# Equivalence of finite dimensional input-output models of solute transport and diffusion in geoscience

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*Abstract*—**We show that for a large class of finite dimensional input-output positive systems that represent networks of transport and diffusion of solute in geological media, there exist equivalent *multi-rate mass transfer* and *multiple interacting continua* representations, which are quite popular in geosciences. Moreover, we provide explicit methods to construct these equivalent representations. The proofs show that controllability property is playing a crucial role. These results contribute to our fundamental understanding on the effect of fine-scale geological structures on the transfer and dispersion of solute.**

*Index Terms*—**Equivalent mass transfer models, positive linear systems, controllability.**

## I. INTRODUCTION

Underground media are characterized by their high surface to volume ratio and by their slow solute movements that overall promote strong water-rock interactions [26], [28]. As a result, water quality strongly evolves with the degradation of anthropogenic contaminants and the dissolution of some minerals. Chemical reactivity is first determined by the residence time of solutes and the input/output behavior of the system, as most reactions are slow and kinetically controlled [27], [21]. Especially important are exchanges between high-flow zones where solutes are transported over long distances with marginal reactivity and low-flow zones in which transport is limited by slow diffusion but reactivity is high because of large residence time [18], [7]. It is for example the case in fractured media where solute velocity can reach some meters per hour in highly transmissive fractures [11], [13] but remains orders of magnitude slower in neighboring pores and smaller fractures giving rise to strong dispersive effects [14], [15]. More generally wide variability of transfer times, high dispersion, and direct interactions between slow diffusion in small pores and fast advection in much larger pores are ubiquitous in soils and aquifers [8]. The dominance of these characteristic features up to some meters to hundreds of meters have prompted the development of numerous simplified models starting from the double-porosity concept [30]. In these models, solutes move quickly by advection in a first porosity with a small volume representing fast-flow channels and slowly by diffusion in a second large homogeneous porosity. Exchanges between the two porosities is diffusion-like. Such models have been widely extended to account not only for one diffusive-like zone but for many of them with different structures and connections to the advective zone [18], [25]. Such extensions are thought to model both the widely varying transfer times and the rich water-rock interactions. The two most famous ones are the Multi-Rate Mass Transfer model (MRMT) [7], [18] and Multiple INteracting Continua model (MINC) [25]. They are made up of an infinity of diffusive zones deriving from analytic solutions of the diffusion equation in layered, cylindrical or spherical impervious inclusions (MRMT) or in series (MINC). Between dual-porosity and these models, many intermediary models of finite dimension have been effectively used and calibrated on synthetic, field, or experimental data showing their relevance and usefulness [10], [2], [23], [31], [32].

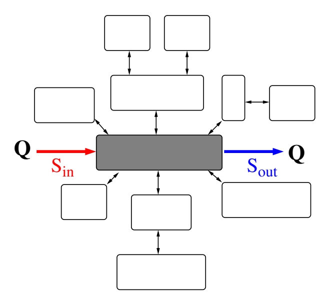


Figure 1. Example of a network with one mobile zone (in grey) and several immobile zones.

Theoretical grounds are however missing to identify classes of equivalent porosity structures, effective calibration capacity on accessible tracer test data, and influence of structure on conservative as well as chemically reactive transport. One can wonder if MRMT and MINC models are not too restrictive to represent real structures. In this work we study the equivalence problem for a wide class of network structures and provide necessary and sufficient conditions, making explicit the mathematical proofs. We stick to the framework of stationary flows (in the mobile zone) and assume water saturation in the immobile zones. We consider a system of $n$ compartments interconnected by diffusion (see Fig. 1) whose water volumes $V_i$ $(i = 1, \cdots, n)$ are assumed to be constant over the time. One reservoir, that we label with the indice 1, is subject to

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an advection of a solute injected at a concentration $S_{in}$ with a water flow rate $Q$, and withdrawn from the same tank 1 at the same water flow rate $Q$ with a concentration $S_{out}$. We call *mobile zone* this particular reservoir and all the others $n-1$ reservoirs are called *immobile zones*. The concentrations $S_i$ ($i=1,\cdots,n$) of the solute in the $n$ tanks are given by the system of $n$ ordinary equations:

$$\begin{array}{rcl} \dot{S}_1 & = & \dfrac{Q}{V_1}(S_{in}-S_1)+\displaystyle\sum_{j=2}^{n}\frac{d_{1j}}{V_1}(S_j-S_1) \\ \dot{S}_i & = & \displaystyle\sum_{j\neq i}\frac{d_{ij}}{V_i}(S_j-S_i) \qquad i=2,\cdots,n \end{array}$$

where the parameters $d_{ij}=d_{ji}$ ($i\neq j$) denote the diffusive exchange rates of solute between reservoirs $i$ and $j$. We assume that the network of reservoirs is connected, i.e. the graph with nodes $P_i$ and edges $\overrightarrow{P_iP_j}$ when $d_{ij}\neq 0$ is strongly connected. For sake of simplicity, we shall assume $Q/V_1=1$, which is always possible by a change of the time scale of the dynamics. Let us adopt an input-output setting in matrix form:

$$\begin{array}{rcl} \dot{X} & = & AX+Bu \\ y & = & CX \end{array} \tag{1}$$

where $X$ denotes the vector of the concentrations $S_i$ ($i=1,\cdots,n$), $u=S_{in}$ the *input* and $y=S_{out}$ the *output*. The column and row matrices $B$ and $C$ are as follows

$$B^t=C=\left[\begin{array}{cccc} 1 & 0 & \ldots & 0 \end{array}\right]$$

Conversely, we consider an input-output system given in the matrix form (1) without the knowledge of the volumes $V_i$ and diffusion parameters $d_{ij}$. This typically happens when the matrix $A$ is identified from experimental measurements of flux and concentrations at different physical locations. We show in Lemma 1.1 that the matrix $A$ has to fulfill the following properties. In Section II, we shall see that how the properties of matrix $A$ allow to reconstruct $V_i$ and $d_{ij}$ (Lemma 2.3).

*Assumptions 1.1:* There exist matrices $V$ and $M$ such that

$$A=-BB^t-V^{-1}M$$

where $V$ is a positive diagonal matrix and $M$ is a symmetric matrix with entries $M_{i,j}$, $i,j=1,\ldots,n$, that fulfills

i. $M$ is irreducible
ii. $M_{i,i}>0$ for any $i$
iii. $M_{i,j}\leq 0$ for any $i\neq j$
iv. $\sum_j M_{i,j}=0$ for any $i$

*Lemma 1.1:* The matrix $A$ associated to a connected network of reservoirs with the first tank as mobile zone (and with $Q/V_1=1$) fulfills Assumption 1.1.

