi_{31} C_3 - (\Phi_{12} + \Phi_{13}) C_1 \\ V_2 \dfrac{dC_2}{dt} = \Phi_{12} C_1 + \Phi_{32} C_3 - (\Phi_{21} + \Phi_{23}) C_2 \\ V_3 \dfrac{dC_3}{dt} = \Phi_{13} C_1 + \Phi_{23} C_2 - (\Phi_{31} + \Phi_{32} + \Phi_0) C_3 \end{cases} \tag{17}$$

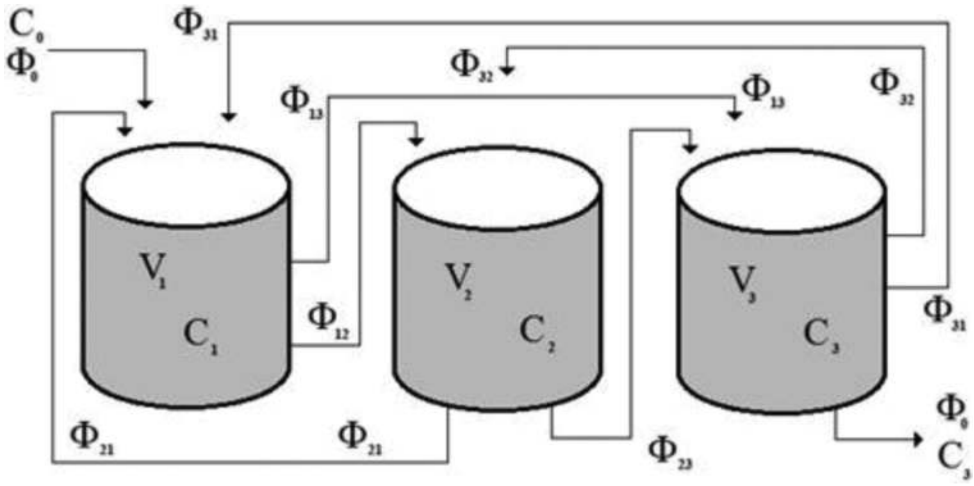

Figure 5. Three tanks with all the possible connections.

Once again, the ODE system can be written as $\frac{d}{dt}\mathbf{C} = \mathbf{A}\mathbf{C} + C_0\mathbf{B}$, where the MP-matrix is:

$$\mathbf{A} = \begin{pmatrix} (-1/V_1)(\Phi_{12}+\Phi_{13}) & \Phi_{21}/V_1 & \Phi_{31}/V_1 \\ \Phi_{12}/V_2 & (-1/V_2)(\Phi_{21}+\Phi_{23}) & \Phi_{32}/V_2 \\ \Phi_{13}/V_3 & \Phi_{23}/V_3 & (-1/V_3)(\Phi_{31}+\Phi_{32}+\Phi_0) \end{pmatrix} \tag{18}$$

In the previous ODE system, the independent vector is:

$$\mathbf{B} = \begin{pmatrix} \Phi_0/V_1 \\ 0 \\ 0 \end{pmatrix} \tag{19}$$

It is easy to observe that the outgoing flux Φ_0 only appears in the last entry of the MP-matrix $\mathbf{A}$ and the incoming flux Φ_0 only is involved in the first entry of vector **B**. These facts—particularly the first one—are relevant when applying the Gershgorin circle theorem, which will be exposed in the next section.

5. The Gershgorin circle theorem

The Gershgorin circle theorem first version was published by S. A. Gershgorin in 1931 [9]. This theorem may be used to bind the spectrum of a complex $n \times n$ matrix, and its statement is the following:

Theorem (Gershgorin)

If A is an $n \times n$ matrix, with entries a_{ij} being $i, j \in \{1, \ldots, n\}$, and $R_i = -\sum_{j \neq i} |a_{ij}|$ is the sum of the non-diagonal entry modules in the ith row, then every eigenvalue of A lies within at least one of the closed disks $\overline{D}(a_{ii}, R_i)$, called Gershgorin disks.

This theorem was widely used in previous book chapters [6, 10, 11] in order to obtain new results about matrices corresponding to chemical problems.

