Abstract. A decomposition principle for nonlinear dynamic compartmental systems is introduced in the present paper. This theory is based on the novel mutually exclusive and exhaustive system and subsystem decomposition methodologies. A deterministic mathematical method is developed for the dynamic analysis of nonlinear compartmental systems based on the proposed theory. The dynamic method enables tracking the evolution of all initial stocks, external inputs, and arbitrary intercompartamental flows as well as the associated storages derived from these stocks, inputs, and flows individually and separately within the system. Multiple system flows and associated storages transmitted from one compartment directly or indirectly to any other or along a given flow path are then analytically characterized, systematically classified, and mathematically formulated. Thus, the dynamic influence of one compartment, in terms of flow and storage transfer, directly or indirectly on any other compartment is ascertained. Consequently, new mathematical system analysis tools are formulated as quantitative system indicators. The proposed mathematical method is then applied to various models from literature to demonstrate its efficiency and wide applicability.

Key words. nonlinear decomposition principle, fundamental matrix solutions, dynamic system and subsystem decomposition, nonlinear dynamic compartmental systems, diac flows and storages, dynamic input-output analysis, dynamic input-output economics, epidemiology, infectious diseases, toxicology, pharmacokinetics, neural networks, chemical and biological systems, control theory, information theory, information diffusion, social networks, traffic flow

AMS subject classifications. 34A34, 35A24, 37C60, 37N25, 37N40, 37G60, 91B74, 92B20, 92C42, 92D30, 92D40, 93C15, 94A15

1. Introduction. Compartmental systems are mathematical abstractions of networks composed of discrete, homogeneous, interconnected components that approximate the behavior of continuous physical systems. The system compartments are interrelated through the flow of a conserved quantity, such as energy, matter, information, or currency between them and their environment based on conservation principles. Therefore, for an accurate quantification of the compartmental system functions, analytic and explicit formulation of system flows and the associated storages generated by these flows are of paramount importance.

Today’s major natural problems involve change, and this makes the need for dynamic and analytical methods of nonlinear system analysis not only appropriate, but also urgent. Dynamic methods for nonlinear compartmental system analysis have remained a long-standing, open problem. Sound rationales are offered in literature for compartmental system analysis, but they are for special cases, such as linear models and static systems [11, 12, 7, 13]. Various mathematical aspects of compartmental systems are studied in literature [9, 1].

This is the first manuscript in literature that potentially addresses the mismatch between the needs for dynamic nonlinear compartmental system analysis and current static and computational simulation methods. The manuscript is structured in three levels: theory, methods, and applications. The underlying novel mathematical theory will be called the nonlinear decomposition principle. The theory is based on the dynamic system and subsystem decomposition methodologies. A deterministic mathematical method is then developed for the dynamic analysis of nonlinear compartmental systems.

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The system decomposition methodology explicitly generates mutually exclusive and exhaustive subsystems, each driven by a single external input and initial stock, that are running within the original system and have the same structures and dynamics as the system itself. Consequently, the composite compartmental throughflows and storages are dynamically decomposed into the subcompartmental subthroughflow and substorage segments based on their constituent external and initial sources. The system decomposition methodology yields the subthroughflow and substorage matrix functions that respectively represent the throughflows and storages derived from the external inputs and initial stocks. Equipped with these matrix measures, the system partitioning ascertain the dynamic distribution of external inputs and initial stocks as well as the organization of the associated storages generated by these inputs and stocks individually and separately within the system. In other words, the system decomposition enables dynamically tracking the evolution of the initial stocks and external inputs as well as the associated storages derived from the stocks and inputs individually and separately within the system. Mathematically, the proposed methodology enables tracking the evolution of the initial conditions, source terms, and associated state variables individually and separately within nonlinear dynamic systems for the first time in literature.

The subsystems are then further decomposed dynamically along a set of mutually exclusive and exhaustive directed subflow paths. The subsystem decomposition methodology yields the transient and the dynamic direct, indirect, acyclic, cycling, and transfer (diact) flows and the associated storages generated by these flows. Arbitrary composite intercompartmental flows and associated storages can dynamically be decomposed into the constituent transient subflow and substorage segments along a given set of subflow paths within the subsystems through this decomposition. These transient subflows and associated substorages represent the dynamic distribution of arbitrary intercompartmental flows and the organization of the associated storages generated by these flows along the given subflow paths. Consequently, the subsystem decomposition enables dynamically tracking the fate of arbitrary intercompartmental flows and associated storages within the subsystems. Therefore, the spread of an arbitrary flow or storage segment from one compartment to the entire system can be determined and monitored. Moreover, a history of compartments visited by arbitrary system flows and storages can also be compiled. Based on the concept of transient flow and storage, the dynamic diact flows and storages transmitted from one compartment, directly or indirectly, to any other in the system are analytically characterized, systematically classified, and mathematically formulated for the quantification of intercompartmental flow and storage dynamics. In summary, the proposed mathematical method, as a whole, decomposes the system flows and storages to the utmost level.

The direct influence of one compartment on another can be determined through the state of the art techniques. The proposed methodology, however, makes the dynamic analysis of both direct and indirect influence of one compartment, in terms of flow and storage transfer, on any other possible in a complex nonlinear system for the first time. This methodology, therefore, constructs a base for the development of dynamic system analysis tools as quantitative system indicators. Multiple such dynamic system measures are formulated and used in the analysis of illustrative models in Section 3 and Appendix E to demonstrate the wide applicability and efficiency of the proposed methodology. The results indicate that the proposed method provides significant advancements in the theory, methodology, and practicality of the current nonlinear dynamic compartmental system analysis.
The applicability of the proposed method extends to various realms regardless of their naturogenic and anthropogenic nature, such as ecology, economics, pharmacokinetics, chemical reaction kinetics, epidemiology, chemical and biomedical systems, neural networks, social networks, and information science. In particular, the proposed methodology can be considered as an extension of input-output economics, developed for static systems several decades ago, to fully nonlinear dynamic compartmental systems for the first time in literature [11, 12]. Essentially, the methodology is applicable to real-world phenomena where compartmental models of conserved quantities can be constructed. Considering hypothetical complex networks with multiple interacting compartments, the compartments can, for example, model species in an ecosystem, financial institutions in a financial system, organs in an organism, molecules in a chemical reaction, neurons in a neural network, or communities in a social network. The conserved quantities that need to be investigated within these systems, then, would be a nutrient, money, a certain drug, a specific type of atom, particular ions, or a piece of information, respectively.

An illustrative SIRS model from epidemiology is analyzed in detail in Section 3, and more case studies are presented from ecosystem ecology in the Appendices. The SIRS model consists of three compartments that represent the populations of three groups: the susceptible or uninfected, $S$, infectious, $I$, and recovered or immune, $R$. The model determines the number of individuals infected with a contagious illness over time [10]. It is shown that, the proposed dynamic system decomposition methodology decomposes each of the composite SIR populations into subpopulations based on their constituent sources of the initial and newborn populations. Consequently, the method enables tracking the evolution of the health states of the newborn or initial SIR populations individually and separately within the total population. The proposed dynamic subsystem decomposition methodology then enables tracking the evolution of the health states of an arbitrary population in any of the SIR groups along a given infection path. Therefore, the effect of an arbitrary population on any other group in terms of the spread of the disease, through not only direct but also indirect interactions, can be ascertained. Consequently, the spread of the disease from an arbitrary population to the entire system can be determined and monitored. It is worth noting for a comparison that the solution to the SIRS model through the state of the art techniques can only provide the composite SIR populations without distinguishing subpopulations based on their constituent sources.

The paper is organized as follows: the mathematical method is introduced in Sections 2.1, 2.2, and 2.5, the nonlinear fundamental matrix solutions and decomposition principle are introduced in Sections 2.3 and 2.4, system analysis is discussed in Section 2.6, and results, examples, discussions, and conclusions follow at the end of the manuscript.

2. Methods. The nonlinear decomposition principle for dynamic compartmental systems is introduced in this section based on the novel dynamic system and subsystem decomposition methodologies. A deterministic mathematical method is then developed for the dynamic analysis of nonlinear compartmental systems. The proposed theory and method construct a base for the formulation of new system analysis tools, such as the fundamental matrices and the diact flows and storages, as quantitative system indicators. These novel concepts and quantities are defined and formulated in this section.

2.1. Compartmental Systems. We assume that components of a physical system are modeled as compartments that are interconnected through flow of energy,
matter, or currency. In such a compartmental model, the state variable \( x_i(t) \) represents the amount of storage in compartment \( i \), and \( f_{ij}(t, x) \) represents the non-negative flow rate from compartment \( j \) to \( i \) at time \( t \) (see Fig. 1).

Let the governing equations for this nonlinear dynamic compartmental system, formulated based on conservation principles, be given as

\[
\dot{x}(t) = \tau(t, x)
\]

with the initial conditions \( x(t_0) = x_0 \). The state vector \( x(t) = [x_1(t), \ldots, x_n(t)]^T \) is a differentiable function for time, \( t \). The function \( \tau(t, x) = [\tau_1(t, x), \ldots, \tau_n(t, x)]^T \) will be called the net throughflow rate vector and expressed as

\[
\tau(t, x) = \hat{\tau}(t, x) - \tilde{\tau}(t, x)
\]

where the respective inward and outward throughflow rate vector functions are

\[
\hat{\tau}(t, x) = [\hat{\tau}_1(t, x), \ldots, \hat{\tau}_n(t, x)]^T \quad \text{and} \quad \tilde{\tau}(t, x) = [\tilde{\tau}_1(t, x), \ldots, \tilde{\tau}_n(t, x)]^T.
\]

The components of the throughflow vectors can further be expanded as

\[
\hat{\tau}_i(t, x) := \sum_{j=0}^{n} f_{ij}(t, x) \quad \text{and} \quad \tilde{\tau}_i(t, x) := \sum_{j=0}^{n} f_{ji}(t, x)
\]

for \( i = 1, \ldots, n \). Index \( j = 0 \) represents the system exterior.

Let \( \Omega \subset \mathbb{R}^n \) be a domain (connected, open set) and \( I \subset \mathbb{R} \) be an open interval. We assume that \( f_{ij}(t, x) \) is a continuous and continuously differentiable function of \( x \) on \( I \times \Omega \). Because of being linear combinations of \( f_{ij}(t, x), \hat{\tau}_i(t, x), \tilde{\tau}_i(t, x) \), and \( \tau_i(t, x) \) have also the same properties. These conditions imply the existence and uniqueness of the solutions to the governing system, Eq 2.2.

We assume the following conditions on the flow rate functions:

\[
f_{ij}(t, x) := q_{ij}^x(t, x) x_j(t), \quad f_{ij}(t, x) \geq 0, \quad \text{and} \quad f_{ii}(t, x) = 0, \quad \forall i, j
\]

where \( q_{ij}^x(t, x) \) has the same properties as \( f_{ij}(t, x) \). The first condition guarantees non-negativity of the state variables, that is, \( x_j(t) \geq 0 \) for all \( j \). The external input and output flow rates, \( z_i(t, x) \) and \( y_i(t, x) \), into and from compartment \( i \) are denoted by

\[
z_i(t, x) := f_{io}(t, x) \quad \text{and} \quad y_i(t, x) := f_{oi}(t, x).
\]

The system can then be rewritten componentwise as

\[
\dot{x}_i(t) = \hat{\tau}_i(t, x) - \tilde{\tau}_i(t, x)
\]

for \( i = 1, \ldots, n \). When the external input and output are separated, the system Eq 2.5 takes the following standard form:

\[
\dot{x}_i(t) = \left( z_i(t, x) + \sum_{j=1}^{n} f_{ij}(t, x) \right) - \left( y_i(t, x) + \sum_{j=1}^{n} f_{ji}(t, x) \right)
\]

with the initial conditions \( x_i(t_0) = x_{i,0} \), for \( i = 1, \ldots, n \). If \( z_i(t, x) > 0 \) or \( x_{i,0} > 0 \) for all \( i \), these positive inputs or initial conditions ensure that the state variables are always strictly positive, \( x_i(t) > 0 \).

The proposed methodology is designed for conservative compartmental systems, as defined below.
DE**NITION 2.1.** A dynamical system will be called compartmental if it can be expressed in the form of Eq. 2.6 with the conditions given in Eq. 2.4. The compartmental system will be called conservative if all internal flow rates add up to zero when the system is closed, that is, when there is neither external input nor output. Formally,

\[
\sum_{i=1}^{n} \dot{x}_i(t) = 0 \quad \text{when} \quad z(t, x) = y(t, x) = 0 \quad \text{on} \quad I
\]

where 0 is the zero vector of size n.

We define the state, input, and output matrix functions as

\[
X(t) := \text{diag}(x(t)), \quad Z(t, x) := \text{diag}(z(t, x)), \quad \text{and} \quad Y(t, x) := \text{diag}(y(t, x)),
\]

respectively. The notation \(\text{diag}(x(t))\) represents the diagonal matrix whose diagonal elements are the elements of vector \(x(t)\), and \(\text{diag}(X(t))\) represents the diagonal matrix whose diagonal elements are the same as the diagonal elements of matrix \(X(t)\). The external input and output vectors are

\[
z(t, x) = [z_1(t, x), \ldots, z_n(t, x)]^T \quad \text{and} \quad y(t, x) = [y_1(t, x), \ldots, y_n(t, x)]^T,
\]

respectively. Clearly,

\[
x(t) = X(t) \mathbf{1}, \quad z(t, x) = Z(t, x) \mathbf{1}, \quad \text{and} \quad y(t, x) = Y(t, x) \mathbf{1}
\]

where \(\mathbf{1}\) is the vector of size \(n\) whose entries are all equal to 1. Excluding the external input and output, we define the flow rate matrix function as the matrix of intercompartmental direct flows:

\[
F(t, x) := (f_{ij}(t, x)).
\]

Using these notations, \(\mathbf{\tau}(t, x)\) and \(\mathbf{\hat{\tau}}(t, x)\), defined in Eq. 2.3, can be expressed in compact form as

\[
\mathbf{\tau}(t, x) = Z(t, x) \mathbf{1} + F(t, x) \mathbf{1} = z(t, x) + F(t, x) \mathbf{1},
\]

\[
\mathbf{\hat{\tau}}(t, x) = Y(t, x) \mathbf{1} + F^T(t, x) \mathbf{1} = y(t, x) + F^T(t, x) \mathbf{1}.
\]

The governing equation, Eq. 2.6, then becomes

\[
\dot{x}(t) = (z(t, x) + F(t, x) \mathbf{1}) - (y(t, x) + F^T(t, x) \mathbf{1})
\]

with the initial conditions \(x(t_0) = x_0\). Separating external inputs from the intercompartmental flows and outputs, the governing equation, Eq. 2.10, takes the following form:

\[
\dot{x}(t) = z(t, x) + F(t, x) \mathbf{1}
\]

where

\[
F(t, x) := F(t, x) - Y(t, x) - \text{diag}(F^T(t, x) \mathbf{1}) = F(t, x) - \mathbf{T}(t, x),
\]

and \(\mathbf{T}(t, x) := \text{diag}(\mathbf{\tau}(t, x)) = Y(t, x) + \text{diag}(F^T(t, x) \mathbf{1})\).
2.2. Dynamic System Decomposition. We introduce the dynamic system decomposition or subcompartmentalization methodology in this section for partitioning the original system into mutually exclusive and exhaustive subsystems. By mutual exclusiveness we mean that transactions are possible only within corresponding subcompartments of the same subsystem. By exhaustiveness we mean that all subsystems sum to the entire system so partitioned (see Figs. 1 and 2). The system decomposition methodology dynamically decomposes composite compartmental throughflows and storages into subcompartmental segments based on their constituent external and initial sources. Therefore, this decomposition ascertains the distribution of external inputs and initial stocks as well as the organization of the associated storages derived from these inputs and stocks individually and separately within the system.

The initial subsystem is driven by all initial stocks. Except the initial subsystem, each subsystem is generated by a single external input. Therefore, the number of subcompartments in each compartment is equal to the number of inputs (or compartments), plus one for the initial stocks. If an input or all initial conditions are zero, the corresponding subsystem is null. Consequently, in a system with $n$ compartments, each compartment has $n + 1$ subcompartments, and, therefore, the system has $n + 1$ subsystems, indexed by $k = 0, \ldots, n$. The initial subsystem ($k = 0$) represents the evolution of the initial stocks, contains no external input, and has the same initial conditions as the original system. The initial conditions for all the other subcompartments are zero. The dynamic system decomposition methodology has two components: state and flow rate decompositions, as introduced in this section.

The initial subsystem will be further decomposed into initial subsystems for a similar analysis of the distribution of intercompartmental flows and the organization of the associated storage derived from the initial stocks. This dynamic initial system decomposition methodology is introduced in Appendix A (see Fig. 1 and 2).

2.2.1. State Decomposition. In this section, we will introduce the state decomposition methodology.

We use the notation of $x_{i_k}(t)$ to represent the $k^{th}$ substate of the $i^{th}$ state variable. Each substate $x_{i_k}(t)$ represents the storage in subcompartment $i_k$ at time $t$, which identifies the portion of the storage in compartment $i$, $x_i(t)$, that is generated by external input into compartment $k \neq 0$, $z_k(t, x)$, during $[t_0, t]$ (see Fig. 1). Therefore, $x_{i_k}(t)$ will also be called substorage function. The $0^{th}$ substate of the $i^{th}$ state, $x_{i_0}(t)$, will be called the initial substorage or substate of $x_i(t)$, and initially it is equal to the initial condition $x_{i,0}$. The initial substates represent the evolution of the initial stocks for $t > t_0$. Therefore, all substate variables are assumed to be zero initially, except the initial substate. Consequently, due to the mutually exclusiveness and exhaustiveness of the system decomposition, we have

$$x_i(t) = \sum_{k=0}^{n} x_{i_k}(t)$$

for $i = 1, \ldots, n$, and the initial conditions are

$$x_{i_k}(t_0) = \begin{cases} x_i(t_0) = x_{i,0}, & k = 0 \\ 0, & k \neq 0 \end{cases}$$

Similar to the original system, the initial subcompartments will further be decomposed into $n$ subcompartments, as explained in Appendix A.1 (see Fig. 2). We will use the notation $x_{i_k,0}(t)$ for the $k^{th}$ substate of the $i^{th}$ initial substate function.
or \( x_{ik}(t) := x_{ik,0}(t) \) for notational convenience. Based on this further decomposition of the initial substates, we also have

\[
(2.15) \quad x_{i0}(t) = x_i(t) = \sum_{k=1}^{n} x_{ik}(t),
\]

for \( i = 1, \ldots, n \), and the corresponding initial conditions become

\[
(2.16) \quad x_{ik}(t_0) = \delta_{ik} x_{i0}(t_0) = \begin{cases} x_{i0}(t_0) = x_{i,0}, & i = k \\ 0, & i \neq k \end{cases}
\]

Let the \( k^{th} \) substate and initial substate vector functions be defined as

\[
(2.17) \quad \mathbf{x}_k(t) := [x_{i_k}(t), \ldots, x_{n_k}(t)]^T, \quad k = 0, \ldots, n \quad \text{and} \quad \mathbf{x}_k(t) := [x_{i_k}(t), \ldots, x_{n_k}(t)]^T, \quad k = 1, \ldots, n.
\]

The vector function \( \mathbf{x}(t) \) of all initial substate and substate variables for the decomposed system will be denoted by

\[
\mathbf{x}(t) := \begin{bmatrix} \mathbf{x}_1^T(t), \ldots, \mathbf{x}_n^T(t) \end{bmatrix}^T = \begin{bmatrix} x_{11}(t), \ldots, x_{n1}(t), x_{12}(t), \ldots, x_{n2}(t), \ldots, x_{1n}(t), \ldots, x_{nn}(t) \end{bmatrix}^T \in \mathbb{R}^{2n^2}.
\]