*Proof:* The matrix $BB^t$ has only one non null term at the first line and first column which represents the advection rate $Q/V_1=1$ at the first tank. The diagonal terms of the matrix $V$ represent the volumes of the $n$ reservoirs, therefore $V$ is a positive diagonal matrix. Condition i. is equivalent to require that the network is connected. The off-diagonal terms $M_{i,j}$ of the matrix $M$ are the opposite of the diffusive exchange rate parameters $d_{ij}$ between reservoirs $i$ and $j$ (equal to 0 if $i$ is not directly connected to $j$), which provides condition iii. The diagonal terms $M_{i,i}$ of the matrix $M$ are the sum of the diffusive terms $d_{ij}$ for the reservoirs $j$ connected to $i$, providing therefore condition ii. and iv. ■

Matrices $A$ that fulfill Assumption 1.1 are compartmental matrices, that have been extensively studied in the literature [20], [29], [22]. In the present work, we focus on two specific structures, MRMT and MINC defined in Section III after giving notation in Section II. Proofs of equivalence of any network structure that fulfills Assumption 1.1 with an MRMT or MINC structure are given in Sections IV and V. Section VI discusses these constructions on two examples. Finally, we draw conclusions with insights for geosciences.

## II. Notations and preliminary results

For sake of simplicity, we introduce the following notations for $X\in\mathbb{R}^n$ and $Z\in\mathcal{M}_{n,n}(\mathbb{R})$

$$\tilde{X}=[X_i]_{i=2,\cdots,n}\ ,\ \tilde{Z}=[Z_{i,j}]_{\substack{i=2,\cdots,n\\ j=2,\cdots,n}}$$

*diag* $(X)$ denotes the diagonal matrix whose diagonal elements are the entries of the vector $X$. We denote by *Vand* $(x_1,\cdots,x_m)$ the (square) Vandermonde matrix and by $\mathbb{1}$ the vector in $\mathbb{R}^n$ whose entries are equal to 1.

Under Assumptions 1.1, the linear system (1) is positive in the sense that for any non-negative initial state and non negative control $u(\cdot)$, state and output are non-negative for any positive time (see [12]). We denote by $\mathcal{C}_{A,B}$ and $\mathcal{O}_{A,C}$ the controllability and observability matrices of the system (1).

*Lemma 2.1:* Under Assumptions 1.1, the symmetric submatrix $\tilde{M}$ is definite positive.

*Proof:* The matrix $\tilde{M}$ is symmetric and consequently it is diagonalizable with real eigenvalues. Its diagonal terms are positive and off-diagonal negative or equal to zero. Furthermore one as

$$\begin{array}{rcl} \tilde{M}_{i,i} & = & M_{i+1,i+1}=-\displaystyle\sum_{j\neq i+1}M_{i+1,j} \\ & = & -\displaystyle\sum_{j\neq i}\tilde{M}_{i,j}-M_{i+1,1}\geq-\sum_{j\neq i}\tilde{M}_{i,j} \end{array}$$

The matrix $\tilde{M}$ is thus (weakly) diagonally dominant. As each irreducible block of the matrix $\tilde{M}$ has to be connected to the mobile zone (otherwise the matrix $A$ won't be irreducible), we deduce that at least one line of each block has to be strictly diagonally dominant. Then, each block is *irreducibly diagonally dominant* and thus invertible by Taussky Theorem (see [19, 6.2.27]). Finally, the usual argument based on Gershgorin discs give the positivity of the eigenvalues. ■

*Lemma 2.2:* Under Assumptions 1.1, the matrix $A$ is non singular. Furthermore, the dynamics admits the unique equilibrium $\mathbb{1}u$, for any constant control $u$.

*Proof:* Let $X$ be a vector such that $AX=0$. Then, one has $BB^tX=-V^{-1}MX$ or equivalently $MX=-V_1X_1B$. Let us decompose the matrix $M$ as follows

$$M=\left[\begin{array}{cc} M_{11} & L \\ L' & \tilde{M} \end{array}\right]$$

where $L$ is a row vector of length $n-1$. Then equality $MX = -V_1X_1B$ amounts to write

$$\left\{ \begin{array}{l} M_{11}X_1 + L\tilde{X} = -V_1X_1 \\ L'X_1 + \tilde{M}\tilde{X} = 0 \end{array} \right.$$

$\tilde{M}$ being invertible (Lemma 2.1), one can write $\tilde{X} = -\tilde{M}^{-1}L'X_1$ and thus $X_1$ has to fulfill

$$(M_{11} - L\tilde{M}^{-1}L')X_1 = -V_1X_1$$

From Assumptions 1.1, one has $M\mathbb{1} = 0$ which gives

$$\left\{ \begin{array}{l} M_{11} + L\tilde{\mathbb{1}} = 0 \\ L' + \tilde{M}\tilde{\mathbb{1}} = 0 \end{array} \right.$$

that implies $M_{11} - L\tilde{M}^{-1}L' = 0$. We conclude that one should have $X_1 = 0$ and then $\tilde{X} = 0$, that is $X = 0$. The matrix $A$ is thus invertible.

Finally, the system admits an unique equilibrium $X^\star = -A^{-1}Bu$ for any constant control $u$. As Assumptions 1.1 imply the equality $A\mathbb{1} = -B$, we deduce that the equilibrium is given by $X^\star = \mathbb{1}u$. ■

*Lemma 2.3:* The matrices $V$ and $M$ can be determined from the matrix $A$ as $V = \mathit{diag}(-B^tA^{-1})$ and $M = -V(A + BB^t)$.

*Proof:* One has $M = -VA - BB^t$. As the matrix $M$ satisfies $\mathbb{1}^tM = 0$, one obtains $\mathbb{1}^tVA + \mathbb{1}^tBB^t = 0$. Remark that the number $\mathbb{1}^tB$ is equal to 1 and as $A$ is invertible by Lemma 2.2, one obtains $\mathbb{1}^tV = -B^tA^{-1}$. The expressions of $V$ and $M$ follow. ■

*Lemma 2.4:* Under Assumptions 1.1, the sub-matrix $\tilde{A}$ is diagonalizable with real negative eigenvalues.