Here, the main purpose is to apply this theorem to MP-matrices as a method to bind their eigenvalues, depending on the characteristics of the MP ODE system, and, even more, the compartment considered.

For instance, if we consider the MP corresponding to **Figure 5**, the first ODE of Eq. (17) can be expressed as $\frac{dC_1}{dt} = \frac{\Phi_0}{V_1} C_0 + \frac{\Phi_{21}}{V_1} C_2 + \frac{\Phi_{31}}{V_1} C_3 - \frac{(\Phi_{12}+\Phi_{13})}{V_1} C_1$

This equation—which obviously corresponds to an input tank—gives the first row of the MP-matrix (Eq. (18)) that can be written as $\begin{pmatrix} -\frac{(\Phi_{12}+\Phi_{13})}{V_1} & \frac{\Phi_{21}}{V_1} & \frac{\Phi_{31}}{V_1} \end{pmatrix}$.

The Gershgorin disk corresponding to this row is centered at $a_{11} = -\frac{(\Phi_{12}+\Phi_{13})}{V_1} < 0$ with radius $R_1 = \frac{\Phi_{21}+\Phi_{31}}{V_1}$.

Now, if a flux balance is performed in this input tank, we have this equation: $\Phi_0 + \Phi_{21} + \Phi_{31} = \Phi_{12} + \Phi_{13}$, and then $\Phi_{21} + \Phi_{31} < \Phi_{12} + \Phi_{13}$ (at least if we consider the nontrivial case $\Phi_0 > 0$). As a consequence of this fact, $|a_{11}| > R_1$, and the Gershgorin disk will look like the one schematized in **Figure 6**.

Now, if the second ODE of Eq. (17) is considered, this equation can be written as $\frac{dC_2}{dt} = \frac{\Phi_{12}}{V_2} C_1 + \frac{\Phi_{32}}{V_2} C_3 - \frac{(\Phi_{21}+\Phi_{23})}{V_2} C_2$.

This internal tank equation corresponds to the second row of the MP-matrix (Eq. (18)): $\begin{pmatrix} \frac{\Phi_{12}}{V_2} & -\frac{(\Phi_{21}+\Phi_{23})}{V_2} & \frac{\Phi_{32}}{V_2} \end{pmatrix}$.

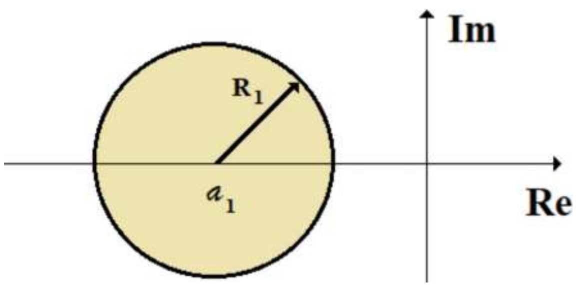

Figure 6. The Gershgorin disk corresponding to an input tank.

The Gershgorin disk corresponding to this row is centered at $a_{22} = -\frac{(\Phi_{21}+\Phi_{23})}{V_2} < 0$ with radius $R_2 = \frac{\Phi_{12}+\Phi_{32}}{V_2}$.

Now, if a flux balance is performed in this internal tank, we have this equation: $\Phi_{12} + \Phi_{32} = \Phi_{21} + \Phi_{23}$, and then $|a_{22}| = R_2$, and the corresponding Gershgorin disk will look like the one schematized in **Figure 7**.

Finally, if the third ODE of Eq. (17) is considered, this equation can be written as $\frac{dC_3}{dt} = \frac{\Phi_{13}}{V_3} C_1 + \frac{\Phi_{23}}{V_3} C_2 - \frac{(\Phi_{31}+\Phi_{32}+\Phi_0)}{V_3} C_3$.

This output tank equation corresponds to the third row of the MP-matrix Eq. (18): $\begin{pmatrix} \frac{\Phi_{13}}{V_3} & \frac{\Phi_{23}}{V_3} & -\frac{(\Phi_{31}+\Phi_{32}+\Phi_0)}{V_3} \end{pmatrix}$.