The state decompositions formulated in Eqs. 2.13 and 2.15 and corresponding initial values in Eqs. 2.14 and 2.16 can then be expressed in vector form as

\[
(2.18) \quad \mathbf{x}(t) := \mathbf{x}_0(t) = \mathbf{x}_1(t) + \ldots + \mathbf{x}_n(t), \quad \mathbf{x}_k(t_0) = x_{k,0} e_k, \quad \mathbf{x}(t_0) = \mathbf{x}_0, \quad \text{and} \quad \mathbf{\bar{x}}(t) := x_1(t) + \ldots + x_n(t), \quad \mathbf{\bar{x}}(t_0) = \mathbf{0}, \quad \mathbf{\bar{x}}(t_0) = \mathbf{0},
\]
for \( k = 1, \ldots, n \), where \( e_k \) is the standard elementary unit vector of size \( n \). The vector functions \( \mathbf{x}(t) \) and \( \bar{\mathbf{x}}(t) \) are the partitions of the state variable \( \mathbf{x}(t) \), which represent the storages derived from the initial stocks and generated by external inputs within the system, respectively. Equations 2.13 and 2.15 also imply that

\[
(2.19) \quad x_i(t) = \sum_{k=1}^{n} x_{ik}(t) + x_{ik}(t) \quad \Rightarrow \quad \dot{x}_i(t) = \sum_{k=1}^{n} \dot{x}_{ik}(t) + \dot{x}_{ik}(t).
\]

In vector notation, that is,

\[
(2.20) \quad \dot{\mathbf{x}}(t) = \dot{\mathbf{x}}(t) + \dot{\mathbf{x}}(t) = (\dot{x}_1(t) + \ldots + \dot{x}_n(t)) + (\dot{x}_1(t) + \ldots + \dot{x}_n(t)).
\]

We define the substate and \( k \text{th} \) substate matrix functions, \( X(t) \) and \( \lambda_k(t) \), as

\[
(2.21) \quad X(t) := (x_{ik}(t)) = [x_1(t) \ldots x_n(t)] \quad \text{and} \quad \lambda_k(t) := \text{diag}(x_k(t))
\]

for \( k = 0, \ldots, n \), together with the initial conditions given in Eq. \ref{eq:init}

\[
(2.22) \quad X(t_0) = 0, \quad \lambda_k(t_0) = 0 \quad \text{for} \quad k \neq 0, \quad \text{and} \quad \lambda_0(t_0) = \text{diag}(x_0).
\]

These matrices will, alternatively, be called the substorage and \( k \text{th} \) substorage matrix functions, respectively. Note that we use the notation 0 for both the \( n \times 1 \) zero vector and \( n \times n \) zero matrix, which should be distinguished from the context. We then have

\[
(2.23) \quad \mathbf{x}(t) = \mathbf{x}(t) + \bar{\mathbf{x}}(t) = x_0(t) + X(t) 1 \quad \text{and} \quad x_k(t) = \lambda_k(t) 1.
\]

The dynamic state decomposition methodology can be schematized as follows:

\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\vdots \\
\dot{x}_n
\end{bmatrix} = \begin{bmatrix}
x_{10} \\
x_{20} \\
\vdots \\
x_{n0}
\end{bmatrix} + \begin{bmatrix}
x_{11} & x_{12} & \cdots & x_{1n} \\
x_{21} & x_{22} & \cdots & x_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
x_{n1} & x_{n2} & \cdots & x_{nn}
\end{bmatrix} \begin{bmatrix}
1 \\
1 \\
\vdots \\
1
\end{bmatrix}
\]

\[
\begin{align*}
\text{2.2.2. Flow Rate Decomposition.} & \quad \text{For a coherent system partitioning, flow rates are also decomposed into flow segments that will be called the subflow rate functions. These subflow rates represent the rate of flow segments between the sub-compartments (see Fig. \ref{fig:substate}).} \\
& \quad \text{We assume that external input } z_i(t, \mathbf{x}) \text{ enters into the system at subcompartment } i_i \text{ (see Fig. 1). Therefore, the input decomposition can be expressed as}
\end{align*}
\]

\[
(2.24) \quad z_{ik}(t, \mathbf{x}) := \delta_{ik} z_i(t, \mathbf{x}) = \begin{cases} 
z_i(t, \mathbf{x}), & i = k \\
0, & i \neq k
\end{cases}
\]

The flow rates, \( f_{ij}(t, \mathbf{x}) \), and output functions, \( y_j(t, \mathbf{x}) \), will also be decomposed into the subflow rate functions. First, we define the flow intensity directed from compartment \( j \) to \( i \) at time \( t \) as

\[
(2.25) \quad q_{ij}^x(t, \mathbf{x}) = \frac{f_{ij}(t, \mathbf{x})}{x_j(t)}
\]
Fig. 2. Schematic representation of a dynamic flow rate decomposition in a three-compartment model system. The figure illustrates the subcompartmentalization of compartment 1 and the corresponding flow rate decomposition from compartment 1 to others, j, $f_{j1}(t,x)$. The figure also illustrates further decomposition of the initial subcompartment and the corresponding initial subflow rate function, $f_{j0i0}(t,x)$ (both dark gray).

for $i = 0, \ldots, n$, $j = 1, \ldots, n$, as formulated in Eq. 2.4. Note that $q_{ij}^x(t,x)$ are sometimes called transfer coefficients, technical coefficients in economics, or stoichiometric coefficients in chemistry. The subflow rates are then defined to be the flow segments proportional to the flow intensities with the proportionality factors of $x_j(t)$. That is,

$$f_{ikj_k}(t,x) := x_j(t) \frac{f_{ij}(t,x)}{x_j(t)} = x_j(t) \frac{f_{ij}(t,x)}{x_j(t)}$$

for $i, k = 0, \ldots, n$ and $j = 1, \ldots, n$. The index 0_k is equivalent to the index 0, and both represent the system exterior. We will use index 0 in both cases for notational convenience. Similar to Eq. 2.4, the functions $f_{ikj_k}(t,x) \geq 0$ represent nonnegative subflow rates from subcompartment $j_k$ to $i_k$ and $f_{ik0}(t,x) = 0$. Due to the mutually exclusiveness and exhaustiveness of the system decomposition and Eq. 2.13, we have

$$f_{ij}(t,x) = \sum_{k=0}^{n} f_{ikj_k}(t,x)$$

for $i, j = 1, \ldots, n$. It can be seen from Eq. 2.26 that flow and subflow intensities between the same compartments in the same flow direction are the same, that is,

$$f_{ikj_k}(t,x) = x_j(t) \frac{f_{ij}(t,x)}{x_j(t)}$$

for $i, k = 0, \ldots, n$ and $j = 1, \ldots, n$ (see Fig. 2).

In Eq. 2.26 above,

$$d_{jk}(x) := \frac{x_j(t)}{x_j(t)}$$

will be called the decomposition factors. It is worth emphasizing that, due to the state decomposition, Eq. 2.13, the decomposition factors form a continuous partition of unity:

$$0 \leq d_{jk}(x) \leq 1 \quad \text{and} \quad \sum_{k=0}^{n} d_{jk}(x) = 1.$$
The decomposition and \( k^{th} \) decomposition matrices, \( D(\mathbf{x}) := (d_{jk}(\mathbf{x})) \) and \( D_k(\mathbf{x}) := \text{diag} ([d_{1k}(\mathbf{x}), \ldots, d_{nk}(\mathbf{x})]) \), can be formulated, accordingly, as

\[
D(\mathbf{x}) = \mathcal{X}^{-1}(t) \mathcal{X}^{-}(t) X(t) \quad \text{and} \quad D_k(\mathbf{x}) = \mathcal{X}^{-1}(t) \mathcal{X}_k(t)
\]  
for \( k = 0, \ldots, n \). Equations 2.23, 2.29 and 2.30 imply that

\[
1 = \mathcal{X}^{-1}(t) \mathcal{X}^{-1}(t) \mathcal{X}_0(t) + \mathcal{X}^{-1}(t) X(t) 1 = D_0(\mathbf{x}) 1 + D(\mathbf{x}) 1.
\]

We define the \( k^{th} \) subflow rate matrix function as

\[
F_k(t, \mathbf{x}) := (f_{ikj}(t, \mathbf{x}))
\]
for \( k = 0, \ldots, n \). Using Eq. 2.26, \( F_k(t, \mathbf{x}) \) can be expressed in matrix form as

\[
F_k(t, \mathbf{x}) = F(t, \mathbf{x}) D_k(\mathbf{x}) = F(t, \mathbf{x}) \mathcal{X}^{-1}(t) \mathcal{X}_k(t).
\]
That is, the \( k^{th} \) decomposition matrix, \( D_k(\mathbf{x}) \), decomposes the compartmental direct flow matrix, \( F(t, \mathbf{x}) \), into the subcompartmental subflow matrices, \( F_k(t, \mathbf{x}) \). Similarly, the \( k^{th} \) output matrix function,

\[
\mathcal{Y}_k(t, \mathbf{x}) := \text{diag} ([f_{0k1}(t, \mathbf{x}), \ldots, f_{0kn}(t, \mathbf{x})]),
\]
can be expressed in matrix form as

\[
\mathcal{Y}_k(t, \mathbf{x}) = \mathcal{Y}(t, \mathbf{x}) D_k(\mathbf{x}) = \mathcal{Y}(t, \mathbf{x}) \mathcal{X}^{-1}(t) \mathcal{X}_k(t),
\]
and the \( k^{th} \) input matrix function can be written as

\[
\mathcal{Z}_k(t, \mathbf{x}) := \text{diag} ([z_{0k1}(t, \mathbf{x}), \ldots, z_{0kn}(t, \mathbf{x})])
\]
for \( k = 0, \ldots, n \). We set \( e_0 = 0 \). The respective \( k^{th} \) output and input vector functions, \( \mathcal{Y}_k(t, \mathbf{x}) \) and \( \mathcal{Z}_k(t, \mathbf{x}) \), can be defined as

\[
\mathcal{Y}_k(t, \mathbf{x}) := \mathcal{Y}_k(t, \mathbf{x}) 1 \quad \text{and} \quad \mathcal{Z}_k(t, \mathbf{x}) := \mathcal{Z}_k(t, \mathbf{x}) 1.
\]

Using these notations, the flow rate decompositions given in Eq. 2.27 and input decomposition formulated in Eq. 2.24 can be written in matrix form as follows:

\[
F(t, \mathbf{x}) = \sum_{k=0}^{n} F_k(t, \mathbf{x}), \quad \mathcal{Y}(t, \mathbf{x}) = \sum_{k=0}^{n} \mathcal{Y}_k(t, \mathbf{x}), \quad \mathcal{Z}(t, \mathbf{x}) = \sum_{k=0}^{n} \mathcal{Z}_k(t, \mathbf{x}).
\]
The equivalence of the flow and subflow rate intensities given in Eq. 2.28 can also be expressed in matrix form as

\[
F(t, \mathbf{x}) \mathcal{X}^{-1}(t) = F_k(t, \mathbf{x}) \mathcal{X}_k^{-1}(t)
\]
for \( k = 0, \ldots, n \).

The flow rate decomposition given in Eq. 2.26 can then be schematized as follows:

\[
\begin{bmatrix}
  f_{11} & \cdots & f_{1n} \\
  f_{21} & \cdots & f_{2n} \\
  \vdots & \ddots & \vdots \\
  f_{n1} & \cdots & f_{nn} \\
\end{bmatrix}
\quad \text{flow rate decomposition} \quad \begin{bmatrix}
  f_{1k1k} & \cdots & f_{1knk} \\
  f_{2k1k} & \cdots & f_{2knk} \\
  \vdots & \ddots & \vdots \\
  f_{nk1k} & \cdots & f_{nnnk} \\
\end{bmatrix}
\]
2.2.3. Domain Decomposition. The dynamic system decomposition methodology uniquely yields new substate variables in a higher dimensional domain from the original ones. We will show in this section that the properties guarantee the existence and uniqueness of the solutions to the decomposed system on the new domain are inherited from those of the original system on the original domain.

There exists a unique decomposition \( \mathbf{x} \) for each \( \mathbf{x} \in \Omega \) with the relationship \( x_i(t) = \sum_{k=1}^{n_i} x_{ik}(t) + x_{ik}(t) \), as given in Eq. 2.19. The new domain that includes these substate variables is denoted by \( \bar{\Omega} \subset \mathbb{R}^{2n^2} \) and will be called the decomposed domain. This process can be represented as

\[
\mathbb{R}^n \supset \Omega \ni \mathbf{x} \xrightarrow{\text{domain decomposition}} \mathbf{x} \in \bar{\Omega} \subset \mathbb{R}^{2n^2}.
\]

There is a one-to-one correspondence between the original and decomposed domains. This correspondence is due to the existence and uniqueness of the governing systems in both the original and decomposed forms as shown further below in this section.

**Proposition 2.2.** The subflow rate functions \( f_{i_k,j_k}(t,\mathbf{x}) \) and \( f_{i_k,j_k}(t,\mathbf{x}) \) are continuous and continuously differentiable in \( \mathbf{x} \) on domain \( \mathcal{I} \times \bar{\Omega} \subset \mathbb{R} \times \mathbb{R}^{2n^2} \).

**Proof.** It is given that \( f_{i,j}(t,\mathbf{x}) \) is continuous and continuously differentiable in \( \mathbf{x} \) on \( \mathcal{I} \times \Omega \subset \mathbb{R} \times \mathbb{R}^n \). Note that, due to Eq. 2.13, \( x_{j_k}(t) \leq x_j(t) \). The decomposition factors \( d_{j_k}(\mathbf{x}) = x_{j_k}(t)/x_j(t) \) are, therefore, well-defined even if \( x_j(t) \to 0 \). Note also that the decomposition factors are continuous and continuously differentiable with respect to \( x_{j_k} \) on \( \mathcal{I} \times \bar{\Omega} \). Therefore,

\[
f_{i_k,j_k}(t,\mathbf{x}) = \frac{x_{j_k}(t)}{x_j(t)} f_{i,j}(t,\mathbf{x})
\]

is also continuous and continuously differentiable in \( x_{j_k} \) on \( \mathcal{I} \times \bar{\Omega} \).

By construction, the subthroughflow functions, \( \bar{r}_{ik}(t,\mathbf{x}) \) and \( \hat{r}_{ik}(t,\mathbf{x}) \), as well as the net subthroughflow function, \( r_{ik}(t,\mathbf{x}) \), are linear combination of \( f_{i_k,j_k}(t,\mathbf{x}) \), as formulated in Eq. 2.44. Therefore, they have the same properties as \( f_{i_k,j_k}(t,\mathbf{x}) \). That is, they are continuous and continuously differentiable in \( \mathbf{x} \) on domain \( \mathcal{I} \times \bar{\Omega} \subset \mathbb{R} \times \mathbb{R}^{2n^2} \). The same arguments with the same conclusions are also valid for \( f_{i_k,j_k}(t,\mathbf{x}), \bar{r}_{ik}(t,\mathbf{x}), \hat{r}_{ik}(t,\mathbf{x}), \) and \( r_{ik}(t,\mathbf{x}) \). \( \square \)

2.2.4. Subsystems. Using the dynamic system decomposition methodology composed of the analytic state and flow rate decomposition components, the system can explicitly be decomposed into mutually exclusive and exhaustive subsystems. The \( k^{th} \) subcompartments of each compartment together with the corresponding \( k^{th} \) substates, subflow rates, inputs, and outputs constitute the \( k^{th} \) subsystem. The subsystems are running within the original system and have the same structure and dynamics as the system itself, except for their external inputs and initial conditions. These otherwise-decoupled subsystems are coupled through the decomposition factors. The initial subsystem is further decomposed into \( n \) subsystems, as formulated in Appendix A.3 (see Fig. 1 and 2).

In Section 2.1, the governing equations are formulated for the original system, Eq. 2.10. In what follows, we will similarly introduce the governing equations for each subsystem. The governing equations for the \( k^{th} \) subsystem can be written in vector form as

\[
\dot{\mathbf{x}}_k(t) = \bar{r}_k(t,\mathbf{x}) - \hat{r}_k(t,\mathbf{x})
\]

\[
= (\mathbf{z}_k(t,\mathbf{x}) + F_k(t,\mathbf{x}) \mathbf{1}) - (\mathbf{y}_k(t,\mathbf{x}) + F^T_k(t,\mathbf{x}) \mathbf{1})
\]
for \( k = 0, \ldots, n \). The initial conditions are \( x_0(t_0) = x_0 \) and \( x_k(t_0) = 0 \) for \( k \neq 0 \).

The \( k^{th} \) inward and outward subthroughflow vectors, \( \tilde{\tau}_k(t, x) \) and \( \hat{\tau}_k(t, x) \), for the \( k^{th} \) subsystem given in Eq. 2.43 can then be expressed as

\[
\begin{align*}
\tilde{\tau}_k(t, x) & := z_k(t, x) + F_k(t, x) 1 \\
& = Z_k(t, x) 1 + F(t, x) \mathcal{X}^{-1}(t) x_k(t), \\
\hat{\tau}_k(t, x) & := y_k(t, x) + F_k^T(t, x) 1 \\
& = \mathcal{Y}(t, x) \mathcal{X}^{-1}(t) \lambda_k(t) 1 + \lambda_k(t) \mathcal{X}^{-1}(t) F^T(t, x) 1 \\
& = (\mathcal{Y}(t, x) + \text{diag}(F^T(t, x) 1)) \mathcal{X}^{-1}(t) x_k(t) \\
& = \mathcal{T}(t, x) \mathcal{X}^{-1}(t) x_k(t).
\end{align*}
\]

The \( k^{th} \) net subthroughflow rate vector, \( \tau_k(t, x) := [\tau_{1k}(t, x), \ldots, \tau_{nk}(t, x)]^T \), becomes

\[
\tau_k(t, x) = \tilde{\tau}_k(t, x) - \hat{\tau}_k(t, x) = z_k(t, x) + A(t, x) x_k(t)
\]

where, using the definition of \( F(t, x) \) given in Eq. 2.12,

\[
A(t, x) := F(t, x) \mathcal{X}^{-1}(t) = (F(t, x) - \mathcal{T}(t, x)) \mathcal{X}^{-1}(t)
\]

\[
= Q^F(t, x) - R^{-1}(t, x),
\]

\( Q^F(t, x) := F(t, x) \mathcal{X}^{-1}(t) \), and \( R^{-1}(t, x) := \mathcal{T}(t, x) \mathcal{X}^{-1}(t) \). Note that, \( A(t, x) \) is the difference of two matrices \( Q^F(t, x) \) and \( R^{-1}(t, x) \) whose entries are the intercompartmental flow intensities and outward throughflow intensities, respectively. We will, therefore, call \( A(t, x) \) the flow intensity matrix. It is sometimes called the compartmental matrix. As indicated earlier in Eq. 2.4, \( Q^F(t, x) \) is called the coefficient matrix in general, but it will be called the storage distribution matrix in the context of the proposed methodology. The novel matrix measure introduced in this work, \( \mathcal{R}(t, x) \), will be called the residence time matrix [4].

The \( k^{th} \) inward and outward subthroughflow matrices, \( \mathcal{T}_k(t, x) := \text{diag}(\tilde{\tau}_k(t, x)) \) and \( \mathcal{H}_k(t, x) := \text{diag}(\hat{\tau}_k(t, x)) \), can be formulated as

\[
\begin{align*}
\mathcal{T}_k(t, x) & = Z_k(t, x) + \text{diag}(F(t, x) \mathcal{X}^{-1}(t) \lambda_k(t) 1), \\
\mathcal{H}_k(t, x) & = \mathcal{T}(t, x) \mathcal{X}^{-1}(t) \lambda_k(t).
\end{align*}
\]

Note that, using Eq. 2.47, \( F_k(t, x) \) defined in Eq. 2.34 can, alternatively, be written in terms of the system flows only:

\[
F_k(t, x) = F(t, x) \mathcal{T}^{-1}(t, x) \mathcal{T}_k(t, x).
\]

We will call \( Q^F(t, x) := F(t, x) \mathcal{T}^{-1}(t, x) \) the flow distribution matrix [4].