*Proof:* Notice first that the matrix $\tilde{A}$ can be written as $\tilde{A} = -\tilde{V}^{-1}\tilde{M}$. The matrix $\tilde{V}$ being diagonal with positive diagonal terms, one can consider its square root $\tilde{V}^{1/2}$, defined as a diagonal matrix with $\sqrt{\tilde{V}_i}$ terms on the diagonal, and its inverse $\tilde{V}^{-1/2}$. Then, one has

$$\tilde{V}^{1/2}\tilde{A}\tilde{V}^{-1/2} = -\tilde{V}^{-1/2}\tilde{M}\tilde{V}^{-1/2}$$

which is symmetric. So $\tilde{A}$ is similar to a symmetric matrix, and thus diagonalizable. Let $\lambda$ be an eigenvalue of $\tilde{A}$. There exist an eigenvector $X \neq 0$ such that

$$\tilde{A}X = \lambda X \Rightarrow X'\tilde{V}(\tilde{A}X) = \lambda X'\tilde{V}X \Leftrightarrow X'\tilde{M}X = -\lambda X'\tilde{V}X$$

As $\tilde{M}$ is definite positive (Lemma 2.1) as well as $\tilde{V}$, we conclude that $\lambda$ has to be negative. ■

*Lemma 2.5:* Under Assumptions 1.1, $(A, B)$ controllable is equivalent to $(A, C)$ observable.

*Proof:* Notice first that one has

$$VAV^{-1} = -BB^t - MV^{-1} = (-BB^t - V^{-1}M)' = A'$$

and by recursion $VA^kV^{-1} = (A')^k$. Then, one can write

$$\begin{array}{rcl} \mathcal{O}'_{A,C} & = & [B, A'B, \cdots, (A')^{n-1}B] \\ & = & V[V^{-1}B, AV^{-1}B, \cdots, A^{n-1}V^{-1}B]. \end{array}$$

But one has $V^{-1}B = V_1^{-1}B$. Thus

$$V_1\mathcal{O}'_{A,C} = V[B, AB, \cdots, A^{n-1}B] = V\mathcal{C}_{A,B}$$

and we conclude $\mathit{rk}(\mathcal{O}_{A,C}) = \mathit{rk}(\mathcal{C}_{A,B})$. ■

## III. The MINC and MRMT configurations

A matrix $A$ that fulfills Assumptions 1.1 and such that the sub-matrix $\tilde{A}$ is diagonal is called a *MRMT (Multi-Rate Mass Transfer)* [18] matrix. It represents a *star* connection of the immobile zones. A tridiagonal matrix $A$ that fulfills Assumptions 1.1 is called a *MINC (Multiple INteracting Continua)* [25] matrix. It represents a *serial connection* of the immobile zones.

*Lemma 3.1:* A MRMT matrix is Hurwitz.

*Proof:* Take a number

$$\gamma > \max\left(\frac{Q}{V_1} + \sum_i \frac{d_{1i}}{V_1}, \frac{d_{12}}{V_2}, \cdots, \frac{d_{1n}}{V_n}\right) .$$

Then the matrix $\gamma I + A$ is an irreducible non-negative matrix. From Perron-Frobenius Theorem [6, Th 1.4], $r = \rho(\gamma I + A)$ is a single eigenvalue of $\gamma I + A$ and there exists a positive eigenvector associated to this eigenvalue. That amounts to claim that there exists a positive eigenvector $X$ of the matrix $A$ for a single (real) eigenvalue $\lambda = r - \gamma$, and furthermore that any other eigenvalue $\mu$ of $A$ is such that $-r < \gamma + \mathit{Re}(\mu) < r$. This implies that one has $\mathit{Re}(\mu) < \lambda$. From the particular structure of MRMT matrix, such a vector $X$ has to fulfill the equalities

$$\begin{array}{rcl} -\dfrac{Q}{V_1} + \displaystyle\sum_{i=2}^{n} \dfrac{d_{1i}}{V_1}(X_i - X_1) & = & \lambda X_1 \\ d_{1i}(X_1 - X_i) & = & \lambda V_iX_i \qquad (i = 2, \cdots, n) \end{array}$$

from which one obtains

$$-\frac{Q}{V_1} = \lambda\left(X_1 + \sum_{i=2}^{n} \frac{V_i}{V_1}X_i\right) .$$

The vector $X$ being positive, we deduce that $\lambda$ is negative. ■

*Remark 3.1:* As $\mathbb{1}u$ is an equilibrium of the system (1) for any constant control $u$, we deduce that $\mathbb{1}u$ is a globally exponentially stable of the dynamics (1).

*Lemma 3.2:* For a minimal representation $(A, B, C)$ where $A$ is MRMT, the eigenvalues of the matrix $\tilde{A}$ are distinct.

*Proof:* The eigenvalues of $\tilde{A}$ for the MRMT structure are $\lambda_i = -d_{1i}/V_i$ $(i = 2, \cdots, n)$. If there exist $i \neq j$ in $\{2, \cdots, n\}$ such that $\lambda_i = \lambda_j = \lambda$, we consider the variable $S_{ij}$ (which does not correspond to a physical concentration)

$$S_{ij} = \frac{V_i}{V_i + V_j}S_i + \frac{V_j}{V_i + V_j}S_j$$

instead of $S_i, S_j$ and write equivalently the dynamics in dimension $n - 1$:

$$\begin{array}{l} \dot{S}_1 = \dfrac{Q}{V_1}(S_{in} - S_1) + \displaystyle\sum_{k \geq 2, k \neq i,j} \dfrac{d_{1k}}{V_1}(S_k - S_1) + \dfrac{d_{1ij}}{V_{ij}}(S_{ij} - S_1) \\ \dot{S}_k = \dfrac{d_{1k}}{V_k}(S_1 - S_k) \qquad k \in \{2, \cdots, n\} \setminus \{i, j\} \\ \dot{S}_{ij} = \dfrac{d_{1ij}}{V_{ij}}(S_1 - S_{ij}) \end{array}$$

with $V_{ij} = V_i + V_j$ and $d_{1ij} = -(V_i + V_j)\lambda$, which show that $(A, B, C)$ is not minimal. ■

In the coming section, we show that any representation that fulfill Assumption 1.1 is equivalent to a MRMT or MINC structure (which are two other positive realizations [5], [24], [4] of the input-output system). Therefore the MINC matrices inherit of the same properties given in Lemmas 3.1 and 3.2. There are many known ways to diagonalize the sub-matrix $\tilde{A}$ or tridiagonalize the whole matrix $A$ to obtain matrices similar to $A$ with an arrow or tridiagonal structure. The remarkable feature we prove is that there exist such transformations that preserve the signs of the entries of the matrices (i.e. Assumption 1.1 is also fulfilled in the new coordinates) so that the equivalent networks have a physical interpretation. In the coming section we first show the equivalence with MRMT and in the following section the equivalence of MRMT with MINC.