The Gershgorin disk corresponding to this row is centered at the point $a_{33} = -\frac{(\Phi_{31}+\Phi_{32}+\Phi_0)}{V_3} < 0$ with radius $R_3 = \frac{\Phi_{13}+\Phi_{23}}{V_3}$.

The flux balance in this case gives $\Phi_{13} + \Phi_{23} = \Phi_{31} + \Phi_{32} + \Phi_0$, and then $|a_{33}| = R_3$, and the corresponding Gershgorin disk will look like as the one schematized in **Figure 7**.

Taking into account all these results, the Gershgorin circles for the MP of **Figure 5** are shown in **Figure 8**.

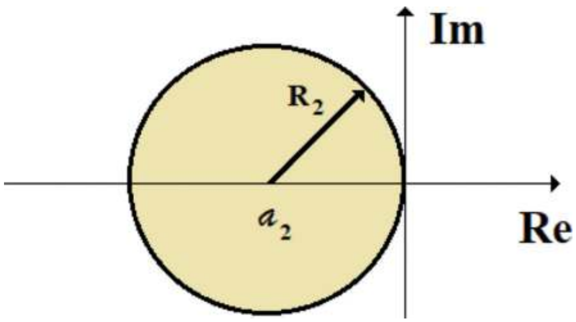

Figure 7. The Gershgorin disk corresponding to an internal tank.

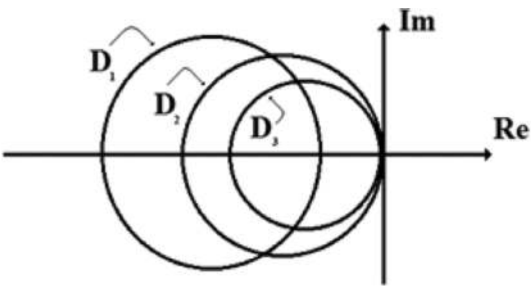

Figure 8. Gershgorin circles for a three-tank system with recirculation.

http://dx.doi.org/10.5772/intechopen.74437

Since every eigenvalue lies within at least one of the Gershgorin disks, it follows that $\mathrm{Re}(\lambda_i) \le 0$, $\forall i = 1, 2, 3$.

In the following section, these results—among others—will be generalized.

6. The general form of MP-matrices and new results

As stated in Section 3, if there is no recirculation, then the ODE system has only negative eigenvalues of the form $\lambda_j = \frac{-\sum_k \Phi_{jk}}{V_j} < 0$, for all $j = 1, 2, \ldots, n$. Then, in this case all the corresponding ODE system solutions will be asymptotically stable.

In a previous work [6], it was proved that in an open MP, with three or less compartments, with or without recirculation, all the corresponding ODE system solutions are asymptotically stable.

It is important to analyze if this result can be generalized or not, when closed systems and/or tanks with more than three compartments are considered. For this purpose, we will start with the following theorem.

Theorem 1

In an open system, if the ith tank is an input one, then the diagonal entry of the ith row is $a_{ii} < 0$ and $|a_{ii}| > R_i$ being $R_i = -\sum_{j \ne i} |a_{ij}|$ the sum of the non-diagonal entry modules of that row.

Proof

If $\Phi_{ai}, \Phi_{bi}, \cdots, \Phi_{ni}$ are the incoming fluxes from other tanks of the system, $\Phi_{iA}, \Phi_{iB}, \cdots, \Phi_{iJ}$ are the outgoing fluxes, and $\Phi_0^1, \Phi_0^2, \cdots, \Phi_0^s$ are the incoming fluxes from outside the system, then the corresponding ODE can be written as

$$V_i \frac{dC_i}{dt} = \Phi_{ai} C_a + \ldots + \Phi_{ni} C_n - \left(\Phi_{iA} + \ldots + \Phi_{iJ}\right) C_i + \Phi_0^1 C_0 + \ldots + \Phi_0^s C_s \tag{20}$$

This equation gives.

$$\frac{dC_i}{dt} = \frac{\Phi_{ai}}{V_i} C_a + \ldots + \frac{\Phi_{ni}}{V_i} C_n - \frac{\sum \Phi_{ij}}{V_i} C_i + \frac{\sum \Phi_0^p}{V_i} C_p \tag{21}$$

Eq. (20) implies that the ith row of the MP-matrix has entries: $\frac{\Phi_{ki}}{V_i}$ for $k \ne i$, $-\frac{\sum \Phi_{ij}}{V_i}$ for $k = i$, and $\frac{\sum \Phi_0^p}{V_i} C_p$ is part of the independent term.