We define the inward and outward subthroughflow matrices, \( \mathcal{T}(t, x) \) and \( \mathcal{H}(t, x) \), as the matrices whose \( k^{th} \) columns are the \( k^{th} \) inward and outward subthroughflow vectors, \( \tilde{\tau}_k(t, x) \) and \( \hat{\tau}_k(t, x) \), \( k = 1, \ldots, n \), respectively:

\[
\begin{align*}
\mathcal{T}(t, x) & := (\tilde{\tau}_1(t, x) \ldots \tilde{\tau}_n(t, x)), \\
\mathcal{H}(t, x) & := (\hat{\tau}_1(t, x) \ldots \hat{\tau}_n(t, x)).
\end{align*}
\]

Using the relationships in Eq. 2.44, these subthroughflow matrices can be expressed in matrix form as

\[
\begin{align*}
\mathcal{T}(t, x) & = Z(t, x) + F(t, x) \mathcal{X}^{-1}(t) X(t), \\
\mathcal{H}(t, x) & = \mathcal{T}(t, x) \mathcal{X}^{-1}(t) X(t).
\end{align*}
\]
We also define the net subthroughflow matrix, $T(t, x)$, as

$$T(t, x) := \hat{T}(t, x) - \bar{T}(t, x) = Z(t, x) + A(t, x) X(t).$$

Due to Eq. 2.50, the decomposition matrix $D(x)$ can be expressed in terms of the subthroughflow functions, instead of the substate functions, as follows:

$$D(x) = X^{-1}(t) X(t) = T^{-1}(t, x) \hat{T}(t, x).$$

Note that, the subthroughflow matrices can be written in the following various forms:

$$\begin{align*}
\hat{T}(t, x) &= F(t, x) D(x) = Q^x(t, x) X(t) = Q^T(t, x) \hat{T}(t, x) \\
\hat{T}(t, x) &= R^{-1}(t, x) X(t)
\end{align*}$$

where $\hat{T}(t, x) = \bar{T}(t, x) - Z(t, x)$ will be called the intercompartmental subthroughflow matrix. These different forms prove useful particularly in the analyses of static systems as introduced by [4, 5].

For each fixed $j$, Eqs. 2.28 or 2.50 imply that

$$\hat{r}_{ji}(t, x) = \frac{\sum_{i=0}^{n} f_{ij}(t, x)}{x_j(t)} = \frac{\sum_{i=0}^{n} f_{ijk}(t, x)}{x_{jk}(t)} = \frac{\hat{r}_{jk}(t, x)}{x_{jk}(t)}$$

for $k = 0, \ldots, n$. This equivalence between the outward throughflow and subthroughflow intensities given in the first and last equalities of Eq. 2.54 can be expressed in matrix form:

$$R^{-1}(t, x) = T(t, x) X^{-1}(t) = \hat{T}_k(t, x) X_k^{-1}(t) = \hat{T}(t, x) X^{-1}(t)$$

where the last equality is derived from Eq. 2.53. This proportionality is used in the derivation of the static diact flows and storages in matrix form by [4] as listed in Table 1. The residence time matrix, $R(t, x)$, has a central role in the integration of various system components and the holistic analysis of the static systems [4].

Equations 2.28 and 2.54 also imply that

$$\frac{\hat{r}_{jk}(t, x)}{\hat{r}_{jl}(t, x)} = \frac{x_{jk}(t)}{x_{jl}(t)} = \frac{f_{ikj}(t, x)}{f_{ikl}(t, x)}$$

for $k, \ell = 0, \ldots, n$. This relationship indicates the proportionality of the parallel subflows and corresponding subthroughflows and substorages. By parallel subflows, we mean the intercompartmental flows that transit through different subcompartments of the same compartment along the same flow path at the same time. The flow path terminology is developed in Appendix C.1.

Using Eq. 2.55, the $k^{th}$ decomposition matrix, $D_k(x)$, can be expressed as

$$D_k(x) = \chi^{-1}(t) \chi_k(t) = T(t, x)^{-1} \hat{T}_k(t, x),$$

similar to the decomposition matrix formulated in Eq. 2.52. It is worth noting that, the decomposition and $k^{th}$ decomposition matrices, $D(x)$ and $D_k(x)$, decompose the compartmental throughflow matrix, $T(t, x)$, into the outward subthroughflow and $k^{th}$ subthroughflow matrices as indicated in Eqs. 2.53 and 2.57, similar to the decomposition of $F(x)$ as formulated in Eq. 2.34. That is,

$$\hat{T}(t, x) = T(t, x) D(x) \quad \text{and} \quad \hat{T}_k(t, x) = T(t, x) D_k(x).$$
It is worth noting also the relationships between the flow and subthroughflow matrices:

\[
\begin{align*}
\mathbf{z}(t, \mathbf{x}) + F(t, \mathbf{x}) \mathbf{1} &= \sum_{k=0}^{n} \mathbf{z}_k(t, \mathbf{x}) + F_k(t, \mathbf{x}) \mathbf{1} = \sum_{k=0}^{n} \hat{\mathbf{r}}_k(t, \mathbf{x}) = \hat{\mathbf{r}}(t, \mathbf{x}) \\
&= \dot{\mathbf{r}}_0(t, \mathbf{x}) + \hat{T}(t, \mathbf{x}) \mathbf{1}, \\
\mathbf{y}(t, \mathbf{x}) + F^T(t, \mathbf{x}) \mathbf{1} &= \sum_{k=0}^{n} \mathbf{y}_k(t, \mathbf{x}) + F^T_k(t, \mathbf{x}) \mathbf{1} = \sum_{k=0}^{n} \hat{\mathbf{r}}_k(t, \mathbf{x}) = \hat{\mathbf{r}}(t, \mathbf{x}) \\
&= \dot{\mathbf{r}}_0(t, \mathbf{x}) + \hat{T}(t, \mathbf{x}) \mathbf{1}.
\end{align*}
\]

The governing equations for the subsystems of the decomposed system can then be written in vector form as

\begin{equation}
(2.59) \quad \dot{\mathbf{x}}_k(t) = \mathbf{z}_k(t, \mathbf{x}) + A(t, \mathbf{x}) \mathbf{x}_k(t)
\end{equation}

with the initial conditions \( \mathbf{x}_0(t_0) = \mathbf{x}_0 \) and \( \mathbf{x}_k(t_0) = \mathbf{0} \) for \( k = 1, \ldots, n \). The governing equations for the decomposed system can similarly be expressed in matrix form using the matrix functions introduced above as follows:

\begin{equation}
(2.60) \quad \begin{align*}
\dot{\mathbf{X}}(t) &= T(t, \mathbf{x}) = \dot{\mathbf{T}}(t, \mathbf{x}) - \hat{T}(t, \mathbf{x}), \quad \mathbf{X}(t_0) = \mathbf{0}, \\
\dot{\mathbf{x}}_0(t) &= \tau_0(t, \mathbf{x}) = \dot{\tau}_0(t, \mathbf{x}) - \hat{\tau}_0(t, \mathbf{x}), \quad \mathbf{x}_0(t_0) = \mathbf{x}_0.
\end{align*}
\end{equation}

This system can also be expressed in terms of the flow intensity matrix, \( A(t, \mathbf{x}) \):

\begin{equation}
(2.61) \quad \begin{align*}
\dot{\mathbf{X}}(t) &= \mathbf{Z}(t, \mathbf{x}) + A(t, \mathbf{x}) \mathbf{X}(t), \quad \mathbf{X}(t_0) = \mathbf{0}, \\
\dot{\mathbf{x}}_0(t) &= A(t, \mathbf{x}) \mathbf{x}_0(t), \quad \mathbf{x}_0(t_0) = \mathbf{x}_0.
\end{align*}
\end{equation}

The system decomposition methodology that yields the governing equations for each subsystem in vector form, Eq. 2.59, or for the entire system in matrix form, Eq. 2.60, can be schematized as follows:

\[
\begin{align*}
\dot{\mathbf{x}}(t) &= \mathbf{r}(t, \mathbf{x}) \\
\dot{\mathbf{x}}_k(t) &= \mathbf{r}_k(t, \mathbf{x}), \quad k = 0, \ldots, n
\end{align*}
\]

**2.2.5. Decomposed System.** For each fixed \( i = 1, \ldots, n \), there are \( n \) governing equations for \( n \) substates, \( x_{i_k}(t) \), and \( n \) equations for \( n \) initial substates, \( \bar{x}_{i_k}(t) \).
Consequently, there are $2n^2$ equations in total; $n^2$ of them are for the substates and the other $n^2$ equations are for the initial substates.

The governing equations for $x_{ik}(t)$ and $x_{ik}(t)$ can be written componentwise as

\begin{equation}
\dot{x}_{ik}(t) = \left( z_{ik}(t, x) + \sum_{j=1}^{n} f_{ij,k}(t, x) \right) - \left( y_{ik}(t, x) + \sum_{j=1}^{n} f_{jk,i}(t, x) \right)
\end{equation}

(2.62) with the initial conditions $x_{ik}(t_0) = 0$, and

\begin{equation}
\dot{x}_{ik}(t) = \left( \sum_{j=1}^{n} f_{ij,k}(t, x) \right) - \left( \sum_{j=1}^{n} f_{jk,i}(t, x) \right)
\end{equation}

(2.63) with the initial conditions $x_{ik}(t_0) = \delta_{i,k} x_{i,0}$, for $i, k = 1, \ldots, n$.

The governing equations for the decomposed system, Eqs. 2.62 and 2.63, are already expressed in vector forms in Eqs. 2.59 and A.42 as follows:

\begin{equation}
\dot{x}_k(t) = z_k(t, x) + A(t, x) x_k(t), \quad x_k(t_0) = 0
\end{equation}

(2.64)\begin{equation}
\dot{x}_k(t) = A(t, x) x_k(t), \quad x_k(t_0) = x_{k,0} e_k
\end{equation}

for $k = 1, \ldots, n$. Summing up the governing equations over $k$ separately for both subsystems and initial subsystems formulated in Eq. 2.64 yields

\begin{equation}
\dot{x}(t) = z(t, x) + A(t, x) \bar{x}(t), \quad \bar{x}(t_0) = 0
\end{equation}

(2.65)\begin{equation}
\dot{x}(t) = A(t, x) \bar{x}(t), \quad \bar{x}(t_0) = 0.
\end{equation}

This system enables the analysis of the evolution of external inputs and initial conditions within the system separately. Adding these two equations side by side gives back the original system, Eq. 2.11, in the following form:

\begin{equation}
\dot{x}(t) = z(t, x) + A(t, x) x(t), \quad x(t_0) = x_0
\end{equation}

(2.66) as $F(t, x) = A(t, x) x(t)$. The decomposition formulated in Eq. 2.65 could directly be obtained from the original system by defining a decomposition with two subsystems—one for external inputs and the other for the initial conditions.

The governing equations, Eqs. 2.62 and 2.63, for the decomposed system are already expressed in matrix form in Eqs. 2.61 and A.44 as follows:

\begin{equation}
\dot{X}(t) = Z(t, x) + A(t, x) X(t), \quad X(t_0) = 0
\end{equation}

(2.67)\begin{equation}
\dot{X}(t) = A(t, x) X(t), \quad X(t_0) = X_0.
\end{equation}

Let a new matrix $X(t)$ be defined, componentwise, as $X_{ik}(t) := x_{ik}(t) + x_{ik}(t)$. The governing equation for $X(t)$ becomes

\begin{equation}
\dot{X}(t) = Z(t, x) + A(t, x) X(t), \quad X(t_0) = X_0
\end{equation}

(2.68) as $Z(t, x) := x_{ik}(t)$. Note that $X_{ik}(t)$ represents composite storage in compartment $i$ that is derived from the initial stock in compartment $k$, $x_{k,0}$, and the external input into compartment $k$, $z_k(t)$. 
2.3. Nonlinear Fundamental Matrix Solutions. In this section, the nonlinear fundamental matrix solutions will be introduced for dynamic compartmental systems. They will be called the fundamental matrix solutions due to the common properties outlined in Theorem 2.4 with fundamental matrix solutions to systems of linear ordinary differential equations. We will first show the existence and uniqueness of the decomposed system in vector form.

**Theorem 2.3.** Let \((t_0, x_0) \in I \times \bar{U}\). There exists a positive integer \(r > 0\) and an interval \(I' = (t_0 - r, t_0 + r) \subset I\) such that the governing equations Eq. 2.64 for the decomposed system has a unique solution passing through \((t_0, x_0)\) on \(I'\).

**Proof.** The net subthroughflow functions \(\tau_{ik}(t, x)\) and \(\tau_{ik}(t, x)\) on the right hand side of the decomposed system Eq. 2.64 are continuous and continuously differentiable for \(x\) on \(I \times \bar{U}\), as shown in Proposition 2.2. The existence and uniqueness of solutions to Eq. 2.64 on \(I'\) is an immediate consequence of Picard’s local existence and uniqueness theorem.

The definitions of nonlinear fundamental matrix solutions and their main properties are outlined in the following theorem.

**Theorem 2.4.** Let \(X(t)\) and \(X(t)\) be the matrix functions defined in Eqs. 2.21 and A.3.  
1. \(X(t)\) and \(X(t)\) are the unique matrix solutions to the decomposed system, Eq. 2.67. They will be called the nonlinear fundamental matrix solutions of Eq. 2.67.
2. For any given \((t_0, x_0) \in I \times \Omega\), the unique solution to the original system, Eq. 2.66, is given by 

\[
x(t) = X(t) \mathbf{1} + X'(t) \mathbf{1}.
\]

That is, \(x(t)\) is the linear combination of the columns of \(X(t)\) and \(X(t)\), where all the combination coefficients are 1.
3. Let \(x_{i0} > 0\) and \(z_i(t, x) > 0\), \(t \in I\), for all \(i\). The column vectors of \(X(t)\) and \(X(t)\) are linearly independent vectors in \(\mathbb{R}^n\). Therefore, both \(X(t)\) and \(X(t)\) are invertible matrices at any time \(t \in I\) under given conditions.

**Proof.** 1. The existence and uniqueness of the solution to the decomposed system in vector form, Eq. 2.64, is shown in Thm. 2.3. The existence and uniqueness of the system in matrix form, Eq. 2.67, follows those of the system Eq. 2.64, by a column-wise comparison of both sides of the matrix equation, Eq. 2.67.
2. By the principle of nonlinear decomposition stated in Thm. 2.5,

\[
x(t) = X(t) \mathbf{1} = X(t) \mathbf{1} + X(t) \mathbf{1} = \sum_{k=1}^{n} x_k(t) + \sum_{k=1}^{n} x_k(t)
\]

is a solution of the original system Eq. 2.66. The uniqueness of this solution follows the uniqueness of the decomposed system Eq. 2.64 as shown in part (1) of this theorem.
3. Let \(x_i(t)\) and \(x_i(t)\) be solution of the decomposed system Eq. 2.64. We would like to show that, for each fixed \(t\), the set of vectors \(\{x_1(t), \ldots, x_n(t)\}\) and \(\{x_1(t), \ldots, x_n(t)\}\) in \(\mathbb{R}^n\) are linearly independent.

We will first show that \(\{x_1(t), \ldots, x_n(t)\}\) is linearly independent set in \(\mathbb{R}^n\) for each fixed \(t \in I\). Suppose that, there exists a \(t_1 \in I\) such that the column
vectors in \( \{x_1(t_1), \ldots, x_n(t_1)\} \) are linearly dependent. There exists then a combination constants \( c_1, \ldots, c_n \) not all zero, such that

\[
0 = c_1 x_1(t_1) + \ldots + c_n x_n(t_1) = X(t_1) c
\]

where \( c = (c_1, \ldots, c_n)^T \in \mathbb{R}^n \). Let

\[
\alpha(t) := c_1 x_1(t) + \ldots + c_n x_n(t) = X(t) c, \quad t \in \mathcal{I}.
\]

Therefore, \( \dot{\alpha}(t) = \dot{X}(t) c \). From the governing matrix equation for \( X(t) \) in Eq. 2.67 and also Eq. 2.70, we have

\[
\dot{\alpha}(t) = Z(t, x) c + A(t, x) \alpha(t), \quad \alpha(t_0) = 0.
\]

Equation 2.69 implies that \( \alpha(t_1) = 0 \). Without loss of generality, assume that \( c_i > 0 \) for some \( i \). We then have

\[
\begin{align*}
\alpha_i(t_0) &= 0, \quad \dot{\alpha}_i(t_0) = c_i z_i(t_0, x) > 0, \quad \text{and} \\
\alpha_i(t_1) &= 0, \quad \dot{\alpha}_i(t_1) = c_i z_i(t_1, x) > 0, \quad \forall i,
\end{align*}
\]

as \( z_i(t, x) > 0 \). Since \( \alpha(t) \) is a differentiable and, therefore, is a continuous function, Eq. 2.72 implies that there exists at least one \( t^* \in (t_0, t_1) \) such that \( \alpha_i(t^*) = 0 \) and \( \dot{\alpha}_i(t^*) < 0 \). Due to Eq. 2.71, this result implies that \( z_i(t^*, x) < 0 \). This contradiction completes the first part of the proof.

Now, we would like to show that \( \{x_1(t), \ldots, x_n(t)\} \) is a linearly independent set in \( \mathbb{R}^n \) for each fixed \( t \in \mathcal{I} \). The condition for this case is that \( x_i(t) > 0, \forall i \). Suppose now that at the same \( t_1 \in \mathcal{I} \), the column vectors in \( \{x_1(t_1), \ldots, x_n(t_1)\} \) are linearly dependent in \( \Omega \). There then exists constants \( \xi_1, \ldots, \xi_n \) not all zero, such that

\[
0 = \xi_1 x_1(t_1) + \ldots + \xi_n x_n(t_1) = \dot{X}(t_1) c
\]

where \( c = (\xi_1, \ldots, \xi_n)^T \in \mathbb{R}^n \). Let

\[
\alpha(t) := \xi_1 x_1(t) + \ldots + \xi_n x_n(t) = X(t) c, \quad t \in \mathcal{I}.
\]

This implies that \( \dot{\alpha}(t) = \dot{X}(t) c \). From the governing matrix equation, Eq. 2.67, for \( X \), and Eq. 2.73, we have

\[
\dot{\alpha}(t) = A(t, x) \alpha(t), \quad \alpha(t_1) = 0.
\]

Due to the uniqueness theorem, Thm. 2.3, \( \alpha(t) = 0, t \in \mathcal{I} \). In particular,

\[
\alpha(t_0) = X(t_0) c = X_0 c = 0 \quad \Rightarrow \quad c = 0
\]

as \( x_i > 0, \forall i \), which is a contradiction.

These two contradictions for each part of the system Eq. 2.67 indicate that neither the set of the column vectors of \( \dot{X}(t) \) nor that of \( X(t) \) can be linearly dependent at any \( t_3 \in \mathcal{I} \). Therefore, the column vectors of \( \dot{X}(t) \) and \( X(t) \) form linearly independent sets, and consequently, the matrices are invertible for all \( t \in \mathcal{I} \). ∎
2.4. Nonlinear Decomposition Principle. We will state the \textit{nonlinear decomposition principle} for dynamic nonlinear compartmental systems in the following theorem. It essentially asserts that the solution for each subsystem also solves the original system, so is any arbitrary combination of these solutions as specified in the theorem.

\textbf{Theorem 2.5.} Let \(d_i(x)\) and \(d_{i_0}(x)\) be the decomposition factors of subsystems and initial subsystems, respectively, based on which the original system, Eq. 2.10, is decomposed into Eq. 2.64. Let also \(x_k(t)\) and \(\bar{x}_k(t)\) be the respective solutions on \(\Omega\) to the \(k\)th subsystem and initial subsystem of the decomposed system with the corresponding external inputs and initial conditions specified in Eq. 2.64. The following combination of the vector functions

\begin{equation}
    x(t) = \sum_{k=1}^{n} \alpha_k x_k(t) + \beta_k \bar{x}_k(t), \quad \alpha_k, \beta_k \in \{0, 1\},
\end{equation}

then is a solution to the original system with the following external inputs and initial conditions on \(\Omega\):

\begin{equation}
    z(t, x) = \sum_{k=1}^{n} \alpha_k z_k(t, x) = \sum_{k=1}^{n} \alpha_k z_k(t, x) e_k \quad \text{and}
\end{equation}

\begin{equation}
    x_0 = x(t_0) = \sum_{k=1}^{n} \beta_k x_k(t_0) = \sum_{k=1}^{n} \beta_k x_{k,0} e_k.
\end{equation}

\textbf{Proof.} Note that, if \(\alpha_k = 0\) or \(\beta_k = 0\) for some \(k\), the corresponding solutions to Eq. 2.64, with the conditions given in Eq. 2.75, become \(x_k(t) = 0\) or \(\bar{x}_k(t) = 0\), respectively. This is because of the fact that the subsystems are driven either by external inputs or initial stocks and, therefore, if there is no source term for a subsystem or the initial condition is zero for an initial subsystem, the corresponding subsystem becomes null—the state variables (and the subflows rates) for that subsystem or initial subsystem become zero.