## IV. Equivalence with MRMT structure

In Proposition 4.1 below we give sufficient conditions for the equivalence, and then show in Proposition 4.2 that it is necessarily fulfilled when the system is controllable.

*Proposition 4.1:* Under Assumption 1.1, take an invertible matrix $P$ such that $P^{-1}\tilde{A}P = \Delta$, where $\Delta$ is diagonal. If all the entries of the vector $P^{-1}\tilde{\mathbb{1}}$ are non-null and the eigenvalues of $\tilde{A}$ are distinct, the matrix

$$R = \begin{bmatrix} 1 & 0 \\ 0 & -P\Delta^{-1} diag\,(P^{-1}A(2:n,1)) \end{bmatrix}$$

is invertible and such that $R^{-1}AR$ is a MRMT matrix.

*Proof:* Take a general matrix $A$ that fulfills Assumption 1.1. From Lemma 2.4, $\tilde{A}$ is diagonalizable with $P$ such that $P^{-1}\tilde{A}P = \Delta$ where $\Delta$ is a diagonal matrix. Let $G$ be the diagonal matrix

$$G = -\Delta^{-1} diag\,(P^{-1}A(2:n,1))$$

and define $\tilde{R} = PG$. Notice that one has $A\mathbb{1} = -B$ from Assumptions 1.1. The $n-1$ lines of this equality gives $A(2:n,1) + \tilde{A}\tilde{\mathbb{1}} = 0$ and one can write

$$\begin{array}{rl} & P^{-1}A(2:n,1) + P^{-1}\tilde{A}\tilde{\mathbb{1}} = 0 \\ \Leftrightarrow & P^{-1}A(2:n,1) + P^{-1}\tilde{A}PP^{-1}\tilde{\mathbb{1}} = 0 \\ \Leftrightarrow & P^{-1}A(2:n,1) + \Delta P^{-1}\tilde{\mathbb{1}} = 0 \end{array}$$

Thus having all the entries of the vector $P^{-1}A(2:n,1)$ non-null is equivalent to have all the entries of the vector $P^{-1}\tilde{\mathbb{1}}$ non null. Then $\tilde{R}$ is invertible and one has

$$\tilde{R}^{-1}\tilde{A}\tilde{R} = G^{-1}P^{-1}\tilde{A}PG = G^{-1}\Delta G = \Delta.$$

One can then consider the matrix $R \in \mathcal{M}_{n,n}$ defined as

$$R = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{R} \end{bmatrix} \quad \text{with} \quad R^{-1} = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{R}^{-1} \end{bmatrix}$$

One has

$$R^{-1}AR = \begin{bmatrix} A_{11} & A(1,2:n)\tilde{R} \\ \tilde{R}^{-1}A(2:n,1) & \Delta \end{bmatrix}$$

We show now that the matrix $R^{-1}AR$ fulfills Assumptions 1.1. One has straightforwardly

$$R^{-1}AR = -B^tB - R^{-1}V^{-1}MR\ .$$

As the irreducibility of the matrix $V^{-1}M$ is preserved by the change of coordinates given by $X \mapsto R^{-1}X$, Property i. is fulfilled. The diagonal terms of $-(R^{-1}AR + BB^t)$ are $-A_{11} - 1$ (which is positive) and the diagonal of $-\Delta$ which is also positive. Property ii. is thus satisfied. We have now to prove that column $\tilde{R}^{-1}A(2:n,1)$ and row $A(1,2:n)\tilde{R}$ are positive to show Property iii. From the definition of the matrix $G$, one has

$$\Delta = -G^{-1} diag\,(P^{-1}A(2:n,1)) = -diag\,(\tilde{R}^{-1}A(2:n,1))$$

and thus one has

$$\tilde{R}^{-1}A(2:n,1) = -\Delta\tilde{\mathbb{1}}$$

As the diagonal terms of $\Delta$ are negative, we deduce that the vector $\tilde{R}^{-1}A(2:n,1)$ is positive. As the matrix $VA$ is symmetric, one can write $V_{11}A(1,2:n) = A(2:n,1)'\tilde{V}$ and then

$$\left(V_{11}A(1,2:n)\tilde{R}\right)' = \tilde{R}'\tilde{V}A(2:n,1) = -\tilde{R}'\tilde{V}\tilde{R}\Delta\tilde{\mathbb{1}}$$

Notice that the matrix $\tilde{R}'\tilde{V}\tilde{R}$ can be written $T'T$ with $T = \tilde{V}^{1/2}\tilde{R}$, and that the matrix $T$ diagonalizes the matrix $S = \tilde{V}^{1/2}\tilde{A}\tilde{V}^{-1/2}$:

$$T^{-1}ST = \tilde{R}^{-1}\tilde{A}\tilde{R} = \Delta$$

The matrix $S$ being symmetric, it is also diagonalizable with a unitary matrix $U$ such that $U'SU = \Delta$. As the eigenvalues of $\tilde{A}$ are distinct, their eigenspaces are one-dimensional and consequently the columns of any matrix that diagonalizes $S$ into $\Delta$ have to be proportional to corresponding eigenvectors. So the matrix $T$ is of the form $UD$ where $D$ is a non-singular diagonal matrix. This implies that the matrix $\tilde{R}'\tilde{V}\tilde{R}$ is equal to $D^2$, which is a positive diagonal matrix. As $-\Delta\tilde{\mathbb{1}}$ is a positive vector, we deduce that the entries of $A(1,2:n)\tilde{R}$ are positive. Remark that $\tilde{\mathbb{1}}$ is necessarily an eigenvector of $\tilde{R}^{-1}$ (or $\tilde{R}$) for the eigenvalue 1: as one has $A\mathbb{1} = -B$, one has also $A(2:n,1) = -\tilde{A}\tilde{\mathbb{1}}$ and then

$$\begin{array}{rcl} \tilde{R}^{-1}\tilde{\mathbb{1}} & = & -\tilde{R}^{-1}\tilde{A}^{-1}A(2:n,1) = -\Delta^{-1}\tilde{R}^{-1}A(2:n,1) \\ & = & -\Delta^{-1}diag\,(\tilde{R}^{-1}A(2:n,1))\tilde{\mathbb{1}} = \tilde{\mathbb{1}} \end{array}$$

Finally, one has

$$(R^{-1}AR + BB^t)\mathbb{1} = R^{-1}A\mathbb{1} + B = -R^{-1}B + B = 0$$

which proves that Property iv. is verified.