A flux balance gives $\sum \Phi_{ki} + \sum \Phi_0^p = \sum \Phi_{ij}$, which implies $\sum \Phi_{ki} < \sum \Phi_{ij}$, and then: $a_{ii} = -\frac{\sum \Phi_{ij}}{V_i} < 0$ and also $R_i = \frac{\sum \Phi_{ki}}{V_i} < \frac{\sum \Phi_{ij}}{V_i} = |a_{ii}|$, which proves the theorem.

Corollary 1

In an open system, being the ith tank an input one, the Gershgorin circle corresponding to the ith row looks like the disk in **Figure 6**.

Corollary 2

If in an open system, all are input tanks, all the eigenvalues satisfy the condition $\mathrm{Re}(\lambda_i) < 0$, and the ODE solutions are asymptotically stable.

Theorem 2

In an open system, if the ith tank is not an input one, then the diagonal entry of the ith row is $a_{ii} < 0$ and $|a_{ii}| = R_i$ being $R_i = -\sum_{j \neq i} |a_{ij}|$ the sum of the non-diagonal entry modules of that row.

Proof

If $\Phi_{ai}, \Phi_{bi}, \cdots, \Phi_{ni}$ are the incoming fluxes from other tanks $(a, b, \cdots, n)$ of the MP system, $\Phi_{iA}, \Phi_{iB}, \cdots, \Phi_{iJ}$ are the outgoing fluxes to other tanks $(A, B, \cdots, J)$, and $\Phi_i^1, \Phi_i^2, \cdots, \Phi_i^s$ are the fluxes from the ith tank to outside the system, then the corresponding ODE can be written as

$$V_i \frac{dC_i}{dt} = \Phi_{ai} C_a + \ldots + \Phi_{ni} C_n - \left(\Phi_{iA} + \ldots + \Phi_{iJ}\right) C_i - \Phi_i^1 C_i - \ldots - \Phi_i^s C_i \tag{22}$$

This equation gives:

$$\frac{dC_i}{dt} = \frac{\Phi_{ai}}{V_i} C_a + \ldots + \frac{\Phi_{ni}}{V_i} C_n - \frac{\sum \Phi_{ij} + \sum \Phi_i^p}{V_i} C_i \tag{23}$$

Eq. (22) implies that the ith row of the MP-matrix has entries $\frac{\Phi_{ki}}{V_i}$ for $k \neq i$ and $-\frac{\sum \Phi_{ij} + \sum \Phi_i^p}{V_i}$ for $k = i$, and this equation does not contribute to the independent term.

In this case a flux balance gives the following equation $\sum \Phi_{ki} = \sum \Phi_{ij} + \sum \Phi_i^p$, then $a_{ii} = -\frac{\sum \Phi_{ij} + \sum \Phi_i^p}{V_i} < 0$, and also $R_i = \frac{\sum \Phi_{ki}}{V_i} = \frac{\sum \Phi_{ij} + \sum \Phi_i^p}{V_i} = |a_{ii}|$, and the theorem is proved.

Corollary 3

In an open system, if the ith tank is not an input one, the Gershgorin circle corresponding to the ith row looks like the disk in **Figure 7**.

Corollary 4

In an open system, the Gershgorin disks look like those of **Figure 8**.

As a consequence of the previous results, the following corollary can be stated.

Corollary 5

In an open system with input and non-input tanks, all the eigenvalues satisfy the condition $\mathrm{Re}(\lambda_i) \leq 0$.

Independently of the previous results, it is easy to observe that all the solutions corresponding to the eigenvalues with $\mathrm{Re}(\lambda_i) < 0$ tend to vanish when $t \to +\infty$.

For this purpose, when analyzing eigenvalues with $\mathrm{Re}(\lambda_i) < 0$, there are two cases to be considered: $\lambda_i \in \mathfrak{R}$ and $\lambda_i \notin \mathfrak{R}$.