Due to the construction of the system decomposition, we have

\begin{equation}
    x(t) = X(t) 1 = X(t) 1 + X(t) 1 = \sum_{k=1}^{n} x_k(t) + x_k(t).
\end{equation}

Therefore, multiplying both sides of the governing equation, Eq. 2.68, by 1 yields the original system in the form of Eq. 2.66 because of the fact that \(F(t, x) 1 = A(t, x) x(t)\). Consequently, if \(x_k\) and \(\bar{x}_k\) are the respective solutions to the \(k\)th subsystem and initial subsystem of the decomposed system, Eq. 2.64, on \(\Omega\), \(x\) is the solution to the original system, Eq. 2.10, on \(\Omega\).

This nonlinear decomposition principle corresponds to the superposition principle for the linear ordinary differential equations. It is in the sense that, the solution to a nonlinear system can be decomposed into \textit{subsolutions}, each of which, as well as any arbitrary combination of them as specified in Thm. 2.5, solves the original system.

2.5. Dynamic Subsystem Decomposition. We will introduce the \textit{dynamic subsystem decomposition} methodology in this section for further partitioning or segmentation of subsystems along a given set of mutually exclusive and exhaustive subflow paths. The subsystem decomposition methodology dynamically decomposes arbitrary composite intercompartmental flows and storages into the constituent transient
subflow and substorage segments along given subflow paths (see Fig. 3). Therefore, the subsystem decomposition determines the distribution of arbitrary intercompartmental flows and the organization of the associated storages generated by these flows within the subsystems. In other words, the subsystem partitioning enables tracking the evolution of arbitrary intercompartmental flows and storages within and monitoring their spread throughout the system.

The dynamic subsystem decomposition methodology will be formulated below using the directed subflow path terminology introduced in Appendix C. The natural subsystem decomposition of each subsystem then yields a mutually exclusive and exhaustive decomposition of the entire system. We will first introduce the transient flows and storages. They will be used for the formulation of the diact flows and storages in the next section.

2.5.1. Transient Flows and Storages. Along a given subflow path \( p_{w_{ik}}^{w_{jk}} = i_k \rightarrow j_k \rightarrow \ell_k \rightarrow n_k \), the transient inflow at subcompartment \( \ell_k \), \( f_{\ell_k}^w(t) \), generated by the local input from \( i_k \) to \( j_k \) during \([t_1, t] \), \( t_1 \geq t_0 \), is the subflow segment that is transmitted from \( j_k \) to \( \ell_k \) at time \( t \). Similarly, the transient outflow generated by the transient inflow at \( \ell_k \) during \([t], t \), \( f_{n_k\ell_k}^w(t) \), is the subflow segment that is transmitted from \( \ell_k \) to the next subcompartment, \( n_k \), along the path at time \( t \). The associated transient substorage in subcompartment \( \ell_k \) at time \( t \), \( x_{n_k\ell_k}^w(t) \), is then the substorage segment governed by the transient inflow and outflow balance during \([t_1, t] \) (see Fig. 3).

The transient outflow at subcompartment \( \ell_k \) at time \( t \), from \( j_k \) to \( n_k \) along subflow path \( p_{w_{nk}}^{w_{jk}} \), \( f_{n_k\ell_k}^w(t) \), can be formulated as

\[
(2.76) \quad f_{n_k\ell_k}^w(t) = \frac{f_{n_k\ell_k}^w(t, x)}{x_{\ell_k}(t)} x_{n_k\ell_k}(t),
\]

similar to Eq. 2.26 or Eq. 2.56, due to the proportionality of parallel subflows, where the transient substorage, \( x_{n_k\ell_k}^w(t) \), is determined by the governing mass balance equation

\[
(2.77) \quad \dot{x}_{n_k\ell_k}^w(t) = f_{n_k\ell_k}^w(t) - \hat{\tau}_{\ell_k}(t, x) x_{n_k\ell_k}(t), \quad x_{n_k\ell_k}(t_1) = 0.
\]

The equivalence of the throughflow and subthroughflow intensities as well as the flow and subflow intensities in the same direction, that is

\[
q_{n_\ell}^w(t, x) = \frac{f_{n_\ell}^w(t, x)}{x_{\ell}(t)} = \frac{f_{n_\ell}^w(t, x)}{x_{\ell}(t)} \quad \text{and} \quad r_{\ell_1}^{-1}(t, x) = \frac{\hat{\tau}_{\ell}(t, x)}{x_{\ell}(t)} = \frac{\hat{\tau}_{\ell}(t, x)}{x_{\ell}(t)}
\]

are given by Eqs. 2.40 and 2.55, for \( \ell, n = 1, \ldots, n \), and \( k = 0, 1, \ldots, n \). Therefore, since the rational expressions in Eqs. 2.76 and 2.77 can be expressed at both compartmental and subcompartmental levels, the subsystem decomposition is actually independent from the state decomposition. That is, the same analysis can be done along flow paths within the system, instead of subflow paths within the subsystems. Note that the initial condition given in Eq. 2.77 for the initial subsystem is \( x_{n_0\ell_0j_0}(t_0) \neq 0 \), and this initial stock is not considered as a transient substorage. The governing equations, Eqs. 2.76 and 2.77, establish the foundation of the dynamic subsystem decomposition. These equations for each subcompartment along a given flow path of interest will then be coupled with the decomposed system, Eqs. 2.62 and 2.63, or the original system, Eq. 2.6, and be solved simultaneously.
inflows, \( \hat{\tau}_i \) and transmitted into the cumulative transient substorages, generated by the composite transfer inflow \( \tau_i \) at subcompartment \( \ell_k \) along subflow path \( p_{nkjk}^w \rightarrow i_k \rightarrow j_k \rightarrow \ell_k \rightarrow n_k \).

Additional relationships for the transient subflows and substorages along self-intersecting subflow paths are formulated in Appendix C.2. The transient subflows and substorages within the initial subsystems can be defined and formulated similarly.

2.5.2. The diact Flows and Storages. Five important transaction types are introduced in this section based on the subsystem decomposition methodology: the diact flows and storages. The transfer flows (denoted by \( t \)) and storages will be formulated in detail below, and parallel derivation for direct (d), indirect (i), cycling (c), and acyclic (a) flows and storages can be found in Appendix D.

The composite transfer flow will be defined as the total intercompartmental transient flow from one compartment, directly or indirectly through other compartments, to another. The composite direct, indirect, acyclic and cycling flow from the initial compartment to the terminal compartment are then defined as the direct, indirect, non-cycling, and cycling segments at the terminal compartment of the composite transfer flow (see Fig. 4). The simple transfer flow will also be defined as the total intercompartmental transient flow from an input-receiving subcompartment, directly or indirectly through other compartments, to another subcompartment. The simple direct, indirect, acyclic, and cycling flow from the initial input-receiving subcompartment to the terminal subcompartment are then defined as the direct, indirect, non-cycling, and cycling segments at the terminal subcompartment of the simple transfer flow (see Fig. 4). The associated simple and composite diact storages are defined as the storages generated by the corresponding diact flows. The simple and composite diact flows and storages at both subcompartmental and compartmental levels are formulated below and in Appendix D.

The composite transfer subflow will be defined as the total intercompartmental transient flow from one subcompartment, directly or indirectly through other subcompartments, to another in the same subsystem. Let \( P^w_{ikjk} \) be the set of mutually exclusive subflow paths \( p^w_{ikjk} \) from subcompartment \( j_k \) directly or indirectly to \( i_k \) in subsystem \( k \). The composite transfer subflow from subcompartment \( j_k \) to \( i_k \), \( \tau^w_{ikjk}(t) \), can be expressed as the sum of the cumulative transient subflows, \( \tau^w_{ik}(t) \), generated by the outward subthroughflow at subcompartment \( j_k \), \( \tau^w_{jk}(t, x) \), during \([t_1, t] \), \( t_1 \geq t_0 \), and transmitted into \( i_k \) at time \( t \) along all subflow paths \( p^w_{ikjk} \in P^w_{ikjk} \). The associated composite transfer substorage, \( x^w_{ikjk}(t) \), at subcompartment \( i_k \) at time \( t \) is the sum of the cumulative transient substorages, \( x^w_{ik}(t) \), generated by the cumulative transient inflows, \( \tau^w_{ik}(t) \), during \([t_1, t] \). Alternatively, \( x^w_{ikjk}(t) \) can be defined as the storage segment generated by the composite transfer inflow \( \tau^w_{ik}(t) \) in subcompartment \( i_k \) during
To distinguish the composite and simple transfer flow and storage matrices, we use a

\[ \tau_{ij}^c(t) = \tau_{ij}^c(t) - \tau_{ij}^s(t), \]

\[ \tau_{ij}^t(t) = \tau_{ij}^t(t), \]

\[ \tau_{ij}^c(t), \]

\[ \tau_{ij}^s(t). \]

These matrix measures \( T_k^s(t) \) and \( X_k^s(t) \) whose \((i, j)\)-elements are \( \tau_{ik,jk}^s(t) \) and \( x_{ik,jk}^s(t) \), respectively. That is,

\[ T_k^s(t) := (\tau_{ik,jk}^s(t)) \quad \text{and} \quad X_k^s(t) := (x_{ik,jk}^s(t)). \]

These matrix measures \( T_k^s(t) \) and \( X_k^s(t) \) are, accordingly, called the \( k \)th composite transfer flow and associated substorage matrix functions. The corresponding composite transfer flow and associated storage matrix functions are \( T^s(t) := (\tau_{ij}^s(t)) \) and \( X^s(t) := (x_{ij}^s(t)) \), respectively.

The simple transfer flows and storages can also be formulated in terms of their composite counterparts as follows:

\[ \tau_{ik}^s(t) = \tau_{ik,kk}^s(t) \quad \text{and} \quad x_{ik}^s(t) = x_{ik,kk}^s(t). \]

To distinguish the composite and simple transfer flow and storage matrices, we use a tilde notation over the simple versions, that is, \( \tilde{T}^s(t) := (\tau_{ik}^s(t)) \) and \( \tilde{X}^s(t) := (x_{ik}^s(t)) \).
The difference between the composite and simple transfer flows, \( \tau^\tau_{ik}(t) \) and \( \tau^\tau_{ik}(t) \), and associated storages, \( x^\tau_{ik}(t) \) and \( x^\tau_{ik}(t) \), is that the composite flow and storage from compartment \( k \) to \( i \) are generated by outward throughflow \( \tau_k(t, x) \) derived from all external inputs, and their simple counterparts from input-receiving subcompartment \( k_k \) to \( i_k \) are generated by outward subthroughflow \( \tau_{ik}(t, x) \) derived from single external input \( z_k(t) \) (see Fig. 4). In that sense, the composite and simple diact flows and storages measure the influence of one compartment on another induced by all and a single external input, respectively.

The simple transfer and indirect subflows can be formulated explicitly. The simple transfer subflow from an input-receiving subcompartment \( k_k \) to \( i_k \) can be expressed as

\[
\tau^\tau_{ik}(t) = \tau^\tau_{ik,k_k}(t) = \sum_{j=1}^{n} f_{ik,jk}(t, x) = \tau_{ik}(t, x) - z_{ik}(t, x) = \tilde{\tau}_{ik}(t, x)
\]

for \( i, k = 1, \ldots, n \). Note that the simple transfer subflow at subcompartment \( i_k \) is equal to the intercompartmental subthroughflow at the same subcompartment. The simple indirect subflow from \( k_k \) to \( i_k \) can then be formulated as

\[
\tau^i_{ik}(t) = \tau^i_{ik,k_k}(t) = \sum_{j=1}^{n} f_{ik,jk}(t, x) = \tau^\tau_{ik}(t) - f_{ik,k_k}(t, x).
\]

Due to the reflexivity of the cycling flow, the simple cycling subflow from an input-receiving subcompartment \( k_k \) to itself can be formulated, in terms of the simple indirect or transfer subflows, as follows:

\[
\tau^c_{k_k}(t) = \tau^c_{k_k,k_k}(t) = \tau^\tau_{k_k}(t) - \tau^i_{k_k}(t) = \sum_{j=1}^{n} f_{k_k,jk}(t, x) = \tilde{\tau}_{k_k}(t, x) - z_k(t, x).
\]

Consequently, the simple acyclic flow from subcompartment \( k_k \) to itself becomes zero:

\[
\tau^a_{k_k}(t) = \tilde{\tau}_{k_k}(t) - \tau^c_{k_k}(t) = 0.
\]

The composite indirect subflow, \( \tau^\tau_{ik,jk}(t) \), from subcompartment \( j_k \) to \( i_k \) can be expressed as the transfer subflow diminished by the direct subflow from \( j_k \) to \( i_k \) at time \( t \). Therefore, it can also be formulated as

\[
\tau^i_{ik,jk}(t) = \tau^\tau_{ik,jk}(t) - f_{ik,jk}(t, x).
\]

Consequently, at the compartmental level, we have

\[
T^\tau(t) = T^d(t) + T^i(t) \quad \text{and} \quad X^\tau(t) = X^d(t) + X^i(t).
\]

There is a functional similarity between \( T^\tau(t) \) and \( T^d(t) = F(t, x) \); the \((i, k)\)—element of \( T^\tau(t) \), \( \tau^\tau_{ik}(t) \), is the indirect flow, while that of \( F(t, x) \), \( \tau^d_{ik}(t) = f_{ik}(t, x) \), is the direct flow from compartment \( k \) to \( i \) at time \( t \). Those elements of \( X^\tau(t) \) and \( X^i(t) \), \( x^\tau_{ik}(t) \) and \( x^i_{ik}(t) \), are then the storages generated by the corresponding direct and indirect flows at time \( t \), respectively.

Therefore, the cycling and acyclic subflows and substorages are related as

\[
\tau^\tau_{ik,jk}(t) = \tau^c_{ik,jk}(t) + \tau^a_{ik,jk}(t) \quad \text{and} \quad x^\tau_{ik,jk}(t) = x^c_{ik,jk}(t) + x^a_{ik,jk}(t).
\]
At the compartmental level, in matrix form, these relationships can be expressed as
\begin{align}
T^c(t) &= T^c(t) + T^s(t) \quad \text{and} \quad X^c(t) = X^c(t) + X^s(t),
\end{align}
similar to Eq. 2.87. The \((i, k)\)-elements of \(T^c(t)\) and \(T^s(t)\), \(r_{ik}^c(t)\) and \(r_{ik}^s(t)\), are the cycling and non-cycling segments of the transfer flow at compartment \(i\) from \(k\). Those elements of \(X^c(t)\) and \(X^s(t)\), \(x_{ik}^c(t)\) and \(x_{ik}^s(t)\), are then the storages generated by the corresponding cycling and acyclic flows at time \(t\), respectively.

The reflexivity of the simple cycling flows and storages formulated in Eq. 2.84 can be extended to their composite counterparts, in matrix form, as follows:
\begin{align}
\text{diag} (T^c(t)) &= \text{diag} (T^s(t)) = \text{diag} (T^s(t)), \\
\text{diag} (X^c(t)) &= \text{diag} (X^s(t)) = \text{diag} (X^s(t)).
\end{align}

All the other simple and composite \textbf{diact} flows and storages can be formulated similar to the composite transfer flows and storages introduced in this section, as presented in Appendix D. The relationships given in Eqs. 2.87, 2.88, and 2.89 can also be expressed in terms of the simple \textbf{diact} flows and storages. The \textbf{diact} subflow and substorage definitions can be extended in parallel to the initial subsystems as well.

\textbf{2.6. System Analysis and Measures.} The dynamic system decomposition methodology yields the subthroughflow and substorage matrices that measure the external influence on system compartments in terms of the flow and storage generation. For the quantification of intercompartmental flow and storage dynamics, the dynamic subsystem decomposition methodology then formulates the transient and dynamic \textbf{diact} flows and storages. These mathematical system analysis tools and their interpretation as quantitative system indicators will be discussed in this section.

The elements of the fundamental matrix solutions, that is, those of the substate and initial substate matrices, \(X(t)\) and \(X(t)\), represent the organization of storages within the system derived from the initial stocks and external inputs, respectively. More specifically, \(x_{ik}(t)\) represents the storage value in compartment \(i\) at time \(t\), derived from the initial stock in compartment \(k\) during time interval \([t_0, t]\). Similarly, \(x_{ki}(t)\) represents the storage in compartment \(i\) at time \(t\) generated by the external input into compartment \(k\), \(z_k(t)\), during \([t_0, t]\) (see Fig. 1). In other words, the proposed methodology can dynamically partition composite compartmental storages into subcompartmental segments based on their constituent initial and external sources. This decomposition enables tracking the evolution of the initial stocks and external inputs, in terms of storage generation, individually and separately within the system. The state variable, \(x_i(t)\), which represents the composite compartmental storage, cannot be used to distinguish the portions of this storage derived from different individual initial and external sources. Therefore, the solution to the decomposed system brings out inferences that cannot be obtained through the analysis of the original system by the state of the art techniques.

The elements of the net subthroughflow and initial subthroughflow rate matrices, \(T(t, x)\) and \(T(t, x)\), represent the distribution of the subthroughflows within the system derived from the initial storages and external inputs, respectively. More specifically, \(r_{ik}(t, x)\) represents the net subthroughflow rate at compartment \(i\) at time \(t\) derived from the initial stock in compartment \(k\) during \([t_0, t]\). Similarly, \(r_{ki}(t, x)\) represents the net subthroughflow rate at compartment \(i\) at time \(t\), generated by the external input into compartment \(k\) during \([t_0, t]\) (see Fig. 2). In other words, the
proposed methodology can dynamically partition composite compartmental through-flows into subcompartmental segments based on their constituent initial and external sources. This decomposition enables tracking the evolution of the initial stocks and external inputs, in terms of flow generation, individually and separately within the system. Thus, the subthroughflow and initial subthroughflow functions of the decomposed system, \( \tau_{i}(t, x) \) and \( \bar{\tau}_{i}(t, x) \), provide more detailed information than the composite throughflow function of the original system, \( \tau_{i}(t, x) \), similar to the state and substate variables, as explained above.

The transient flows and associated storages transmitted along given flow paths are also formulated systematically, through subsystem decomposition methodology. Arbitrary composite intercompartmental flows and storages are dynamically decomposed into the constituent transient subflow segments and substorage portions in each compartment along a given set of subflow paths. Therefore, the dynamic subsystem decomposition determines the distribution of arbitrary intercompartmental flows and the organization of the associated storages generated by these flows along given subflow paths within the subsystems. In other words, the subsystem decomposition enables dynamically tracking the fate of arbitrary intercompartmental flows and associated storages within the subsystems. Consequently, the proposed methodology determines the dynamic influence of one compartment, through direct or indirect interactions, on any other in a complex network. Moreover, a history of compartments visited by arbitrary system flows and storages can also be compiled. The dynamic direct, indirect, acyclic, cycling, transfer (diact) flows and storages transmitted from one compartment, directly or indirectly, to any other—including itself—within the system are also formulated for the quantification of intercompartmental flow and storage dynamics.

The proposed methodology constructs a base for the formulation of multiple dynamic and static mathematical system analysis tools of matrix, vector, and scalar types as quantitative system indicators, other than the ones listed above. The system measures and indices for the diact effect, utility, exposure, residence time, as well as the corresponding system efficiency, stress, and resilience have recently been developed by \[3\] in the context of ecosystem ecology. The static versions of these system analysis tools have also been introduced in separate works \[4, 5\].

3. Results. The proposed methodology is applied to various compartmental models from literature in this section and in Appendix E. The results and their interpretations are presented.

3.1. Case Study. The SIR model is one of the simplest compartmental models in epidemiology which consists of three compartments that represent the populations of three groups: the susceptible or uninfected, \( x_1 = S \), infectious, \( x_2 = I \), and recovered or immune, \( x_3 = R \). The model determines the number of individuals infected with a contagious illness over time. It is reasonably predictive for infectious diseases transmitted from individual to individual. The first SIR model was proposed in its simplest form by \[10\].

In this section, we will analyze a modified version of SIR model. More specifically, it is called the SIRS model for waning immunity with demographics. The model parameters are adopted from \[2\] and the modeling assumptions can be deduced from the model formulation below or can be readily found in the literature \[2, 6\].