■

*Proposition 4.2:* Under Assumptions 1.1, the entries of the vector $P^{-1}\tilde{\mathbb{1}}$ are non null for any $P$ such that $P^{-1}\tilde{A}P = \Delta$ with $\Delta$ diagonal, when the pair $(A,B)$ is controllable. Furthermore, the eigenvalues of $\tilde{A}$ are distinct.

*Proof:* From Lemma 2.4, $\tilde{A}$ is diagonalizable with $P$ such that $P^{-1}\tilde{A}P = \Delta$ where $\Delta$ is a diagonal matrix. Posit $X = P^{-1}\tilde{\mathbb{1}}$. One has

$$P^{-1}\tilde{A}^kP = \Delta^k \implies P^{-1}\tilde{A}^k\tilde{\mathbb{1}} = \Delta^kX\ , \quad k = 1, \cdots$$

This implies

$$P^{-1}\left[\tilde{\mathbb{1}},\tilde{A}\tilde{\mathbb{1}},\cdots,\tilde{A}^{n-1}\tilde{\mathbb{1}}\right]=\mathit{diag}\,(X)Vand(\lambda_1,\cdots,\lambda_n)$$

or equivalently

$$P^{-1}\mathcal{C}_{\tilde{A},\tilde{\mathbb{1}}}=\mathit{diag}\,(X)Vand(\lambda_1,\cdots,\lambda_{n-1})$$

We deduce that when $\mathcal{C}_{\tilde{A},\tilde{\mathbb{1}}}$ is full rank, $\mathit{diag}\,(X)$ and $Vand(\lambda_1,\cdots,\lambda_{n-1})$ are non-singular, that is all the entries of $X$ are non-null and the eigenvalues $\lambda_1,\cdots,\lambda_{n-1}$ are distinct. We show now that the controllability of the pair $(A,B)$ implies that the pair $(\tilde{A},\tilde{\mathbb{1}})$ is also controllable.

From the property $A\mathbb{1}=-B$, one can write

$$A=\begin{bmatrix} A_{11} & L \\ -\tilde{A}\tilde{\mathbb{1}} & \tilde{A}\end{bmatrix}$$

where $L$ is a row vector of length $n-1$. Then one has

$$A\mathbb{1}=\begin{bmatrix} -1 \\ \tilde{0}\end{bmatrix},\quad A^2\mathbb{1}=\begin{bmatrix} -A_{11} \\ \tilde{A}\tilde{\mathbb{1}}\end{bmatrix},$$

$$A^3\mathbb{1}=\begin{bmatrix} -A_{11}^2+L\tilde{A}\tilde{\mathbb{1}} \\ A_{11}\tilde{A}\tilde{\mathbb{1}}+\tilde{A}^2\mathbb{1}\end{bmatrix}$$

that are of the form

$$A^k\mathbb{1}=\begin{bmatrix} \alpha_k \\ P_k\end{bmatrix}\text{ with } P_k=\tilde{A}^{k-1}\mathbb{1}+\sum_{j\leq k-2}\beta_{k,j}\tilde{A}^j\mathbb{1}\ ,$$

for $k=2,3$. By recursion, one obtains

$$\begin{aligned} P_{k+1} &= -\alpha_k\tilde{A}\tilde{\mathbb{1}}+\tilde{A}^k\mathbb{1}+\sum_{j\leq k-2}\beta_{k,j}\tilde{A}^{j+1}\mathbb{1} \\ &= \tilde{A}^k\mathbb{1}+\sum_{j\leq k-1}\beta_{k+1,j}\tilde{A}^j\mathbb{1}\end{aligned}$$

for $k=2,\cdots$. Then, one can write

$$-\mathcal{C}_{A,B}=\mathcal{C}_{A,A\mathbb{1}}=\begin{bmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_n \\ \tilde{0} & P_2 & \cdots & P_n\end{bmatrix}$$

from which one deduces

$$\begin{aligned} \mathit{rk}\,(\mathcal{C}_{A,B})=n &\Rightarrow \mathit{rk}\,(P_2,\cdots,P_n)=n-1 \\ &\Rightarrow \mathit{rk}\,(\tilde{A}\mathbb{1},\cdots\tilde{A}^{n-1}\mathbb{1})=n-1\end{aligned}$$

One can also write $[\tilde{A}\mathbb{1},\cdots\tilde{A}^{n-1}\mathbb{1}]=\tilde{A}\mathcal{C}_{\tilde{A},\tilde{\mathbb{1}}}$ and as $\tilde{A}$ is invertible (Lemma 2.4), we finally obtain that $\mathcal{C}_{\tilde{A},\tilde{\mathbb{1}}}$ is full rank. ■

## V. Equivalence with MINC structure

As we have shown in Sec. IV that a system (1) that fulfills Assumption 1.1 with $(A,B)$ controllable is equivalent to a MRMT structure, we consider such systems only, that is

$$A=\begin{bmatrix} A_{11} & A(1,2:n) \\ A(2:n,1) & \Delta\end{bmatrix}$$

where $\Delta$ is a diagonal matrix (of size $n-1$) with distinct negative eigenvalues. We denote by $V$ the associated diagonal matrix given by Lemma 2.3. We shall use the tridiagonalization Lanczos algorithm [17]: for a symmetric matrix $S$ and a unit vector $q_1$, consider the sequence $\pi_k=(\beta_k,q_k,r_k)$ as

- $\beta_0=0$, $q_0=0$, $r_0=q_1$,
- if $\beta_k\neq 0$, define $q_{k+1}=r_k/\beta_k$, $\alpha_{k+1}=q_{k+1}'Sq_{k+1}$, $r_{k+1}=(S-\alpha_{k+1}I)q_{k+1}-\beta_kq_k$ and $\beta_{k+1}=||r_{k+1}||$.

*Lemma 5.1:* The Lanczos algorithm applied to the matrix $\Delta$ with $q_1=A(2:n,1)/||A(2:n,1)||$ provides an orthogonal unitary matrix $Q=[q_1\cdots q_{n-1}]$ such that $Q'\Delta Q$ is symmetric tridiagonal with positive terms on the sub- (or super-) diagonal.