In the first case, the corresponding ODE solutions are a linear combination of the functions $\{\exp(-\lambda_i t),\ t\exp(-\lambda_i t),\ t^2\exp(-\lambda_i t), \ldots,\ t^q\exp(-\lambda_i t)\}$, where the number q depends on the algebraic and geometric multiplicity of λ_i (i.e., $AM(\lambda_i)$ and $GM(\lambda_i)$). Taking into account that $\lambda_i < 0$, it follows that $t^n\exp(-\lambda_i t) \underset{t\to+\infty}{\to} 0, \forall n = 0,\ 1, \ldots,\ q$.

In the second case—which really happens, as it will be observed later—we have $\lambda_i = a + bi\ \notin \mathfrak{R}$ (with $a < 0, b \neq 0$). The ODE solutions are a linear combination of $\{\exp(-at)\cos(bt),\ \exp(-at)\sin(bt), \ldots,\ t^q\exp(-at)\cos(bt),\ t^q\exp(-at)\sin(bt)\}$, where the number q depends on $AM(\lambda_i)$ and $GM(\lambda_i)$ as in the other case. It is easy to prove that $t^n\exp(-at)\cos(bt) \underset{t\to+\infty}{\to} 0$ and $t^n\exp(-at)\sin(bt) \underset{t\to+\infty}{\to} 0, \forall n = 0,\ 1, \ldots,\ q$, since $a < 0$.

According to the position of the Gershgorin disks for an MP-matrix (see **Figure 8**), the ODE solutions corresponding to an eigenvalue λ_i, with $\mathrm{Re}(\lambda_i) = 0$, can be analyzed.

For this purpose it is important to observe that if an eigenvalue λ_i satisfies $\mathrm{Re}(\lambda_i) = 0$, then it must be $\lambda_i = 0$, since the Gershgorin disks look like those in **Figure 8**.

In this case the ODE solutions are a linear combination of the following functions: $\{\exp(-0t),\ t\exp(-0t),\ t^2\exp(-0t), \ldots,\ t^q\exp(-0t)\} = \{1,\ t,\ t^2, \ldots,\ t^q\}$, where the number q depends on $AM(0)$ and $GM(0)$. In other words, the corresponding solutions are polynomial, and so, they will not tend to vanish nor remain bounded when $t \to +\infty$, unless $AM(0) = MG(0)$, and the polynomial becomes a constant.

Considering all these results, it is obvious that the stability of the ODE system solutions will depend exclusively on $AM(0)$ and $GM(0)$.

7. Several questions and a conjecture

In the previous section, some particular cases with $\lambda_i = 0$ and/or $\lambda_i = a + bi\ \notin \mathfrak{R}$ (with $a < 0, b \neq 0$) were considered. A first question to analyze is if there exists an MP that satisfies any of these conditions. For this purpose, let us consider the closed MP of **Figure 9**, in which ODE system can be written as $\frac{d}{dt}\mathbf{C} = \mathbf{AC}$, and the corresponding MP-matrix is $\begin{pmatrix} -a & 0 & a \\ b & -b & 0 \\ 0 & c & -c \end{pmatrix}$, being $a = \frac{\Phi}{V_1}$, $b = \frac{\Phi}{V_2}$, and $c = \frac{\Phi}{V_3}$. If Φ and V_i are chosen such that $a = 1$,

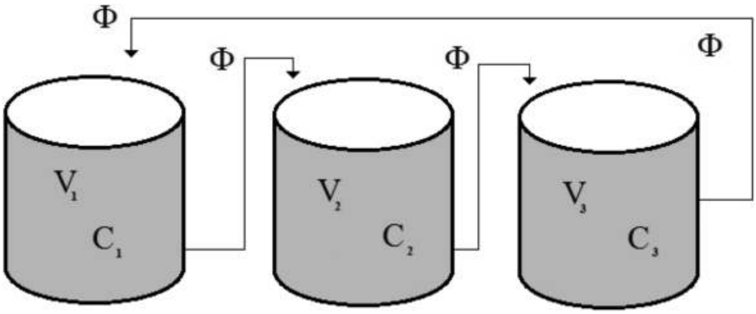

Figure 9. Three tanks with all the possible connections.