The proposed methodology is applied to the following dynamic compartmental
system, governing a laboratory population of mice infected with microbes:

\[
\begin{aligned}
\frac{dx_1}{dt} &= \alpha + \nu x_3 - \beta x_1 x_2 - \mu x_1 \\
\frac{dx_2}{dt} &= \beta x_1 x_2 - (\gamma + \sigma + \mu) x_2 \\
\frac{dx_3}{dt} &= \gamma x_2 - (\nu + \mu) x_3
\end{aligned}
\]

(3.1)

with the initial conditions \( x(t_0) = [10, 10, 0]^T \). The total initial population is given to be 20 by [2], but the initial population for each group is not specified individually. They are, therefore, arbitrarily chosen in this work. The model parameters are the birth rate (or daily rate of input of susceptible mice) \( \alpha = 0.33 \), the natural mortality rate \( \mu = 0.006 \), the mortality rate caused by the disease \( \sigma = 0.06 \), the infection rate \( \beta = 0.0056 \), the recovery rate \( \gamma = 0.04 \), and the immunity loss rate \( \nu = 0.021 \). All parameters are in units of [day\(^{-1}\)] (see Fig. 5).

The system flow regime can be expressed in matrix form as

\[
F(t, x) = \begin{bmatrix}
0 & 0 & \nu x_3 \\
\beta x_1 x_2 & 0 & 0 \\
0 & \gamma x_2 & 0
\end{bmatrix}, \quad z(t, x) = \begin{bmatrix}
\alpha \\
0 \\
0
\end{bmatrix}, \quad y(t, x) = \begin{bmatrix}
\mu x_1 \\
(\mu + \sigma) x_2 \\
\mu x_3
\end{bmatrix}.
\]

The decomposed system can then be expressed in the following matrix form:

\[
\begin{aligned}
\dot{X}(t) &= Z(t, x) + A(t, x) X(t), \quad X(t_0) = 0, \\
\dot{X}(t) &= A(t, x) X(t), \quad X(t_0) = X_0.
\end{aligned}
\]

(3.2)

The fundamental substate matrices, \( X(t) = (x_{ik}(t)) \) and \( \dot{X}(t) = (\dot{x}_{ik}(t)) \), the state, external output, and input matrices, \( \dot{X}(t) = \text{diag}(\dot{x}(t)) \), \( Y(t, x) = \text{diag}(y(t, x)) \), and \( Z(t, x) = \text{diag}(z(t, x)) \), as well as the flow intensity matrix,

\[
A(t, x) = (F(t, x) - T(t, x)) X^{-1}(t)
\]

where \( T(t, x) = Y(t, x) + \text{diag}(F^T(t, x), \mathbf{1}) \) are defined above in the Methods Section.

The numerical results for the state variables \( x(t) \), \( \dot{x}(t) \), and \( \ddot{x}(t) \) are presented in Fig. 6. It can be seen that the oscillatory behavior of the real data is better
approximated by the total population function, $x_1(t) + x_2(t) + x_3(t)$, presented in Fig. 6, than the corresponding graph presented by [2] (cf. solid dots in Fig. 1(d) in [2]). Moreover, the proposed methodology enables tracking the evolution of the initial and newborn populations individually and separately within the system, as presented in Fig. 6. It is worth emphasizing that such individual analysis of the initial and newborn populations separately within a nonlinear dynamic system cannot be done through the state of the art techniques.

![Fig. 6](image1.png)

**Fig. 6.** Numerical results for the evolution of the state variables $x(t)$, initial populations, $x(t)$, and populations generated by external inputs, $x(t)$ (Example 3.1).

The fundamental matrices, that is, the substate and initial substate matrix functions, $X(t)$ and $X(t)$, are also presented in Fig. 7. Note that the substate functions for the $3^{rd}$ initial subsystem and $2^{nd}$ and $3^{rd}$ subsystems are identically zero because of the zero initial condition, $x_{30} = 0$, and external inputs, $z_2(t) = z_3(t) = 0$. That is,

$$x_{ik}(t) = 0 \quad \text{and} \quad x_{ik}(t) = 0 \quad \text{for} \quad k = 2, 3 \quad \text{and} \quad i = 1, 2, 3.$$

Since there is only one nonzero input in this model ($z_1(t) > 0$), $x_1(t) = x_{11}(t)$, $x_2(t) = x_{21}(t)$, and $x_3(t) = x_{31}(t)$, as presented in Figs. 6 and 7. The initial substate and substate variables $x_{21}(t)$ and $x_{21}(t)$, for example, represent the population in compartment 2 at time $t$, which is derived from the initial population in compartment 1, $x_{10}$, and external input into compartment 1, $z_1(t)$, during $[t_0, t]$, respectively. Biologically, $x_{21}(t)$ can be interpreted as the population of the infected mice at time $t$, that had initially been susceptible and then infected sometime during $[t_0, t]$. Similarly, $x_{21}(t)$ represents the population of the infected mice at time $t$, which were born (or introduced) susceptible and then infected during $[t_0, t]$.

![Fig. 7](image2.png)

**Fig. 7.** Graphical representations of the initial substate and substate functions $x_{ik}(t)$ and $x_{ik}(t)$ for all $i, k$. The substates that are equal to zero are not labeled. (Example 3.1).
In general terms, the state variable \( x_i(t) \) of the original system, Eq. 3.1, for SIR group dynamics represents the population in group \( i \) at time \( t \) with the initial population, \( x_i(t_0) \). It cannot be used to distinguish the subpopulations generated by either newborn (the only external input in this model, \( z_1(t) \)) or derived from the initial SIR populations (initial conditions, \( x_{i0} \)). On the other hand, the state variable \( x_{ik}(t) \) of the decomposed system, Eq. 3.2, for SIR subgroup dynamics represents the subpopulation in group \( i \) at time \( t \), which is transferred from the newborn population in group \( S \) during \([t_0, t] \). Similarly, the state variable of the decomposed system, \( x_{ik}(t) \), represents the subpopulation in group \( i \) at time \( t \), which is transferred from the initial population in group \( k \), \( x_k(t_0) \), during \([t_0, t] \). Parallel interpretations are possible for the throughput function of the original system, \( \tau_i(t, x) \), and the subthroughflow functions of the decomposed system, \( \hat{\tau}_{ik}(t, x), \hat{\tau}_{ik}(t, x), \hat{\tau}_{ik}(t, x) \), and \( \hat{\tau}_{ik}(t, x) \), as well.

The proposed dynamic system decomposition methodology, consequently, enables compiling a health history of the newborn or initial SIR populations by tracking the evolution of their health states individually and separately. Note that, the solution to the original system through the state of the art techniques can only provide the evolution of their health states individually and separately. Such classification and characterization of the subpopulations in each SIR group as presented above are not possible through the application of the state of the art techniques.

The transient substorage functions at compartment 2 along closed subflow path \( p_{2,1}^1 := 0_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \) are computed as an application of the proposed dynamic subsystem decomposition methodology. The links on this path that directly contribute to the cumulative transient substorage \( x_{21}^1(t) \) are numbered with red cycle numbers, \( m \), in the extended subflow path diagram below:

\[
p_{2,1}^1 = 0_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow \cdots
\]

The cumulative transient subsubstorage function \( x_{21}^3(t) \) at subcompartment 2 along \( p_{2,1}^1 \) will be approximated by three terms \((m_1 = 3)\) using Eq. C.1:

\[
x_{21}^3(t) = \sum_{m=1}^3 x_{31,21}^m(t) = x_{31,21}^{1,1}(t) + x_{31,21}^{1,2}(t) + x_{31,21}^{1,3}(t).
\]

The governing equations Eqs. 2.76 and 2.77 for the transient substorage functions, \( x_{31,21}^{1,m}(t) \), are solved simultaneously with the decomposed system Eq. 2.67. Numerical results are presented in Fig. 8. Since the subflow path \( p_{2,1}^3 \) covers the entire flow regime in subsystem 1, \( x_{21}(t) \) and \( x_{21}^3(t) \) must be the same. They, however, are approximately equal as presented in Fig. 8, that is, \( x_{21}^3(t) \cong x_{21}(t) \). The difference is caused by the truncation errors in the computation of the cumulative transient subflow, and larger \( m_1 \) values improve the approximation. Since subflow path \( p_{2,1}^3 \) represents the complete flow regime in subsystem 1 and it is closed, \( x_{21}^3(t) \) is also the simple cycling subflow at subcompartment 2, that is \( x_{21}^3(t) = x_{21}^3(t) = x_{21}^1(t) \).

Biologically, the transient substorage functions, \( x_{31,21}^{1,m}(t) \), represent the population of the mice at time \( t \) that are infected \( m \) times after being recovered during \([t_0, t] \). These populations are decreasing with increasing \( m \) values, as expected. Such classification and characterization of the subpopulations in each SIR group as presented above are not possible through the application of the state of the art techniques.

Along the following subflow paths of finite length,

\[
p_{01}^2 := 0_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \Rightarrow 0_1,
\]

\[
p_{01}^3 := 0_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \rightarrow 3_1 \rightarrow 1_1 \rightarrow 2_1 \Rightarrow 0_1,
\]
the transient subflow rate functions can be computed using the governing equations Eqs. 2.76 and 2.77 similar to the transient storages as discussed above (see Fig. 5). Note that the paths represent the death (external output) of the newborn mice (external input) following two complete infection cycles (after three infections). The only difference between them is the last links which represent the death due to the disease ($\sigma$) and the natural death ($\mu$). The numerical results for these transient external output rates at compartment 2, $f_{0,211}(t)$ and $f_{0,211}(t)$, which correspond to these last two links, are depicted in Fig. 8. Because of the corresponding parameter values, $\sigma$ and $\mu$, the death rate due to the disease is 10 times higher than that due to the natural death. These rate functions can biologically be interpreted as the number of mice that were born during $[0, t]$ and die per day at time $t$ after being repeatedly recovered and getting infected for the third time. More specifically, one of these transient output rates at $t = 500$ days, $f_{0,211}(500) = 0.027$, for example, indicates that 2.7 out of 100 mice that were born during $[0, 500]$ die per day on the 500th day of the experiment due to the disease, after getting infected three times.

The proposed dynamic subsystem decomposition methodology, consequently, enables compiling a history of the health states of an arbitrary population in any of the $SIR$ groups along a given infection path. Therefore, the effect of the arbitrary population on any other group in terms of the spread of the disease, through not only direct but also indirect interactions, can be determined. As a result, the spread of the disease from an arbitrary population to the entire population can dynamically be determined and monitored.

The system approaches an epidemic equilibrium as presented in the graphs of Fig. 7 after about 450 days. At this steady state, the system information becomes

$$(3.3) \quad F = \begin{bmatrix} 0 & 0 & 0.20 \\ 0.53 & 0 & 0 \\ 0 & 0.20 & 0 \end{bmatrix}, \quad x = \begin{bmatrix} 18.93 \\ 5.00 \\ 9.52 \end{bmatrix}, \quad y = \begin{bmatrix} 0 \\ 0.33 \\ 0 \end{bmatrix}, \quad z = \begin{bmatrix} 0.33 \\ 0 \\ 0 \end{bmatrix}.$$  

The components of the output vector implies that, at steady state, the only external output occurs from compartment 2; $y_2 = 0.33$. This biologically means that, at steady state, the model accounts for only death caused by the disease.

The static $\text{diact}$ flows and storages in matrix form are listed in Table 1 as formulated by [4]. For this SIRS model, the composite indirect flow rate and storage
matrices become

\[
T^i = \begin{bmatrix}
0.20 & 0.20 & 0 \\
0 & 0.20 & 0.20 \\
0.20 & 0 & 0.08
\end{bmatrix}
\quad \text{and} \quad
X^i = \begin{bmatrix}
7.14 & 7.14 & 0 \\
0 & 1.89 & 1.89 \\
9.52 & 0 & 3.59
\end{bmatrix}.
\]

The zero entries of the matrices indicate that there is no indirect flow, and therefore, associated storage generation in the corresponding flow direction. For example, the \((1, 3)\)–entry of \(T^i\) is \(\tau_{13}^i = 0\), which indicates that although there is a direct flow from the recovered population to the susceptible group, \(f_{13} = 0.20\), there is no indirect flow in the same direction through the infectious population at the epidemic equilibrium. Moreover, due to reflexivity, the diagonal elements of these matrices represent the cycling flows and storages. The cycling flow rate at compartment 3, \(\tau_3^i = \tau_{33}^i = 0.08\), indicates that 0.08 recovered mice become susceptible by losing immunity, get infected, and recovered again per day. In other words, about 8 mice complete such a recovery cycle within a 100 day period. This cycling flow constantly maintains the cycling storage of \(x_3^i = x_{33}^i = 3.59\) mice within the recovered mice population. The other static diactic flows and associated storages can similarly be computed and interpreted accordingly.

Evidently, the detailed information and inferences enabled by the proposed methodology cannot be obtained by analyzing the original system through the state of the art techniques.

4. Discussion. We introduced a nonlinear decomposition principle for dynamic compartmental systems based on the novel system decomposition methodology in the present paper. A deterministic mathematical method is then developed for dynamic analysis of nonlinear compartmental systems. The method is applied to various models from literature to demonstrate its efficiency and wide applicability. The results indicate that the proposed theory and methodology provides significant advancements in the theory, methodology, and practicality of the current nonlinear dynamic compartmental system analysis.

Many natural phenomena can be modeled through compartmental systems. Although good rationales are offered in the literature for the analysis of compartmental networks, they are mainly for special cases, such as linear models and static systems. Realistically, nature is always on the move and its systems are constantly changing to meet ever-renewing circumstances. Therefore, the need for dynamic analysis of nonlinear compartmental systems has always been present.

This is the first manuscript in literature that proposes a theory and develops a comprehensive method for holistic analysis of nonlinear dynamic compartmental systems. The proposed theory is based on the dynamic system and subsystem decomposition methodologies. The original nonlinear compartmental system is decomposed into mutually exclusive and exhaustive subsystems through the system decomposition methodology. The subsystems are then further decomposed along a given set of mutually exclusive and exhaustive subflow paths through the subsystem decomposition methodology. While the dynamic system decomposition formulates the distribution of external inputs and initial stocks as well as the organization of the associated storages generated by the inputs and stocks individually and separately within the system, the dynamic subsystem decomposition formulates the distribution of intercompartmental flows and the organization of associated storages within the subsystems. The proposed mathematical method, therefore, as a whole, yields the dynamic decomposition of system flows and storages to the utmost level.
The system decomposition methodology yields the subthroughflow and substorage matrix functions that respectively represent the flows at and storages in each compartment separately derived from individual external inputs and initial stocks. More specifically, the composite compartmental storage and throughflow, $x_i(t)$ and $\tau_i(t)$, are dynamically partitioned into the subcompartmental substorage and subthroughflow segments, $x_{ik}(t)$ and $\tau_{ik}(t)$ ($x_{ik}(t)$ and $\tau_{ik}(t)$), respectively, based on their constituent external (initial) sources, $z_k(t)$ ($x_{in}$). In other words, this methodology enables tracking the evolution of external inputs and initial stocks as well as associated storages individually and separately within the system. The subsystem decomposition methodology then yields the transient and the dynamic direct, indirect, acyclic, cycling, and transfer (diact) flows and associated storages transmitted along a given flow path or from one compartment, directly or indirectly, to any other. The subsystem partitioning, therefore, enables tracking the fate of arbitrary intercompartmental flows and associated storages along given subflow paths within the subsystems. Therefore, the spread of an arbitrary flow or storage segment from one compartment to the entire system can be determined and monitored. Moreover, a history of compartments visited by arbitrary system flows and storages can also be compiled.

The proposed dynamic methodology also constructs a base for the development of new mathematical system analysis tools as quantitative system indicators. Multiple novel measures, such as the substorage, subthroughflow, diact flow and storage matrices, are introduced in the present manuscript. The illustrative case studies in Section 3 and Appendix E demonstrate efficiency and wide applicability of the proposed methodology and measures. More dynamic and static measures and indices have recently been introduced in the context of ecosystem ecology by \[3, 5, 4\].

In summary, we consider that the proposed mathematical theory and methodology brings a novel, formal, deterministic, complex system theory to the service of urgent natural problems of the day.

Appendices. The dynamic system and subsystem decomposition methodologies for the initial subsystem in parallel to the decomposition of the original system, the applications of the proposed method to special cases, such as linear and static models, and additional method formulations and examples are presented in this section.

Appendix A. Initial System Decomposition.

The dynamic system decomposition methodology is introduced in Section 2.2. In order to analyze the flow distribution and the storage organization derived from the initial stocks individually and separately within the system, the initial subsystem will further be decomposed into initial subsystems in parallel to the system decomposition. With some abuse of terminology, we will call the subsystems of the initial subsystem the initial subsystems, instead of the initial sub-sub-systems (see Fig. 1 and 2). The initial system decomposition methodology dynamically decomposes the composite subthroughflows and substorages within the initial subsystem into segments based on their constituent initial stocks. In other words, the initial system decomposition enables dynamically tracking the evolution of the initial stocks individually and separately within the system.

Each initial subsystem is driven by an initial stock. Therefore, if there is no initial stock in a compartment, that is, the initial condition is zero, the corresponding initial subsystem is null. The number of initial subsystems, therefore, is equal to the number of initial conditions (or compartments). Therefore, there are $n$ initial subsystems, one for each initial condition, indexed by $k = 1, \ldots, n$. The dynamic initial subsystem decomposition methodology is introduced in this section.
A.1. Initial State Decomposition. Similar to the original system, the initial subcompartments can further be decomposed into \( n \) subcompartments (see Fig. 2). We will use the notation \( x_{ik_0}(t) \) for \( k^\text{th} \) state of \( i^\text{th} \) initial state or \( x_{ik}(t) \) for notational convenience. Based on this further decomposition of the initial states, we have

\[
x_{i0}(t) = \bar{x}_i(t) = \sum_{k=1}^{n} x_{ik}(t)
\]

for \( i = 1, \ldots, n \), and the corresponding initial conditions are

\[
\bar{x}_{ik_0}(t_0) = \delta_{ik_0} x_{i0}(t_0) = \begin{cases} x_{i0}(t_0) = x_{i0}, & i = k \\ 0, & i \neq k \end{cases}
\]

The \textit{initial state matrix} function is then defined as

\[
X(t) := (x_{ik}(t)) = \begin{bmatrix} x_1(t) & \cdots & x_n(t) \end{bmatrix}.
\]

We also define the \textit{initial state} and the \( k^\text{th} \) \textit{initial state matrix} functions, \( X(t) \) and \( X_k(t) \), as

\[
X(t) := X_0(t) = \text{diag} (\bar{x}(t)) \quad \text{and} \quad X_k(t) := \text{diag} (\bar{x}_k(t))
\]

for \( k = 1, \ldots, n \). These matrices will, alternatively, be called the \textit{initial substorage} and \( k^\text{th} \textit{initial substorage matrix} \) functions, respectively. The initial conditions of these matrices given in Eq. A.2 can be expressed in matrix form as

\[
X(t_0) = X_0(t_0) = X_k(t_0) = \text{diag}(\bar{x}_0) \quad \text{and} \quad X_k(t_0) := \text{diag} (x_{k,0} e_k).
\]

Note that

\[
\bar{x}(t) = X(t) \mathbf{1} \quad \text{and} \quad \bar{x}_k(t) = X_k(t) \mathbf{1}.
\]

The state decomposition methodology for the initial subsystem can be summarized as follows:

\[
\mathbf{x}_0 = \bar{x}(t) = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_n \end{bmatrix} \quad \text{state decomposition} \quad X(t) = \begin{bmatrix} \bar{x}_{11} & \bar{x}_{12} & \cdots & \bar{x}_{1n} \\ \bar{x}_{21} & \bar{x}_{22} & \cdots & \bar{x}_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{x}_{n1} & \bar{x}_{n2} & \cdots & \bar{x}_{nn} \end{bmatrix}
\]

A.2. Initial Flow Rate Decomposition. Similar to the flow rate decomposition of the original system introduced in Section 2.2.2, the initial flow rates are also decomposed into \textit{initial subflow rates} that represent the rate of subflow segments between the initial subcompartments (see Fig. 2).