*Proof:* We recall from [17, Th 10.1.1] that when $\mathcal{C}_{S,q_1}$ is full rank, $\pi_k$ is defined up to $n_S=\text{size}(S)$ and the orthonormal matrix $Q=[q_1\cdots q_{n_S}]$ is such that $Q'AQ$ is symmetric tridiagonal with positive terms on the sub-diagonal. As the matrix $\Delta$ is diagonal, one has

$$\mathcal{C}_{\Delta,q_1}=\mathit{Vand}\,(\lambda_1,\cdots,\lambda_{n-1})\mathit{diag}\,(q_1)$$

where $\lambda_i$ $(i=1,\cdots,n-1)$ are the diagonal elements of $\Delta$. Furthermore, as Assumptions 1.1 imply the equality $A\mathbb{1}=-B$, one has

$$q_1^t=-\frac{1}{\sqrt{\sum_{i=1}^{n-1}\lambda_i}}\begin{bmatrix}\lambda_1 & \cdots & \lambda_{n-1}\end{bmatrix}$$

As $\lambda_i$ are all distinct and non null, $q_1$ is a non null vector and the matrices $\mathit{Vand}\,(\lambda_1,\cdots,\lambda_{n-1})$, $\mathit{diag}\,(q_1)$ are full rank. Therefore $\mathcal{C}_{\Delta,q_1}$ is full rank. ■

*Proposition 5.1:* Let $A$ be a MRMT matrix such that $(A,B)$ is controllable. Let $Q$ be the orthogonal matrix given by the Lanczos algorithm applied to $\Delta$ with $q_1=A(2:n,1)/||A(2:n,1)||$. Let $U$ be the upper triangular matrix with positive diagonal entries given by the Cholesky decomposition of the symmetric matrix $Q'\tilde{V}Q$. Then the matrix

$$T=\begin{bmatrix} 1 & 0 \\ 0 & QU^{-1}\end{bmatrix}$$

is such that $T^{-1}AT$ is symmetric tridiagonal with positive entries on the sub- (or super-)diagonal.

*Proof:* Lemma 5.1 provides the existence of the matrix $Q$ such that $Q'\Delta Q$ is tridiagonal with positive terms on the sub- and super-diagonal. For convenience, we define the matrices

$$P=\begin{bmatrix} 1 & 0 \\ 0 & Q\end{bmatrix}\quad\text{and}\quad W=\begin{bmatrix} 1 & 0 \\ 0 & U\end{bmatrix}.$$

Clearly, $P$ is orthogonal, $W$ is upper triangular with positive diagonal, and one has $T=PW^{-1}$. Consider the matrix

$$P'AP=\begin{bmatrix} A_{11} & A(1,2:n)Q \\ Q'A(2:n,1) & Q'\Delta Q\end{bmatrix}.$$

For the particular choice of the first column of $Q$, one has

$$Q'A(2:n,1)=\frac{B}{||A(2:n,1)||}$$

and $Q'\Delta Q$ is triangular with positive sub-diagonal. Therefore, $P'AP$ is an upper Hessenberg matrix with positive entries on its sub-diagonal. Consider then

$$\begin{aligned} P'\mathcal{C}_{A,B} &= P'[B,AB,A^2B,\cdots] \\ &= [P'B,(P'AP)P'B,(P'A^2P)P'B,\cdots]\end{aligned}$$

Notice that one has $P'B = B$ and obtains recursively

$$\begin{array}{rcl} (P'AP)B & = & [\star, h_2, 0, \cdots\cdots, 0]^t \\ (P'A^2P)B & = & [\star, \star, h_3, 0, \cdots, 0]^t \\ \vdots & & \end{array}$$

where the numbers $h_i$ are positive. $P'\mathcal{C}_{A,B}$ is thus upper triangular with positive diagonal, as the matrix $W$. Then $T^{-1}\mathcal{C}_{A,B} = WP'\mathcal{C}_{A,B}$ is also upper triangular with positive entries on its diagonal. We then use a result about tridiagonalization of SISO systems [16, Lemma 2.2] that ensures that $T^{-1}AT$ is tridiagonal with positive entries on its sub-diagonal. Let us show that $T^{-1}AT$ is also symmetric. One has

$$T^{-1}AT = \begin{bmatrix} A_{11} & A(1,2:n)QU^{-1} \\ UQ'A(2:n,1) & UQ'\Delta QU^{-1} \end{bmatrix}$$

As the matrix $VA$ is symmetric by Assumption 1.1, one can write

$$\begin{array}{rcl} \left(A(1,2:n)QU^{-1}\right)' & = & \frac{1}{V_1}(U^{-1})'Q'\tilde{V}A(2:n,1) \\ & = & \frac{1}{V_1}(U^{-1})'U'UQ'A(2:n,1) \\ & = & \frac{1}{V_1}UQ'A(2:n,1) \end{array}$$

and as we have chosen $V_1 = 1$ we obtain $\left(A(1,2:n)QU^{-1}\right)' = UQ'A(2:n,1)$. Consider now the sub-matrix $UQ'\Delta QU^{-1}$. Notice first that the decomposition $Q'\tilde{V}Q = U'U$ implies the equalities $U' = Q'\tilde{V}QU^{-1}$ and $(U^{-1})' = UQ'\tilde{V}^{-1}Q$. Then on can write

$$\begin{array}{rcl} \left(UQ'\Delta QU^{-1}\right)' & = & (U^{-1})'Q'\Delta QU' \\ & = & (UQ'\tilde{V}^{-1}Q)Q'\Delta Q(Q'\tilde{V}QU^{-1}) \\ & = & UQ'\tilde{V}^{-1}\Delta\tilde{V}QU^{-1} \\ & = & UQ'\Delta QU^{-1} \end{array}$$

■

*Proposition 5.2:* The vector $X = T^{-1}\mathbb{1}$, where the matrix $T$ is provided by Proposition 5.1, is positive.

*Proof:* The matrices $A + BB'$ and $T^{-1}AT + BB'$ have non-negative entries outside their main diagonals. So there exists a number $\gamma > 0$ such that $I + \frac{1}{\gamma}(A + BB')$ and $I + \frac{1}{\gamma}(T^{-1}AT + BB')$ are non-negative matrices.