$b = 2$, and $c = 3$, it is easy to show that the eigenvalues are $\lambda_1 = 0$ and $\lambda_{2,3} = -3 \pm i\sqrt{2}$, which prove that null and/or complex eigenvalues are possible.

Other questions are not so simple like the previous one. The next two examples propose challenging problems that deserve to be studied:

Question 1:

Is it possible to find an MP-matrix with an eigenvalue $\lambda_i = 0$ such that $AM(0) > 1$?

Question 2:

Is it possible to find an MP-matrix such that $AM(0) > GM(0)$?

Question 3:

Is it possible to find an MP-matrix with complex eigenvalues in an open system?

Finally, it is interesting to observe that all cases analyzed here with $\lambda_i = 0$ correspond to closed systems. Moreover, in a previous book chapter [6], it was proved that $\mathrm{Re}(\lambda_i) \leq 0 \;, \forall i$, in any MP open system with three tanks or less. Taking into account all these facts, it can be conjectured that in an open system, all the MP-matrix eigenvalues have negative real part and as a consequence, all the solutions are asymptotically stable.

8. Conclusions

Mixing problems are interesting sources for applied research in mathematical modeling, ODE, and linear algebra, and—as it was shown—their behavior depends on how they are connected. It has been proved that null eigenvalues are not expected in open systems with three or less components, and $\mathrm{Re}(\lambda_i) \leq 0, \forall i$ is a general conclusion for open MP-matrices that can be obtained by applying the Gershgorin circle theorem.

As a final remark, all the MP differential equation systems considered in this chapter have stable or asymptotically stable solutions. Nevertheless, this situation may change depending on the answers to the questions and the conjecture presented in the last section, giving a challenging proposal for further research on this topic.

Acknowledgements

The author wishes to thank Marjorie Chaves for her assistance and support in this work.

Author details

Victor Martinez-Luaces

Address all correspondence to: victoreml@gmail.com

Faculty of Engineering, UdelaR, Montevideo, Uruguay

References

[1] Braun M. Differential Equations and their Applications. 3rd ed. New York: Springer; 2013. 546 p. DOI: 10.1007/978-1-4684-9229-3

[2] Groestch C. Inverse Problems: Activities for Undergraduates. Washington D.C.: Mathematical Association of America; 1999. 222 p

[3] Martinez-Luaces V. Engaging secondary school and university teachers in modelling: Some experiences in South American countries. International Journal of Mathematical Education in Science and Technology. 2005;**36**(2–3):193-205

[4] Martinez-Luaces V. Inverse-modelling problems in chemical engineering courses. In: Proceedings of the Southern Hemisphere Conference on Undergraduate Mathematics and Statistics Teaching and Learning. (Delta ´07); 26–30 November 2007; Calafate: Argentina. pp. 111-118

[5] Martinez-Luaces V. Modelling and inverse-modelling: Experiences with O.D.E. Linear systems in engineering courses. International Journal of Mathematical Education in Science and Technology. 2009;**40**(2):259-268

[6] Martinez-Luaces V. Matrices in chemical problems: Characterization, properties and consequences about the stability of ODE Systems. In: Baswell A, editor. Advances in Mathematics Research. New York: Nova Publishers; 2017. pp. 1-33

[7] Zill D. Differential Equations with Boundary-Value Problems. 9th ed. Boston: Cengage Learning; 2016. 630 p

[8] Boelkins M, Goldberg J, Potter M. Differential Equations with Linear Algebra. New York: Oxford University Press; 2009. 576 p

[9] Varga R. Geršgorin and His Circles. Berlin, Germany: Springer-Verlag; 2004

[10] Martinez-Luaces V. First order chemical kinetics matrices and stability of O.D.E. systems. In: Kyrchei I, editor. Advances in Linear Algebra Research. New York: Nova Publishers; 2015. pp. 325-343

[11] Martinez-Luaces V. Qualitative behavior of concentration curves in first order chemical kinetics mechanisms. In: Taylor J, editor. Advances in Chemistry Research. New York: Nova Publishers; 2017. pp. 139-169