For notational convenience, we set

\[
f_{ij}(t, \mathbf{x}) := f_{i_0,j_0}(t, \mathbf{x}), \quad z_i(t, \mathbf{x}) := f_{i0}(t, \mathbf{x}), \quad \text{and} \quad y_j(t, \mathbf{x}) := f_{0j}(t, \mathbf{x})
\]

for \( i, j = 1, \ldots, n \). We define the \textit{initial subflow rate, input, and output matrix} functions as

\[
F(t, \mathbf{x}) := F_0(t, \mathbf{x}), \quad Z(t, \mathbf{x}) := Z_0(t, \mathbf{x}) = \mathbf{0}, \quad \text{and} \quad \mathcal{Y}(t, \mathbf{x}) := \mathcal{Y}_0(t, \mathbf{x}).
\]
We will use the notation \( f_{ik,jk} (t, x) \) for flow rate from initial substate \( x_{jk} (t) \) to \( x_{ik} (t) \) for notational convenience, for \( i, j, k = 1, \ldots, n \). In particular, \( z_{ik} (t, x) := f_{ik,0} (t, x) = 0 \) and \( y_{jk} (t, x) := f_{0j,k} (t, x) \).

The initial subflow rate decomposition can then be formulated as

\[
(A.9) \quad f_{ik,jk} (t, x) := \frac{x_{jk} (t)}{x_j (t)} \bar{f}_{ij} (t, x) = \frac{x_{jk} (t)}{x_j (t)} f_{ij} (t, x)
\]

for \( i, j, k = 1, \ldots, n \), because of Eq. 2.28. Due to the state decomposition, Eq. A.1, we also have

\[
(A.10) \quad f_{ij} (t, x) = \sum_{k=1}^{n} f_{ik,jk} (t, x)
\]

for \( i, j = 1, \ldots, n \). It can be seen from Eq. A.9 that the initial flow and subflow rate intensities between the same compartments in the same flow direction are the same, that is

\[
(A.11) \quad \frac{f_{ik,jk} (t, x)}{x_{jk} (t)} = \frac{f_{ij} (t, x)}{x_j (t)} = \frac{f_{ik,jk} (t, x)}{x_{jk} (t)} = \frac{f_{ij} (t, x)}{x_j (t)}
\]

for \( i, j, k = 1, \ldots, n \) (see Fig. 2). The last two equalities are due to Eq. 2.28.

The decomposition factors, \( d_{ik} (x) \), for the initial subflow rates with the following definition and properties

\[
(A.12) \quad d_{ik} (x) := \frac{x_{jk} (t)}{x_j (t)}, \quad 0 \leq d_{ik} (x) \leq 1, \quad \text{and} \quad \sum_{k=0}^{n} d_{jk} (x) = 1,
\]

form another continuous partition of unity. Note also that, due to Eq. A.1, \( x_{jk} (t) \leq x_j (t) \). The decomposition factors are, therefore, well-defined even if \( x_j (t) \rightarrow 0 \). The respective initial decomposition and \( k^{th} \) initial decomposition matrices, \( D(x) := (d_{jk} (x)) \) and \( D_k (x) = \text{diag} ([d_{1k} (x), \ldots, d_{nk} (x)]) \), for the initial subsystems can be formulated, accordingly, as

\[
(A.13) \quad D(x) = X^{-1} (t) X (t) \quad \text{and} \quad D_k (x) := X^{-1} (t) X_k (t)
\]

for \( k = 1, \ldots, n \). Equations A.6 and A.12 imply that

\[
(A.14) \quad 1 = X^{-1} (t) x_0 (t) = X^{-1} (t) X (t) 1 = D(x) 1.
\]

From Eqs. 2.32 and A.14, we also have

\[
(A.15) \quad x(t) = x(t) + \bar{x}(t) = X(t) 1 + X(t) 1,
\]

similar to Eq. 2.23.

We define the \( k^{th} \) initial subflow rate matrix function as

\[
(A.16) \quad F_k (t, x) := \left( f_{ik,jk} (t, x) \right)
\]

for \( k = 1, \ldots, n \). Using Eq. A.9, \( F_k (t, x) \) can be expressed in various matrix forms:

\[
(A.17) \quad F_k (t, x) = F(t, x) D_k (x) = F(t, x) X^{-1} (t) X_k (t) = F(t, x) X^{-1} (t) X_k (t).
\]
That is, the $k^{th}$ initial decomposition matrix, $D_k(x)$, decomposes the direct initial flow matrix, $F(t,x)$, into the initial subflow matrices, $F_k(t,x)$. The last equality is derived from Eqs. A.4 and 2.34, as these equations imply that

$$F(t,x) = F_0(t,x) = F(t,x) \mathcal{X}^{-1}(t) \mathcal{X}_0(t) = F(t,x) \mathcal{X}^{-1}(t) \mathcal{X}(t).$$

Similarly, the $k^{th}$ initial output matrix function,

$${\bar{y}}_k(t,x) := \text{diag} \left([f_{01k}(t,x), \ldots, f_{0nk}(t,x)]\right),$$

can be expressed in matrix form as

$${\bar{y}}_k(t,x) = \mathcal{Y}(t,x) D_k(x) = \mathcal{Y}(t,x) \mathcal{X}^{-1}(t) \mathcal{X}_k(t) = \mathcal{Y}(t,x) \mathcal{X}^{-1}(t) \mathcal{X}_k(t)$$

and the $k^{th}$ initial input matrix function becomes

$$Z_k(t,x) = 0$$

for $k = 1, \ldots, n$. The initial output and $k^{th}$ output vectors, $y(t,x)$ and $y_k(t,x)$, for the $k^{th}$ initial subsystem can be defined as follows:

$$y(t,x) := \mathcal{Y}(t,x) 1 \quad \text{and} \quad y_k(t,x) := \bar{y}_k(t,x) 1.$$

Clearly, the initial input and $k^{th}$ input vectors are $z(t,x) := Z(t,x) 1 = 0$ and $z_k(t,x) := Z_k(t,x) 1 = 0$.

Using these notations, the flow rate decompositions given in Eq. A.10 can be expressed in matrix form:

$$F(t,x) = \sum_{k=1}^{n} F_k(t,x), \quad \mathcal{Y}(t,x) = \sum_{k=1}^{n} \bar{y}_k(t,x), \quad Z(t,x) = \sum_{k=1}^{n} Z_k(t,x) = 0.$$

The equivalence of the flow, initial flow, and initial subflow rate intensities given in Eq. A.11 can also be expressed in matrix form as follows:

$$F_k(t,x) \mathcal{X}_k^{-1}(t) = F(t,x) \mathcal{X}^{-1}(t) = F_0(t,x) \mathcal{X}_0^{-1}(t) = F(t,x) \mathcal{X}^{-1}(t)$$

for $k = 1, \ldots, n$, similar to Eq. 2.40. Equations 2.48 and A.24 also imply that the flow and storage distribution matrices for both subsystems and initial subsystems are the same. That is,

$$Q^r(t,x) := F(t,x) \mathcal{X}^{-1}(t) = Q^r(t,x)$$

$$Q^r(t,x) := F(t,x) \mathcal{T}^{-1}(t) = Q^r(t,x)$$

The initial flow rate decomposition methodology for the initial subsystem given in Eq. A.9 can be schematized as follows:

$$\begin{bmatrix}
  f_{11} & \cdots & f_{1n} \\
  f_{21} & \cdots & f_{2n} \\
  \vdots & \ddots & \vdots \\
  f_{n1} & \cdots & f_{nn}
\end{bmatrix}
\begin{bmatrix}
  x_{1k}(t) \\
  x_{2k}(t) \\
  \vdots \\
  x_{nk}(t)
\end{bmatrix}
= \begin{bmatrix}
  f_{1k1k} & \cdots & f_{1knk} \\
  f_{2k1k} & \cdots & f_{2knk} \\
  \vdots & \ddots & \vdots \\
  f_{nk1k} & \cdots & f_{nknn}
\end{bmatrix}
\begin{bmatrix}
  f_{11k} & \cdots & f_{1nk} \\
  f_{21k} & \cdots & f_{2nk} \\
  \vdots & \ddots & \vdots \\
  f_{nk1} & \cdots & f_{nnk}
\end{bmatrix}$$
A.3. Initial Subsystems. Using the dynamic initial system decomposition methodology composed of the analytic state and flow rate decomposition components, the initial system can explicitly be decomposed into mutually exclusive and exhaustive initial subsystems, each of which is driven by a single initial stock (see Fig. 1 and 2).

The $k^{th}$ subcompartments of each initial subcompartment together with the corresponding $k^{th}$ initial substates, initial subflow rates, inputs, and outputs constitute the $k^{th}$ initial subsystem. Therefore, the system decomposition methodology generates mutually exclusive and exhaustive subsystems that are running within the initial subsystem and have the same structure and dynamics as the initial subsystem itself, except for their initial conditions. These otherwise-decoupled subsystems are coupled through the decomposition factors. Therefore, in a system with $n$ compartments, each initial subcompartment has $n$ subcompartments. Consequently, the system has $n$ initial subsystems indexed by $k = 1, \ldots , n$. The substorage of each of these $n$ initial subcompartments is derived from a single initial stock. If any of the initial conditions is zero, the corresponding initial subsystem becomes null.

Similar to the governing equations for the original system Eq. 2.10, the governing equations for the initial subsystem can be written in the following vector form

$$\dot{X}(t) = F(t, X) - F(t, \hat{X}(t), X(t_0) = X_0$$

as given in Eq. 2.43 where $X(t) = x_0$, $\bar{\tau}(t, X) = \tau_0(t, X)$, and $\bar{\tau}(t, X) = \tau_0(t, X)$. The governing equations for the $k^{th}$ initial subsystem can then be written in vector form as

$$\dot{X}_k(t) = \bar{\tau}_k(t, X) - \hat{\tau}_k(t, X)$$

$$= F_k(t, X) \mathcal{X}^{-1}(t) x_k(t) - F_k(t, \hat{x}_k(t), X(t_0) = x_{k,0} e_k$$

for $k = 1, \ldots , n$. The corresponding initial conditions become $x_k(t_0) = x_{k,0} e_k$.

The $k^{th}$ inward and outward subthroughflow vectors, $\bar{\tau}_k(t, X)$ and $\hat{\tau}_k(t, X)$, for the $k^{th}$ initial subsystem given in Eq. A.27 can then be expressed in the following forms:

$$\bar{\tau}_k(t, X) := F_k(t, X) 1$$

$$= F(t, X) \mathcal{X}^{-1}(t) x_k(t)$$

$$= F(t, x) \mathcal{X}^{-1}(t) x_k(t)$$

$$= F_k(t, X) \mathcal{X}^{-1}(t) x_k(t)$$

$$\hat{\tau}_k(t, X) := y_k(t, X) + F_k^T(t, X) 1$$

$$= \mathcal{Y}(t, X) \mathcal{X}^{-1}(t) \mathcal{X}_k(t) 1 + \mathcal{Y}_k(t) \mathcal{X}^{-1}(t) F_k^T(t, X) 1$$

$$= (\mathcal{Y}(t, x) + \text{diag}(F(t, x) 1)) \mathcal{X}^{-1}(t) x_k(t)$$

The $k^{th}$ net subthroughflow rate vector, $\tau_k(t, X) = [\tau_{1k}(t, X), \ldots , \tau_{nk}(t, X)]^T$, for the initial subsystem then becomes

$$\tau_k(t, X) := \bar{\tau}_k(t, X) - \hat{\tau}_k(t, X) = A(t, x) x_k(t).$$

The $k^{th}$ inward and outward subthroughflow matrices, $\bar{\tau}_k(t, X) := \text{diag}(\bar{\tau}_k(t, X))$ and $\hat{\tau}_k(t, X) := \text{diag}(\hat{\tau}_k(t, X))$, for the $k^{th}$ initial subsystem can be expressed as

$$\bar{\tau}_k(t, X) = \mathcal{F}(t, x) \mathcal{X}^{-1}(t) \mathcal{X}_k(t) 1$$

$$\hat{\tau}_k(t, X) = \mathcal{T}(t, x) \mathcal{X}^{-1}(t) \mathcal{X}_k(t).$$
Note that, using Eq. A.30, \( F_k(t, x) \) given in Eq. A.17 can, alternatively, be written in terms of the system flows only:

\[
F_k(t, x) = F(t, x) T^{-1}(t, x) \hat{T}_k(t, x).
\]

We define the inward and outward subthroughflow matrices, \( \hat{T}(t, x) \) and \( \hat{T}(t, x) \), for the initial subsystems as the matrices whose \( k \)th columns are the inward and outward initial subthroughflow vectors, \( \hat{\tau}_k(t, x) \) and \( \hat{\tau}_k(t, x) \), \( k = 1, \ldots, n \), respectively:

\[
\hat{T}(t, x) := (\hat{\tau}_{jk}(t, x)) = [\hat{\tau}_1(t, x) \cdots \hat{\tau}_n(t, x)],
\]

\[
\hat{T}(t, x) := (\hat{\tau}_{jk}(t, x)) = [\hat{\tau}_1(t, x) \cdots \hat{\tau}_n(t, x)].
\]

Using the relationships in Eq. A.28, these subthroughflow matrices for the initial subsystems can be expressed in matrix form as

\[
\hat{T}(t, x) = F(t, x) \mathcal{X}^{-1}(t) X(t),
\]

\[
\hat{\tau}(t, x) = T(t, x) \mathcal{X}^{-1}(t) X(t).
\]

We then define the net subthroughflow matrix, \( T(t, x) \), for the initial subsystems as follows:

\[
T(t, x) := \hat{T}(t, x) - \hat{T}(t, x) = A(t, x) X(t).
\]

Due to Eq. A.33, the decomposition matrix \( D(x) \) can be expressed in terms of the subthroughflow functions instead of the substate functions:

\[
D(x) = \mathcal{X}^{-1}(t) X(t) = T^{-1}(t, x) \hat{T}(t, x).
\]

Note that, using the notations developed above, the initial subthroughflow matrices can be written in various forms as follows:

\[
\hat{T}(t, x) = F(t, x) D(x) = Q^\tau(t, x) \mathcal{X}(t) = Q^\tau(t, x) \hat{T}(t, x)
\]

\[
\hat{T}(t, x) = R^{-1}(t, x) X(t).
\]

For each fixed \( j \), Eqs. A.9 or A.33 imply that

\[
\frac{\hat{\tau}_{jk}(t, x)}{x_{jk}(t)} = \frac{\hat{\tau}_{jk}(t, x)}{x_{jk}(t)} = \frac{\sum_{i=0}^{n} f_{ij}(t, x)}{x_{jk}(t)} \frac{\sum_{i=0}^{n} f_{ij}(t, x)}{x_{jk}(t)} = \frac{\hat{\tau}_{jk}(t, x)}{x_{jk}(t)}
\]

for \( k = 1, \ldots, n \). This equivalence of outward throughflow and subthroughflow intensities for the initial subsystems given in the second and last equalities of Eq. A.37 can be expressed in matrix form:

\[
R^{-1}(t, x) = T(t, x) \mathcal{X}^{-1}(t) = \hat{T}_0(t, x) \mathcal{X}_0^{-1}(t)
\]

\[
= \hat{T}(t, x) \mathcal{X}^{-1}(t) = \hat{T}_k(t, x) \mathcal{X}_k^{-1}(t) = \hat{T}(t, x) \mathcal{X}^{-1}(t)
\]

where the last equality is derived from Eq. A.36. Equations A.9, A.37, and 2.54 also imply that

\[
\frac{\hat{\tau}_{jk}(t, x)}{\hat{\tau}_{jk}(t, x)} = \frac{\hat{\tau}_{jk}(t, x)}{\hat{\tau}_{jk}(t, x)} = \frac{x_{jk}(t)}{x_{jk}(t)} = \frac{f_{ij}(t, x)}{f_{ij}(t, x)}
\]

\[
\frac{\hat{\tau}_{jk}(t, x)}{\hat{\tau}_{jk}(t, x)} = \frac{\hat{\tau}_{jk}(t, x)}{\hat{\tau}_{jk}(t, x)} = \frac{x_{jk}(t)}{x_{jk}(t)} = \frac{f_{ij}(t, x)}{f_{ij}(t, x)}
\]
for \( k, \ell = 1, \ldots, n \). This relationship indicates the proportionality of the parallel initial subflows and corresponding subthroughflows and substorages.

Using Eq. A.38, the \( k^{th} \) initial decomposition matrix, \( \bar{D}_k(x) \), can be written as

\[
(\text{A.40}) \quad \bar{D}_k(x) = \mathcal{X}^{-1}(t) \mathcal{X}_k(t) = \mathcal{T}(t, x)^{-1} \bar{T}_k(t, x),
\]

similar to the initial decomposition matrix, as formulated in Eq. A.35. It is worth noting that the initial decomposition and \( k^{th} \) initial decomposition matrices, \( \bar{D}(x) \) and \( \bar{D}_k(x) \), decompose the compartmental throughflow matrix, \( \mathcal{T}(t, x) \), into the outward initial subthroughflow and \( k^{th} \) initial subthroughflow matrices as indicated in Eqs. A.36 and A.40, similar to the decomposition of \( \bar{F}(t, x) \) as formulated in Eq. A.17. That is,

\[
(\text{A.41}) \quad \bar{T}(t, x) = \mathcal{T}(t, x) \bar{D}(x) \quad \text{and} \quad \bar{T}_k(t, x) = \mathcal{T}(t, x) \bar{D}_k(x).
\]

It is worth noting also the relationships given below between the flow and subthroughflow matrices for the initial subsystems:

\[
\bar{F}(t, x) 1 = \sum_{k=1}^{n} \bar{F}_k(t, x) 1 = \sum_{k=1}^{n} \bar{\tau}_k(t, x) = \bar{\tau}(t, x) = \bar{T}(t, x) 1,
\]

\[
\mathbf{y}(t, x) + \bar{F}^T(t, x) 1 = \sum_{k=1}^{n} \mathbf{y}_k(t, x) + \mathbf{F}_k^T(t, x) 1 = \sum_{k=1}^{n} \bar{\tau}_k(t, x) = \bar{\tau}(t, x)
\]

\[
= \bar{T}(t, x) 1.
\]

The governing equations for the initial subsystems of the decomposed system, Eq. 2.63, can then be written in vector form as

\[
(\text{A.42}) \quad \dot{x}_k(t) = A(t, x) x_k(t), \quad x_k(t_0) = x_{k,0} e_k
\]

for \( k = 1, \ldots, n \). In matrix form, the governing equations become

\[
(\text{A.43}) \quad \dot{X}(t) = \mathcal{T}(t, x) = \bar{T}(t, x) - \bar{T}(t, x), \quad X(t_0) = X_0.
\]

This system can also be expressed in terms of the flow intensity matrix, \( A(t, x) \):

\[
(\text{A.44}) \quad \dot{X}(t) = A(t, x) X(t), \quad X(t_0) = X_0.
\]

The system decomposition methodology that yields the governing equations for each initial subsystem in vector form, Eq. A.42, or for the entire initial system in matrix form, Eq. A.43, can be schematized as follows:
\( \hat{x}(t) = \tau(t, \mathbf{x}) \)

\( \hat{x}_k(t) = \tau_k(t, \mathbf{x}), \quad k = 1, \ldots, n \)

\[
\begin{bmatrix}
\dot{x}_1 \\
\dot{x}_2 \\
\vdots \\
\dot{x}_n
\end{bmatrix}
= \begin{bmatrix}
I_1 \\
I_2 \\
\vdots \\
I_n
\end{bmatrix}
\]

\[\text{vector form}\]

\[
\begin{bmatrix}
\dot{x}_{11} & \cdots & \dot{x}_{1n} \\
\dot{x}_{21} & \cdots & \dot{x}_{2n} \\
\vdots & \ddots & \vdots \\
\dot{x}_{n1} & \cdots & \dot{x}_{nn}
\end{bmatrix}
= \begin{bmatrix}
I_{11} & \cdots & I_{1n} \\
I_{21} & \cdots & I_{2n} \\
\vdots & \ddots & \vdots \\
I_{n1} & \cdots & I_{nn}
\end{bmatrix}
\]

\[\text{matrix form}\]

\[\dot{X}(t) = T(t, \mathbf{x})\]

**Appendix B. Analytic Solution to Linear Systems.**

In this section, we analyze linear dynamic compartmental systems. For linear systems, the original system of governing equations, Eq. 2.66, takes the following compact form:

\[ (B.1) \quad \dot{x}(t) = z(t) + A(t)x(t), \quad x(t_0) = x_0. \]

The system partitioning methodology yields a linear system, if the original system is linear. That is, the decomposed system, Eq. 2.67, is also linear:

\[ (B.2) \quad \dot{X}(t) = Z(t) + A(t)X(t), \quad X(t_0) = 0, \]

\[ \dot{X}(t) = A(t)X(t), \quad X(t_0) = X_0. \]

Let \( V(t) \) be the fundamental matrix solution of the system Eq. B.1, that is, the unique solution of the system

\[ (B.3) \quad \dot{V}(t) = A(t)V(t), \quad V(t_0) = I. \]

The solutions for \( X(t) \) and \( \dot{X}(t) \) in terms of \( V(t) \) become

\[ (B.4) \quad X(t) = \int_{t_0}^t V(t) V^{-1}(\tau) Z(\tau) d\tau \quad \text{and} \quad \dot{X}(t) = V(t) X_0. \]

Therefore, we have the following observation.