By Assumption 1.1, one has $A\mathbb{1} = -B$, which implies the property

$$\left(I + \frac{1}{\gamma}(A + BB')\right)\mathbb{1} = \mathbb{1}\ .$$

Thus $I + \frac{1}{\gamma}(A+BB')$ is a stochastic matrix, and we know that its maximal eigenvalue is 1 [6, Th 5.3]. As $I + \frac{1}{\gamma}(A + BB')$ and $I + \frac{1}{\gamma}(T^{-1}AT + BB')$ are similar:

$$T^{-1}\left(I + \frac{1}{\gamma}(T^{-1}AT + BB')\right)T = I + \frac{1}{\gamma}(A + BB'),$$

the maximal eigenvalue of $I + \frac{1}{\gamma}(T^{-1}AT + BB')$ is also 1. Furthermore, as $A + BB'$ is irreducible by Assumption 1.1, $I + \frac{1}{\gamma}(T^{-1}AT + BB')$ is also irreducible. The property $A\mathbb{1} = -B$ implies

$$\begin{aligned} \left(I + \frac{1}{\gamma}(T^{-1}AT + BB')\right)X &= X + \frac{1}{\gamma}(T^{-1}A\mathbb{1} + B) \\ &= X + \frac{1}{\gamma}(-T^{-1}B + B) = X \end{aligned}$$

So $X$ is an eigenvector of $I + \frac{1}{\gamma}(T^{-1}AT + BB')$ for its maximal eigenvalue 1. Finally, notice that $X = T^{-1}\mathbb{1}$ implies that the first entry of $X$ is equal to 1. Then, by Perron-Frobenius Theorem [6, Th 1.4], we conclude that $X$ is a positive vector. ■

*Proposition 5.3:* Let $A$ be a MRMT matrix such that $(A, B)$ is controllable and $R = T\mathit{diag}\,(T^{-1}\mathbb{1})$, where $T$ is provided by Proposition 5.1. Then $(R^{-1}AR, B, C)$ is an equivalent representation where $R^{-1}AR$ is a MINC matrix.

*Proof:* Let $X = T^{-1}\mathbb{1}$ and $\bar{A} = R^{-1}AR$. Define $\bar{V} = \mathit{diag}\,(X)^2$ and $\bar{M} = -\bar{V}(\bar{A} + BB')$. As $A + BB'$ is irreducible by Assumption 1.1, the similar matrix $\bar{A} + BB'$ is also irreducible, as well as $\bar{M}$ because $V$ is a diagonal invertible matrix. By Proposition 5.1, $T^{-1}AT$ is a symmetric tridiagonal matrix with positive terms on the sub- or super-diagonal. By Proposition 5.2, $X$ is a positive vector, and thus $\bar{A} = \mathit{diag}\,(X)^{-1}(T^{-1}AT)\mathit{diag}\,(X)$ is also a tridiagonal matrix with the same signs outside the diagonal. Thus, $\bar{M}$ is a tridiagonal matrix with negative terms on sub- or super-diagonal. Moreover, one has $\bar{B} = R^{-1}B = B$ and $\bar{C} = CR = C$. Finally, to show that $(\bar{A}, \bar{B}, \bar{C})$ is a MINC representation, we have to prove that $\bar{M}$ is symmetric with $\bar{M}\mathbb{1} = 0$. One has

$$\begin{array}{rcl} \bar{M} & = & -\mathit{diag}\,(X)^2(\mathit{diag}\,(X)^{-1}T^{-1}AT\mathit{diag}\,(X) + BB') \\ & = & -\mathit{diag}\,(X)T^{-1}AT\mathit{diag}\,(X) - X_1^2.BB'. \end{array}$$

where $X_1 = 1$. The matrix $\bar{M}$ is thus symmetric. One has also

$$\begin{array}{rcl} \bar{M}\mathbb{1} & = & -\mathit{diag}\,(X)T^{-1}AT\mathit{diag}\,(X)\mathbb{1} - BB'\mathbb{1} \\ & = & -\mathit{diag}\,(X)T^{-1}ATX - B \\ & = & -\mathit{diag}\,(X)T^{-1}AT(T^{-1}\mathbb{1}) - B \\ & = & -\mathit{diag}\,(X)T^{-1}A\mathbb{1} - B \\ & = & \mathit{diag}\,(X)T^{-1}B - B \\ & = & \mathit{diag}\,(X)B - B = 0 \end{array}$$

■

*Remark 5.1:* One can easily show that the volumes matrix $\bar{V}$ of an equivalent representation can be determined as $\bar{V} = R^tVR$, where $R$ is the transformation matrix.

## VI. Examples and discussion

We first give an example that illustrates the necessity of the controllability property for the equivalence construction. We present a second example that shows that MRMT or MINC forms can be efficient ways to obtain reduced models.

Consider a network of 4 tanks with $V_1 = 1$, $V_2 = 1$, $V_3 = 2$, $V_4 = 3$ and $d_{12} = 1$, $d_{13} = 2$, $d_{14} = 3$, $d_{23} = 3$, $d_{24} = 3$:

$$A = \begin{bmatrix} -7 & 1 & 2 & 3 \\ 1 & -7 & 3 & 3 \\ 1 & \frac{3}{2} & -\frac{5}{2} & 0 \\ 1 & 1 & 0 & -2 \end{bmatrix}$$

At the first look, this structure does not exhibit any special property or symmetry that could make believe that it is non minimal. One has $\tilde{A}\tilde{\mathbb{1}} = -\tilde{\mathbb{1}}$ but here $A$ satisfies $A(2:4,1) = \tilde{\mathbb{1}}$. Consequently the vector $A(2:4,1)$ is an eigenvector of the matrix $\tilde{A}$ for the eigenvalue $-1$. If the multiplicity of $-1$ was more than 1, then $\lambda = -9.5$ should be an eigenvalue of $\tilde{A}$, as the trace of $\tilde{A}$ is $-11.5$. But an eigenvector $X$ of $\tilde{A}$ fulfills

$$\begin{array}{rcl} -7X_1 + 3X_2 + 3X_3 & = & \lambda X_1 \\ 1.5X_1 - 2.5X_2 & = & \lambda X_2 \\ X_1 - 2X_3 & = & \lambda X_3 \end{array}$$

one should have $(\lambda + 7)X_1 - 3X_2 - 3X_3 = 0$ with

$$X_2 = \frac{1.5}{\lambda + 2.5} X_1 \ , \ X_3 = \frac{1}{\lambda + 2} X_1 \quad (\text{and } X_1 \neq 0)$$

which is not possible for $\lambda = -9.5$. Then, any matrix $P$ that diagonalizes $\tilde{A}$ should have one column proportional to the eigenvector $\tilde{\mathbb{1}}$, which amounts to have $P^{-1}\tilde{\mathbb{1}}$ with exactly one non-null entry. Thus one cannot apply Proposition 4.1 to obtain an equivalent MRMT system of the same dimension. The pair $(A, B)$ is indeed non controllable, even though the matrix $\tilde{A}$ has distinct eigenvalues, as one has

$$AB = \begin{bmatrix} -7 \\ 1 \\ 1 \\ 1 \end{bmatrix} , \ A^2B = \begin{bmatrix} 55 \\ -8 \\ -8 \\ -8 \end{bmatrix} = -B - 8AB$$

from which one deduce $rk\,(\mathcal{C}_{A,B}) = 2$. This system admits a minimal representation of dimension 2 that can be found by gathering the immobile zones in one of volume $\bar{V} = V_2 + V_3 + V_4 = 6$ and solute concentration

$$\bar{S} = \frac{V_2S_2 + V_3S_3 + V_4S_4}{\bar{V}} = \frac{S_2 + 2S_3 + 3S_4}{6}$$