**Remark B.1.** The initial substate matrix of the decomposed system, \( X(t) \), scaled by the nonzero matrix of the initial conditions, \( X_0 > 0 \), is the fundamental matrix solution to the original linear system, Eq. B.1. That is, \( V(t) = X(t) X_0^{-1} \).

The solution for \( X(t) \) can then be expressed, in terms of the fundamental matrix solution, as

\[ (B.5) \quad X(t) = \int_{t_0}^t X(t) X^{-1}(\tau) Z(\tau) d\tau. \]

For linear systems, Eq. 2.68 becomes

\[ (B.6) \quad \dot{X}(t) = Z(t) + A(t)X(t), \quad X(t_0) = X_0. \]
The solution for $X(t)$ can be written, in terms of $\bar{X}(t)$:

$$X(t) = X(t) + \bar{X}(t) = X(t) + \int_{t_0}^{t} X(t) X^{-1}(\tau) Z(\tau) \, d\tau.$$

Multiplying both sides by 1, we get

$$x(t) = x_0(t) + \int_{t_0}^{t} X(t) X^{-1}(\tau) z(\tau) \, d\tau,$$

which is the general solution to the original system, Eq. B.1.

For the particular case of constant diagonalizable flow intensity matrix $A(t) = A$, the fundamental matrix solution can be written in the following form:

$$V(t) = \exp \left( \int_{t_0}^{t} A \, ds \right) = e^{(t-t_0)A} = U e^{(t-t_0)\Lambda} U^{-1}$$

where $U$ is the matrix whose columns are the eigenvectors of $A$, and $\Lambda$ is the diagonal matrix whose diagonal elements are the corresponding eigenvalues of $A$. The solution for the matrix equation given in Eq. B.7 then becomes

$$X(t) = X(t) + \bar{X}(t) = e^{(t-t_0)A} X_0 + \int_{t_0}^{t} e^{(t-r)A} Z(\tau) \, d\tau.$$

Consequently, Eq. B.8 takes the following form:

$$x(t) = e^{(t-t_0)A} x_0 + \int_{t_0}^{t} e^{(t-r)A} z(\tau) \, d\tau.$$

For linear systems, the governing equation for the subsystem decomposition, Eq. 2.77, can be solved explicitly for $x_{w,n,k,j,k}(t)$ as well. The solution becomes

$$x_{w,n,k,j,k}(t) = \int_{t_1}^{t} e^{-\int_{s}^{t} r_{\ell}^{-1}(s') x(s') \, ds'} \int_{\ell}^{w} f_{\ell,k,j,k}(s) \, ds$$

where the outward throughflow intensity function $r_{\ell}^{-1}(t, x) = \hat{\tau}_{\ell}(t, x)/x_{\ell}(t)$ is defined in Eq. 2.55. Equation B.12 formulates the transient storage $x_{w,n,k,j,k}(t)$ generated by the transient inflow, $f_{\ell}^{w}(t, x_{\ell}, k)$, at subcompartment $\ell$, at any time $t \geq t_1$ (see Fig. 3).

**B.1. Static Compartamental System Analysis.** At steady state, the time derivatives of the state variables are zero. That is,

$$X(t) = \dot{X}(t) = 0.$$

Clearly, if the decomposed system, Eq. 2.67, is at steady state, the original system, Eq. 2.11, is also at steady state, due to Eq. 2.19. Since $A$ is a strictly diagonally dominant constant matrix, it is invertible, and

$$T = T = 0 \quad \Rightarrow \quad X = -A^{-1} Z \quad \text{and} \quad X = 0$$

because of the relationships given in Eq. 2.67. The static systems can be decomposed and analyzed based on both external inputs and outputs. The proposed methodology for static systems in both input- and output-orientations have recently been introduced and their duality is demonstrated by [4, 5].

**Appendix C. Dynamic Subsystem Decomposition.**

The dynamic subsystem decomposition methodology is introduced in Section 2.5. The method formulation is based on the concept of directed subflow paths, which will be detailed below.
C.1. Subflow Paths. A \textit{link} will be defined as the connection between two system compartments that represents direct transactions between them. A link constitutes a \textit{step} along a given flow path from one subcompartment to another. A \textit{directed subflow path} in a subsystem will then be defined as a chain of connected links initiated at one subcompartment and ending in another of the same subsystem. The number of links or steps along a directed subflow path is called the \textit{length} of the pathway. The \textit{connection} of a subflow path to the ambient subsystem is defined as the initial and only subcompartment on the path that receives inflow. The transient subflow and substorage computations along a subflow path must start at its connection. The link to the connection which represents the only inflow into the path will be called the \textit{local input} and the source of this input will be called the \textit{local source}. The outflow from the terminal subcompartment of the path will be called the \textit{local output}. The environment can be taken as the local source or terminal subcompartment.

A subflow path $j_k \Rightarrow \tau_k \Rightarrow \ell_k \Rightarrow n_k \Rightarrow \cdots$ in subsystem $k$ with connection $j_k$ and the \textit{local source} $i_k$ will be represented by $i_k \Rightarrow \tau_k \Rightarrow j_k^* \Rightarrow \ell_k \Rightarrow n_k \Rightarrow \cdots$. The connection is marked with red superscript ($*$), and the local input with red arrow. A subflow link that does not directly contribute to the particular subflow or substorage in question will be represented by ($\Rightarrow$) symbol. If the local input or output are external input or output, the corresponding subcompartments on the pathway will be denoted by $0_k$. Therefore, $0_k$ indicates that the local input is external input $z_k(t)$, and, since there is no external input for the initial subsystem, $0_0$ indicates that the local input is zero. Assuming that the terminal subcompartment of the path partially defined above is $v_k$, the complete subflow path will be represented by $p_{v_k,j_k} = i_k \Rightarrow \tau_k \Rightarrow j_k^* \Rightarrow \ell_k \Rightarrow n_k \Rightarrow \cdots \Rightarrow v_k$. If the initial and terminal subcompartments are the same, say $\ell_k$, a simpler notation will be used for the path $p_{\ell_k}$. For more than one path in the same subsystem, the path number will be represented by superscript $w$: $p_{v_k,j_k}^w$. Having the connection and local source be the same, that is, having a path of type $i_k \Rightarrow i_k^* \Rightarrow \cdots$ implies that the local input is the subthroughflow into that subcompartment, $\tilde{r}_{i_k}(t,x)$.

The subsystems can be decomposed into subflows and the associated substorages generated by these subflows along a set of mutually exclusive and exhaustive directed subflow paths. By \textit{mutually exclusive} subflow paths, we mean that no given subflow path in a subsystem is a \textit{subpath}, that is, completely inside of another path in the same subsystem. The \textit{exhaustiveness}, in this context, means that such mutually exclusive subflow paths all together sum to the entire subsystem so partitioned. A subflow path that does not self intersect will be called the \textit{linear path}, and the one with the same initial and terminal subcompartment will be called the \textit{closed path}. A subflow path composed of linear and closed subpaths will be called the \textit{mixed type path}. We will use the notation of $P_k$ for a set of mutually exclusive and exhaustive subflow paths in subsystem $k$, and $w_k$ for the number of paths in this set.

Each subsystem can be partitioned along a set of mutually exclusive and exhaustive subflow paths as follows: For subsystem $k$, the connections of all subflow paths can be taken to be subcompartment $k$, with the local input being external input $z_k(t)$. The terminal subcompartments of the linear paths are the ones with external output, and those of the closed and mixed type paths can be taken as the first (and the last) subcompartments of the closed subpaths. The cumulative transient outflow at the last subcompartment of a closed subpath will be considered as the local output. Consequently, the number of subflow paths in a subsystem obtained by this partitioning is equal to the number of local outputs. This subsystem partitioning will be called the \textit{natural subsystem decomposition}. The natural subsystem decomposition of all subsystems yields a mutually exclusive and exhaustive decomposition of the entire...
system.

C.2. Transient Flows and Storages. The transient subflows and substorages are defined for linear subflow paths in Section 2.5. Additional relationships will be formulated in this section.

Self-intersecting directed flow paths are common within compartmental systems. The transient inflow and outflow and associated transient substorage change with each cycle along such paths. The cumulative values are obtained by summing up all transient subflows and substorages at the corresponding subcompartments with each cycle. The number of terms in these summations depends on the number of times the directed path intersects itself. In particular, transient subflows cycle along directed closed paths repeatedly and indefinitely. Therefore, in this case, the summations yield infinite series of functions that are convergent pointwise in time, due to their construction.

The sum of the transient inflows from subcompartment \( j_k \) to \( \ell_k \) and the outflows from \( \ell_k \) to \( n_k \) generated at subcompartment \( \ell_k \) at time \( t \) by the local input into the connection of a given self-intersecting subflow path \( p_{w_{jk}}^{w} \) during \([t_1, t] \), \( t_1 \geq t_0 \), will respectively be called the inward and outward cumulative transient subflow at subcompartment \( \ell_k \) at time \( t \). The associated storage generated by the inward cumulative transient subflow will be called cumulative transient substorage. These inward and outward cumulative transient subflows will be denoted by \( \hat{x}_{\ell_k}^{w}(t) \) and \( \hat{x}_{n_k \ell k j_k}^{w}(t) \), respectively, and associated cumulative transient substorage by \( x_{n_k \ell k j_k}^{w}(t) \). They can be formulated as

\[
(C.1) \quad x_{\ell_k}^{w}(t) := \sum_{m=1}^{m_w} x_{n_k \ell_k j_k}^{w,m}(t), \quad \hat{x}_{\ell_k}^{w}(t) := \sum_{m=1}^{m_w} f_{\ell_k j_k i_k}^{w,m}(t), \quad \hat{x}_{n_k \ell k j_k}^{w}(t) := \sum_{m=1}^{m_w} f_{n_k \ell_k j_k}^{w,m}(t)
\]

for \( k = 0, 1, \ldots, n \), where the superscript \( m \) represents the cycle number, and \( m_w \) is the number of cycles, that is, the number of times the path \( p_{w_{jk}}^{w} \) intersects itself. Large number of terms, \( m_w \), in computation of these summations reduce truncation errors and, thus, improve the approximations. If a given path is not self-intersecting at \( x_{\ell_k} \) \((m = 1)\), we write

\[
\hat{x}_{\ell_k}^{w}(t) = x_{n_k \ell_k j_k}^{w}(t), \quad \hat{x}_{n_k \ell k j_k}^{w}(t) = f_{\ell_k j_k i_k}^{w}(t), \quad \hat{x}_{n_k \ell k j_k}^{w}(t) = f_{n_k \ell_k j_k}^{w}(t).
\]

Let \( P_k \) be the set of mutually exclusive and exhaustive subflow paths of the natural decomposition of subsystem \( k \), and \( w_k \) be the number of paths in this set. We also have

\[
x_{\ell_k}(t) := \sum_{w=1}^{w_k} x_{\ell_k}^{w}(t), \quad \hat{x}_{\ell_k}(t, x) := \sum_{w=1}^{w_k} \hat{x}_{\ell_k}^{w}(t), \quad \hat{x}_{\ell_k}(t) := \sum_{w=1}^{w_k} \hat{x}_{\ell_k}^{w}(t).
\]

That is, due to the mutually exclusiveness and exhaustiveness of the subsystem decomposition, the sum of the cumulative transient subflows and substorages are equal to the subthroughflows and substorages, respectively.

C.3. Static Subsystem Decomposition. The static version of the dynamic subsystem decomposition introduced in Eqs. 2.76 and 2.77 is formulated by \([4]\). Since the time derivatives of the state variables are zero at steady state, we set \( x_{n_k \ell_k j_k}^{w}(t) = 0 \) in Eq. 2.77. Then, the static transient outflow \( f_{n_k \ell_k j_k}^{w} \) at subcompartment \( \ell_k \), from \( j_k \) to \( n_k \) along subflow path \( p_{n_k j_k}^{w} \), and the transient substorage \( x_{n_k \ell_k j_k}^{w} \) generated at
\[ x_{n_k,\ell_k}^{w, f_{k, i_k}} = x_{\ell_k}^{f_{k, i_k}} \text{ and } f_{n_k,\ell_k}^{w, f_{k, i_k}} = \frac{f_{n_k,\ell_k}^{w, f_{k, i_k}}}{x_{\ell_k}^{f_{k, i_k}}}. \]

Appendix D. The diact Flows and Storages.

The diact transaction types are introduced in Sec. 2.5.2 based on the proposed dynamic subsystem decomposition methodology. The detailed formulation of diact flows and the associated storages generated by these flows are presented in this section. The diact flows and storages within the initial subsystems can be formulated similarly.

Let \( P_{\ell_k}^{d_k,j_k} \) and \( P_{\ell_k}^{i_k,j_k} \) be defined as the sets of mutually exclusive direct and indirect subflow paths \( p_{\ell_k}^{w, f_{k, i_k}} \) from subcompartment \( j_k \), directly and indirectly, to \( i_k \), respectively. The sets \( P_{\ell_k}^{c_k,j_k} \) and \( P_{\ell_k}^{c_k,j_k} \) are also defined as the sets of mutually exclusive cycling and acyclic subflow paths \( p_{\ell_k}^{w, f_{k, i_k}} \) from \( j_k \) to \( i_k \) with a closed and linear subpath at terminal subcompartment \( i_k \), respectively. The cycling subflow set, \( P_{\ell_k}^{c_k,j_k} \), can alternatively be defined as the set of mutually exclusive subflow paths \( p_{\ell_k}^{w, f_{k, i_k}} \) from subcompartment \( i_k \) indirectly back to itself. The number of subflow paths in \( P_{\ell_k}^{c_k,j_k} \) will be denoted by \( w_k \), where the superscript (*) represents any of the diact symbols.

The composite transfer flows, associated storages, and corresponding matrix measures are formulated in Eqs. 2.78, 2.79, and 2.80, using the transfer subflow set, \( P_{\ell_k}^{c_k,j_k} \). All the other simple and composite diact flows, associated storages, and matrix functions can then be formulated similarly by substituting the corresponding diact flows and storages for their composite transfer counterparts in these equations and by using the corresponding diact subflow sets instead. A compact derivation of the diact flows and storages are presented below.

The composite diact subflow will be defined as the transfer subflow from one subcompartment to another in the same subsystem along the subflow paths in \( P_{\ell_k}^{c_k,j_k} \). More specifically, the composite diact subflow from subcompartment \( j_k \) to \( i_k \), \( \tau_{i_k,j_k}^{*} \) \((t)\), is defined as the sum of the cumulative transient subflows, \( \tau_{i_k,j_k}^{*} \) \((t)\), generated by the outward subthroughflow at subcompartment \( j_k \), \( \tau_{j_k}^{*} \) \((t,x)\), during \([t_1, t]\), \( t_1 \geq t_0 \), and transmitted into \( i_k \) at time \( t \) along all subflow paths \( P_{\ell_k}^{c_k,j_k} \in P_{\ell_k}^{c_k,j_k} \). The associated composite diact substorage, \( x_{i_k,j_k}^{*} \) \((t)\), at subcompartment \( i_k \) at time \( t \) is the sum of the cumulative transient substorages, \( x_{i_k,j_k}^{*} \) \((t)\), generated by the cumulative transient inflows, \( \tau_{i_k}^{*} \) \((t)\), during \([t_1, t]\). Alternatively, \( x_{i_k,j_k}^{*} \) \((t)\) can be defined as the storage segment generated by the composite diact inflow \( \tau_{i_k,j_k}^{*} \) \((t)\) in subcompartment \( i_k \) during \([t_1, t]\). The simple diact subflows can be defined similar to the their composite
counterparts except for the following differences: the local inputs for the simple and composite diact subflows are $\tilde{r}_{ik}(t, x)$ and $\tilde{r}_{j_k}(t, x)$, and the corresponding subflow sets are $P_{ik}^w$ and $P_{j_k}^w$, respectively. Note that, for the cycling case, the first entrance of the transient subflows and substorages into $i_k$ are not considered as cycling subflow and substorages. Figure 9 depicts the complementary nature of the indirect (or acyclic) and cycling subflows.

The composite diact subflows and substorages can then be formulated as

$$
\tau_{i_k}^w(t) := \sum_{w=1}^{w_k} \tau_{i_k}^w(t) \quad \text{and} \quad x_{i_k}^w(t) := \sum_{w=1}^{w_k} x_{i_k}^w(t)
$$

where $w_k$ is the number of subflow paths $p_{ik}^w \in P_{ik}^w$. The sum of all composite diact subflows and substorages from subcompartment $j_k$ to $i_k$ for each subsystem $k$ will be called the composite diact flow and storage at time $t$, $\tau_{ij}^*(t)$ and $x_{ij}^*(t)$, from compartment $j$ to $i$:

$$
\tau_{ij}^*(t) := \sum_{k=0}^{n} \tau_{i_k,j_k}^*(t) \quad \text{and} \quad x_{ij}^*(t) := \sum_{k=0}^{n} x_{i_k,j_k}^*(t).
$$

For notational convenience, we define $n \times n$ matrix functions $T_k^*(t)$ and $X_k^*(t)$ whose $(i, j)$—elements are $\tau_{i_k,j_k}^*(t)$ and $x_{i_k,j_k}^*(t)$, respectively. That is,

$$
T_k^*(t) := (\tau_{i_k,j_k}^*(t)) \quad \text{and} \quad X_k^*(t) := (x_{i_k,j_k}^*(t)).
$$

These matrix measures $T_k^*(t)$ and $X_k^*(t)$ are called the $k^{th}$ composite diact subflow and associated substorage matrix functions. The corresponding composite diact flow and associated storage matrix measures are $T^*(t) := (\tau_{ij}^*(t))$ and $X^*(t) := (x_{ij}^*(t))$, respectively.

The composite diact compartmental throughflow and storage matrices and vectors can then be formulated as

$$
T^*(t) := \text{diag} (T^*(t) 1) \Rightarrow \tau^*(t) := T^*(t) 1 \quad \text{and} \quad X^*(t) := \text{diag} (X^*(t) 1) \Rightarrow x^*(t) := X^*(t) 1.
$$

The simple diact flows and storages can also be formulated in terms of their composite counterparts as follows:

$$
\tau_{ik}^*(t) = \tau_{ik,k_k}(t) \quad \text{and} \quad x_{ik}^*(t) = x_{ik,k_k}(t).
$$

To distinguish the composite and simple transfer flow and storage matrices, we use a tilde notation over the simple versions, that is, $\tilde{T}^*(t) := (\tau_{ik}^*(t))$ and $\tilde{X}^*(t) := (x_{ik}^*(t))$.

The difference between the composite and simple diact flows, $\tau_{ik}^*(t)$ and $\tilde{\tau}_{ik}(t)$, and storages, $x_{ik}^*(t)$ and $\tilde{x}_{ik}(t)$, is that the composite flow and storage from compartment $k$ to $i$ are generated by outward throughflow $\tau_k(t, x)$ derived from all external inputs and their simple counterparts from input-receiving subcompartment $k_k$ to $i_k$ are generated by outward subthroughflow $\tilde{\tau}_{k_k}(t, x)$ derived from single external input $z_k(t)$ (see Fig. 4). In that sense, the composite and simple diact flows and storages measure the influence of one compartment on another induced by all and single external inputs, respectively.
The input-oriented, flow-based diact flow and storage distribution and the simple and composite diact (sub)flow and (sub)storage matrices. The superscript (*) in each equation represents any of the diact symbols.

| diact | Flow and storage distribution matrices | Flows | Storages |
|-------|---------------------------------------|-------|----------|
| d     | $N^d = F^T T^{-1}$                     |       |          |
| i     | $N^i = (N - I) N^{-1} - F^T T^{-1}$    |       |          |
| a     | $N^a = (N^{-1} N - I) N^{-1}$          | $T^* = N^* T$ | $X^* = S^* T$ |
| c     | $N^c = (N - N^{-1} N) N^{-1}$          | $T^*_e = N^* T_e$ | $X^*_e = S^* T_e$ |
| t     | $N^t = (N - I) N^{-1}$                 |       |          |

D.1. Static diact Flows and Storages. The static diact flows and storages are introduced by [4], using Eq. 2.56, as listed in matrix form in Table 1. All quantities in the table are the static counterparts of their dynamic versions introduced in the present paper. For invertible matrix $Z$, we also define

$$N := \hat{T} Z^{-1}, \quad N' := \text{diag}(N), \quad \text{and} \quad T := \text{diag}(\hat{T}).$$

See Example E.2 for application of these formulations to a static ecological model.