One can check that $(S_1, \bar{S})$ are solutions of the system

$$\begin{array}{rcl} \dot{S}_1 & = & -7S_1 + 6\bar{S} + u \\ \dot{\bar{S}} & = & S_1 - \bar{S} \end{array}$$

Consider now the network of 5 unitary volumes with

$$A = \begin{bmatrix} -3 & 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 \\ 1 & 0 & -3 & 1 & 1 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 1 & 1 & -2 \end{bmatrix}.$$

One can check that the pair $(A, B)$ is controllable. Then, the constructions of Sections IV and V give the following equivalent MRMT and MINC matrices:

$$A_{MRMT} \simeq \begin{bmatrix} -4 & 0.33 & 0.17 & 1 & 1.5 \\ 8.2 & -8.2 & 0 & 0 & 0 \\ 3.3 & 0 & -3.3 & 0 & 0 \\ 1 & 0 & 0 & -1 & 0 \\ 0.52 & 0 & 0 & 0 & -0.52 \end{bmatrix},$$

$$A_{MINC} \simeq \begin{bmatrix} -4 & 3 & 0 & 0 & 0 \\ 1.7 & -5 & 3.3 & 0 & 0 \\ 0 & 3.6 & -4.1 & 0.53 & 0 \\ 0 & 0 & 2.5 & -2.9 & 0.45 \\ 0 & 0 & 0 & 0.95 & -0.95 \end{bmatrix}.$$

Differently to that original network, the magnitude of the values of volumes and diffusive exchange rates are significantly different among compartments, opening the door of possible model reduction dropping some compartments.

For the equivalent MRMT structure, one obtains $V_1 = 1$, $V_2 \simeq 0.04$, $V_3 \simeq 0.05$, $V_4 = 1$, $V_5 \simeq 2.9$, $d_{12} \simeq 0.33$, $d_{13} \simeq 0.17$, $d_{14} = 1$, $d_{15} \simeq 1.5$, and notices that zones 2 and 3 are of relatively small volumes (compared to the total volume of the system which is equal to 5) and connected to the mobile zone with relatively small diffusive parameters. Then, one may expect to have a good approximation with a reduced MRMT model dropping zones 2 and 3. Keeping the volumes $V_1$, $V_4$, $V_5$ with the parameters $d_{14}$, $d_{15}$, one obtains the 3 compartments MRMT matrix

$$\tilde{A}_{MRMT} \simeq \begin{bmatrix} -3.5 & 1 & 1.5 \\ 1 & -1 & 0 \\ 0 & 0.5 & -0.5 \end{bmatrix}.$$

For the equivalent MINC structure, one obtains $V_1 = 1$, $V_2 \simeq 1.8$, $V_3 \simeq 1.7$, $V_4 \simeq 0.36$, $V_5 \simeq 0.17$, $d_{12} = 3$, $d_{23} = 6$, $d_{34} \simeq 0.89$, $d_{45} \simeq 0.16$. Here, one notices that the two last volumes are relatively small and connected with relatively small diffusion terms. Keeping the volumes $V_1$, $V_2$, $V_3$ with the parameters $d_{12}$, $d_{23}$, one obtains the reduced model

$$\tilde{A}_{MINC} \simeq \begin{bmatrix} -4 & 3 & 0 \\ 1.67 & -5 & 3.33 \\ 0 & 3.6 & -3.6 \end{bmatrix}.$$

The Nyquist diagrams associated to the original model $A$ and the reduced $\tilde{A}_{MRMT}$, $\tilde{A}_{MINC}$ are reported on Fig. 2, showing the quality of the approximation with only three compartments derived from the MRMT or MINC representations. There exist many reduction methods in the literature, but a reduction through MRMT or MINC has the advantage to obtain easily reduced models with a physical meaning.

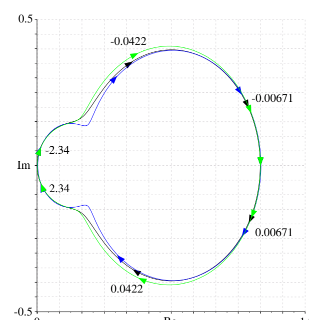


Figure 2. Nyquist diagrams for $A$ (black), $\tilde{A}_{MRMT}$ (blue), $\tilde{A}_{MINC}$ (green)

## VII. Conclusion

We have shown that a general network structure admits equivalent "star" (MRMT) or "series" (MINC) structures, that are commonly considered in geosciences to represent soil porosity in mass transfers. In this way, we reconcile these two approaches. Practically, this means that when the structure is unknown, or partially known, one can use equivalently the most convenient structure to identify the parameters or use some a priori knowledge. We have also shown the crucial role played by the controllability property of the model. Although there is no particular control issue in the representations of mass transfers, controllability is a necessary condition to obtain equivalence with the multi-rate mass transfer (MRMT) structures of depth one, introduced by Haggerty and Gorelick in 1995 [18], or the multiple interacting continua structure (MINC) [25]. This condition is related to the minimal representation, that is not necessarily fulfilled for such structures even for non-singular irreducible network matrices with distinct eigenvalues. Examples of equivalent MRMT and MINC representations have shown that it provides also a simple and efficient technique to obtain reduced models.

From a geosciences view point, this analysis shows the existence of both identifiable and non-identifiable porosity structures from data. Input-output signals are typical of conservative tracer tests where non-reactive tracers are injected in an upstream well and analyzed in a downstream well [13]. Identifiable structures could thus be calibrated on tracer tests [1]. The identified structure is however not unique as shown on examples, meaning that a porosity structure cannot be fully characterized by a tracer test. This is an advantage rather than a drawback as the porosity structure should support both conservative and reactive transport [10], [9].

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