Appendix E. Case Studies.

A linear dynamic and a static model from ecosystem ecology are analyzed in this section. The linear dynamic model is solved analytically through the proposed methodology. The static model is used for an application of the static version of the proposed dynamic methodology.

E.1. Case Study. In this example, a linear model introduced by [8] is solved analytically. This linear dynamic model has two state variables, $x_1(t)$ and $x_2(t)$ (see Fig. 10). The external input, $z(t) = [z_1(t, x), z_2(t, x)]^T$, output, $y(t, x) = [y_1(t, x), y_2(t, x)]^T$, and the rate functions, $F(t, x)$, are given as

$$F(t, x) = \begin{bmatrix} 0 & 2/3 x_2 \\ 4/3 x_1 & 0 \end{bmatrix}, \quad y(t, x) = \begin{bmatrix} 1/3 x_1 \\ 5/3 x_2 \end{bmatrix}, \quad \text{and} \quad z(t, x) = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}.$$

The input, output, and state matrices becomes

$$Z(t, x) = \begin{bmatrix} z_1 & 0 \\ 0 & z_2 \end{bmatrix}, \quad Y(t, x) = \begin{bmatrix} 1/3 x_1 & 0 \\ 0 & 5/3 x_2 \end{bmatrix}, \quad \text{and} \quad X(t, x) = \begin{bmatrix} x_1 & 0 \\ 0 & x_2 \end{bmatrix}.$$

Componentwise, the governing equations, Eq. 2.6, take the following form:

$$\dot{x}_1(t) = z_1(t) + \frac{2}{3} x_2(t) - \left(\frac{4}{3} + \frac{1}{3}\right) x_1(t)$$

$$\dot{x}_2(t) = z_2(t) + \frac{4}{3} x_1(t) - \left(\frac{2}{3} + \frac{5}{3}\right) x_2(t)$$

with the initial conditions $x_0 = [x_{1,0}, x_{2,0}]^T = [3, 3]^T$. In vector form, using the notation of Eq. 2.10, the governing equations can be expressed as

$$\begin{cases} \dot{x}(t) = (z(t, x) + F(t, x) 1) - (y(t, x) + F^T(t, x) 1) \\ x(t_0) = x_0 \end{cases}$$
In matrix form, as given in Eq. 2.66, the governing system of equations becomes

\( \dot{x}(t) = z(t) + A x(t), \quad x(t_0) = x_0 \)

where \( A \) is the constant flow intensity matrix given in Eq. 2.46:

\( A = (F - T) X^{-1}. \)

It can be written explicitly as

\( A = \begin{bmatrix} -\left( \frac{4}{3} + \frac{1}{3} \right) & \frac{2}{3} \\ \frac{4}{3} & -\left( \frac{2}{3} + \frac{5}{3} \right) \end{bmatrix} = \begin{bmatrix} -\frac{5}{3} & \frac{2}{3} \\ \frac{4}{3} & -\frac{7}{3} \end{bmatrix}. \)

For the following state decomposition,

\( x_i(t) = \sum_{k=0}^{2} x_{ik}(t), \)

the substate and subflow rate functions become

\[
X(t) = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix}, \\
F_k(t, x) = \begin{bmatrix} f_{1k,1} & f_{1k,2} \\ f_{2k,1} & f_{2k,2} \end{bmatrix} = \begin{bmatrix} 0 & \frac{2}{3} d_{2k} x_2 \\ \frac{4}{3} d_{1k} x_1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & \frac{2}{3} x_{2k} \\ \frac{4}{3} x_{1k} & 0 \end{bmatrix}, \\
z_k(t, x) = \begin{bmatrix} z_{1k} \\ z_{2k} \end{bmatrix} = \begin{bmatrix} \delta_{1k} z_1 \\ \delta_{2k} z_2 \end{bmatrix} = \begin{bmatrix} \delta_{1k} \\ \delta_{2k} \end{bmatrix}, \\
y_k(t, x) = \begin{bmatrix} y_{1k} \\ y_{2k} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} d_{1k} x_1 \\ \frac{5}{3} d_{2k} x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} x_{1k} \\ \frac{5}{3} x_{2k} \end{bmatrix}. 
\]

The decomposed system, Eq. 2.62, can be expressed as

\[
\dot{x}_{1k}(t) = z_{1k}(t) + \frac{2}{3} x_{2k}(t) - \left( \frac{4}{3} + \frac{1}{3} \right) x_{1k}(t) \\
\dot{x}_{2k}(t) = z_{2k}(t) + \frac{4}{3} x_{1k}(t) - \left( \frac{2}{3} + \frac{5}{3} \right) x_{2k}(t)
\]

with the initial conditions \( x_{ik}(t_0) = 0 \) for \( i, k = 1, 2 \).

Similarly, for the following decomposition of the initial subsystem \( (k = 0) \),

\( x_i(t) = \sum_{k=1}^{2} x_{ik}(t), \)
the initial subflow rate functions become
\[
X(t) = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{bmatrix},
\]
(12)
F_k(t, x) = \begin{bmatrix} f_{11,1} \\ f_{21,1} \end{bmatrix}, \quad \begin{bmatrix} f_{11,2} \\ f_{21,2} \end{bmatrix} = \begin{bmatrix} \frac{4}{3} d_{11} x_1 & 0 \\ 0 & \frac{4}{3} x_{1,2} \end{bmatrix} = \begin{bmatrix} 0 & \frac{2}{3} x_{2,2} \\ \frac{2}{3} x_{2,2} & 0 \end{bmatrix},
\]
(13)
\[
z_k(t, x) = \begin{bmatrix} z_{1k} \\ z_{2k} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},
\]
(14)
\[
y_k(t, x) = \begin{bmatrix} y_{1k} \\ y_{2k} \end{bmatrix} = \begin{bmatrix} \frac{1}{3} d_{11} x_1 \\ \frac{5}{3} d_{22} x_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{3} x_{1,1} \\ \frac{5}{3} x_{2,2} \end{bmatrix}.
\]
(15)
The initial subsystem decomposition yields the following governing equations, as formulated in Eq. 2.63:
\[
\dot{x}_{1k}(t) = \frac{2}{3} x_{2k}(t) - \left( \frac{4}{3} + \frac{1}{3} \right) x_{1k}(t),
\]
(16)
\[
\dot{x}_{2k}(t) = \frac{4}{3} x_{1k}(t) - \left( \frac{2}{3} + \frac{5}{3} \right) x_{2k}(t)
\]
with the initial conditions \( x_{1k}(t_0) = x_{1,k,n}(t_0) = 3 \delta_{ik} \) for \( i, k = 1, 2 \). Thus, there are \( 2n^2 = 8 \) equations in the decomposed system; \( n^2 = 4 \) of them are for the substates and the other \( n^2 \) equations are for the initial substates.

The governing equations for the decomposed system can be written in vector form, as given in Eq. 2.64:
\[
\dot{x}_k(t) = z_k + A x_k(t), \quad x_k(t_0) = 0,
\]
(17)
\[
\dot{x}_k(t) = A x_k(t), \quad x_k(t_0) = x_{k,0} e_k,
\]
for \( k = 1, 2 \) or in matrix form, as given in Eq. 2.67:
\[
\dot{X}(t) = Z + A X(t), \quad X(t_0) = 0,
\]
(18)
\[
\dot{X}(t) = A X(t), \quad X(t_0) = X_0.
\]

The governing system, Eq. E.15, is linear. It can, therefore, be solved analytically as formulated in Section B. Since the flow intensity matrix, \( A \), is constant, the fundamental matrix solution becomes
\[
V(t) = \begin{bmatrix} 2e^{-t} + e^{-3t} \\ \frac{2}{3} e^{-t} + e^{-3t} \end{bmatrix},
\]
(19)
as formulated in Eq. B.9. The solution for the matrix equation, Eq. E.15, as formulated in Eq. B.4, then becomes
\[
X(t) = \begin{bmatrix} 2e^{-t} + e^{-3t} \\ 2e^{-t} - 2e^{-3t} \end{bmatrix} = \begin{bmatrix} e^{-t} - e^{-3t} \\ e^{-t} + 2e^{-3t} \end{bmatrix},
\]
(20)
\[
X(t) = \begin{bmatrix} \frac{7}{9} e^{-t} + \frac{8}{9} e^{-3t} \\ \frac{2}{9} e^{-t} - \frac{7}{9} e^{-3t} \end{bmatrix}.
\]
(21)
Therefore, the solution to the original system is
\[
x(t) = X(t) \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 2e^{-t} + 1 \\ 2e^{-t} + 1 \end{bmatrix}.
It can easily be seen that the dynamic solution, Eq. (E.17), converges to this steady state solution as \( t \to \infty \).

We also analyze the system with a time dependent input \( z(t) = [3 + \sin(t), 3 + \sin(2t)]^T \). The initial substate matrix, \( X(t) \), is the same as the one given in Eq. (E.17) for the constant input case above. Similar computations leads us to the following initial substate vector and substate matrix components:

\[
\begin{align*}
X_{11}(t) &= x_{21}(t) = 3 e^{-t}, \\
X_{12}(t) &= \frac{7}{3} - \frac{11 \cos(t)}{30} + \frac{13 \sin(t)}{30} - \frac{5 e^{-t}}{3} + \frac{3 e^{-3t}}{10}, \\
X_{14}(t) &= \frac{2}{3} - \frac{16 \cos(2t)}{195} - \frac{2 \sin(2t)}{195} - \frac{13 e^{-t}}{15} + \frac{11 e^{-3t}}{39}, \\
X_{21}(t) &= \frac{4}{3} - \frac{4 \cos(t)}{15} + \frac{2 \sin(t)}{15} - \frac{5 e^{-t}}{3} + \frac{3 e^{-3t}}{5}, \\
X_{22}(t) &= \frac{5}{3} - \frac{46 \cos(2t)}{195} + \frac{43 \sin(2t)}{195} - \frac{13 e^{-t}}{15} - \frac{22 e^{-3t}}{39}.
\end{align*}
\]

The solutions to the system, given in Eq. (E.17), for the constant external input case are the same as the ones given by [8]. The authors, however, did not provide an explicit solution for the time-dependent input case for a comparison. At steady state, the solution for the substate matrix becomes,

\[
\lim_{t \to \infty} X(t) = \begin{bmatrix}
\frac{7}{3} - \frac{11 \cos(t)}{30} + \frac{13 \sin(t)}{30} & \frac{2}{3} - \frac{16 \cos(2t)}{195} - \frac{2 \sin(2t)}{195} \\
\frac{4}{3} - \frac{4 \cos(t)}{15} + \frac{2 \sin(t)}{15} & \frac{5}{3} - \frac{46 \cos(2t)}{195} + \frac{43 \sin(2t)}{195}
\end{bmatrix}.
\]

Similarly, the elements of the initial subthroughflow vector and the subthroughflow matrix are

\[
\begin{align*}
\hat{\tau}_{11}(t) &= 2 e^{-t}, \quad \hat{\tau}_{21}(t) = 4 e^{-t}, \\
\hat{\tau}_{12}(t) &= 35 \cos(t) + 49 \sin(t) - 10 e^{-t} + 2 e^{-3t}, \\
\hat{\tau}_{14}(t) &= \frac{742}{585} - \frac{184 \cos^2(t)}{585} + \frac{86 \sin(2t)}{585} - \frac{26 e^{-t}}{45} - \frac{44 e^{-3t}}{117}, \\
\hat{\tau}_{21}(t) &= \frac{28}{9} - \frac{22 \cos(t)}{45} + \frac{26 \sin(t)}{45} - \frac{20 e^{-t}}{9} - \frac{2 e^{-3t}}{5}, \\
\hat{\tau}_{22}(t) &= \frac{2339}{585} - \frac{128 \cos^2(t)}{585} + \frac{577 \sin(2t)}{585} - \frac{52 e^{-t}}{45} + \frac{44 e^{-3t}}{117}.
\end{align*}
\]

Graphical representations of the substate and the inward subthroughflow matrices, \( X(t) \) and \( \hat{T}(t) \), given in Eqs. (E.21) and (E.23), are depicted in Fig. 11. Using these
matrices, the dynamic distribution of external inputs as inward throughflows and the organization of the associated storages generated by the inputs within the system can be analyzed individually and separately.

The simple cycling flows and the associated storages generated by these flows are also calculated below, as an application of the subsystem partitioning methodology. The sets of mutually exclusive subflow paths from subcompartment $k_k$ to $1_k$ with a closed subpath at $1_k$, $P_{1-k}^c$, are given as $P_{1-k}^c = \{p_{1-k}^1, p_{1-k}^2\}$, $P_{2-k}^c = \{p_{2-k}^1, p_{2-k}^2\}$, where $p_{1-k}^1 := 0_0 \rightarrow 1_0 \leadsto 2_0 \rightarrow 1_0$, $p_{1-k}^2 := 0_0 \rightarrow 2_0 \rightarrow 1_0 \leadsto 2_0 \rightarrow 1_0$, $p_{2-k}^1 := 0_2 \rightarrow 2_2 \rightarrow 1_2 \rightarrow 2_2$, and $p_{2-k}^2 := 0_2 \rightarrow 2_2 \rightarrow 1_2 \leadsto 2_2 \rightarrow 1_2$ (see Fig. 10). For the subflow paths in $P_{1-k}^c$, the cycling flows are derived from the initial stocks and for the ones in $P_{2-k}^c$, the flows are generated by the respective environmental inputs of $z_1(t)$ and $z_2(t)$. The sets of subflow paths for $P_{k-k}^c$, $k = 0, 1, 2$, can similarly be defined.

The simple cycling subflow at subcompartment $1_2$ along the only subflow path in subsystem 2 ($w_2 = 1$) $p_{1-2}^1 \in P_{1-2}^c$ and associated storages are

$$
\tau_{1-2}^w = \sum_{w=1}^1 \tau_{1-2}^{w}(t) = \tau_{1-2}^1(t) \quad \text{and} \quad x_{1-2}^w(t) = \sum_{w=1}^1 x_{1-2}^{w}(t) = x_{1-2}^1(t),
$$

as formulated in Eq. 2.78. The links contributing to the cycling flow along the path are marked with red cycle numbers in the extended subflow diagram below:

$$
p_{1-2}^1 = 0_2 \rightarrow 2_2 \leadsto 1_2 \rightarrow 2_2 \rightarrow 1_2 \leadsto 2_2 \rightarrow 1_2 \leadsto \cdots
$$

Note that the first flow entrance into $1_2$ is not considered as cycling flow. The cumulative transient inflow $\tau_{1-2}^1(t)$ and substorage $x_{1-2}^1(t)$ can be approximated by two terms ($m_1 = 2$) along the closed subpath as formulated in Eq. C.1:

$$
x_{1-2}^1(t) = \sum_{m=1}^2 x_{2-1-2-2}^{1,m}(t) \approx x_{2-1-2-2}^{1,1}(t) + x_{2-1-2-2}^{1,2}(t),
$$

$$
\tau_{1-2}^1(t) = \sum_{m=1}^2 \tau_{1-2}^{1,m}(t) \approx \tau_{1-2}^{1,1}(t) + \tau_{1-2}^{1,2}(t).
$$

The governing equations for the transient subflows and associated substorage functions, $f_{1-2}^{1,m}(t)$ and $x_{2-1-2}^{w,m}(t)$ as well as the other transient subflows and substorages involved in Eq. E.24, as formulated in Eqs. 2.76 and 2.77, are coupled and solved.
simultaneously together with the decomposed system, Eqs. 2.62 and 2.63. The numerical results for the cycling flow and associated storage functions

\[(E.24) \quad \tau^c_i(t) = \sum_{k=0}^{2} \tau^c_{ik}(t) \quad \text{and} \quad x^c_i(t) = \sum_{k=0}^{2} x^c_{ik}(t)\]

for \(i = 1, 2\), are presented in Fig. 11.

Note that, due to the reflexivity of cycling flows, the same computations can be done more practically in only two steps using the sets of closed subflow paths, \(P^c_{ik}\), instead (for example, along \(P^c_{11} := 1_1 \rightsquigarrow 1_1 \rightsquigarrow 2_1 \rightarrow 1_1\) in subcompartment 1).

**E.2. Case Study.** To demonstrate an application of the static version of the proposed dynamic methodology, a commonly studied ecosystem network proposed by [15] is used as an example in this section. This ecosystem has already been analyzed in detail by [4, 5].

Cone Spring is a small, shallow spring-brook located in Louisa County, Iowa. The study area consists of 116 m². The network has 5 compartments representing 1—Plants, 2—Detritus, 3—Bacteria, 4—Detritus Feeders, and 5—Carnivores. These compartments are connected by the transaction of energy between them. The conserved quantity needs to be investigated within the system is energy. The system flow information is given as follows:

\[
F = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
8881 & 0 & 1600 & 200 & 167 \\
0 & 5205 & 0 & 0 & 0 \\
0 & 2309 & 75 & 0 & 0 \\
0 & 0 & 0 & 370 & 0
\end{bmatrix}, \quad y = \begin{bmatrix}
2303 \\
3969 \\
3530 \\
1814 \\
203
\end{bmatrix}, \quad z = \begin{bmatrix}
11184 \\
635 \\
0 \\
0 \\
0
\end{bmatrix}.
\]

The unit for energy flows and storages are kkal x m⁻² x y⁻¹ and kkal x m⁻², respectively.

The system decomposition methodology yields the subthroughflow matrix as

\[
T = \begin{bmatrix}
11184 & 0 & 0 & 0 & 0 \\
10717 & 766 & 0 & 0 & 0 \\
4858 & 347 & 0 & 0 & 0 \\
2225 & 159 & 0 & 0 & 0 \\
345 & 25 & 0 & 0 & 0
\end{bmatrix}.
\]

The subsystem decomposition methodology yields the diact flows and storages as given in Table 1. The direct flow matrix is \(T^d = F\). The composite indirect flow matrix becomes

\[
T^i = \begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
1835.74 & 1967.00 & 63.02 & 226.41 & 31.04 \\
4857.67 & 0 & 753.81 & 193.28 & 89.76 \\
2224.91 & 75.00 & 334.40 & 88.52 & 41.11 \\
345.31 & 370.00 & 63.53 & 0 & 6.38
\end{bmatrix}.
\]

Note the \(\tau^i_{21} = \tau^i_{54} = 0\). This is because of the fact that there is no indirect flow from compartment 2 to 3 or from 4 to 5 (see Fig. 12). There is no indirect flow to
The Cone Spring model is also studied by [14] for similar purposes. The authors defined a matrix called the total flow matrix. Although the derivation rationales are different, the transfer flow matrix given in Eq. E.25 is equivalent to this total flow matrix.

As listed in Table 1, the simple cycling and acyclic subflow matrices can also be expressed as follows:

\[
\bar{T}^c = \begin{bmatrix}
  0 & 0 & 0 & 0 & 0 \\
  0 & 11184 & 0 & 0 & 0 \\
  1835.74 & 131.26 & 0 & 0 & 0 \\
  703.51 & 50.30 & 0 & 0 & 0 \\
  82.62 & 5.91 & 0 & 0 & 0 \\
  5.96 & 0.43 & 0 & 0 & 0
\end{bmatrix}
\quad \text{and} \quad
\bar{T}^a = \begin{bmatrix}
  11184 & 0 & 0 & 0 & 0 \\
  8881 & 635 & 0 & 0 & 0 \\
  4154.16 & 297.03 & 0 & 0 & 0 \\
  2142.30 & 153.18 & 0 & 0 & 0 \\
  339.35 & 24.26 & 0 & 0 & 0
\end{bmatrix}.
\]

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