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Interval enclosures for reachable sets of chemical kinetic flow systems. Part 1: Sparse transformation

Aditya Tulsyan, Paul I. Barton *

Process Systems Engineering Laboratory, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

HIGHLIGHTS

- Considers the problem of computing reachable sets for CSTRs under uncertainty.
- Proposes a linear transformation to project CSTR dynamics onto subspaces.
- The transformation is based on oblique projections onto subspaces.
- The transformation is invertible and leads to a sparse system representation.

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ABSTRACT

Computing reachable sets for continuous-stirred tank reactors (CSTRs) under uncertainty is crucial for designing efficient model-based control strategies or developing robust process monitoring protocols. This paper, the first in the three-part series, develops a linear transformation to project the dynamics of a CSTR reaction system onto a transformed state space. The proposed transformation is invertible, and leads to a "sparse" system representation in the transformed state space – a property crucial for the methods developed to compute reachable sets of CSTR reaction systems. The second and third papers in this series discuss how the transformation developed here can be used to compute effectively outer interval approximations to the reachable sets of CSTR reaction systems. To this effect, two new bounding methods – direct and indirect-bounding methods – are proposed in the second and third paper, respectively, to compute tight interval enclosures for the reachable sets of CSTR reaction systems. Several numerical examples are also provided to demonstrate efficacy of the proposed direct and indirect-bounding methods.

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1. Introduction

The dynamics of chemical reaction kinetics in a continuous stirred tank reactor (CSTR) of constant volume V can be modeled using a set of ordinary differential equations (ODEs) given by

$$\dot{\mathbf{x}}(t,\mathbf{u}) = \mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{1}{V}u_{\mathrm{o}}(t)\mathbf{x}(t,\mathbf{u}),$$

where $\mathbf{x}$ is the concentrations of the species in the CSTR, $\mathbf{S}$ and $\mathbf{W}$ are the stoichiometric and concentration matrices, $\mathbf{r}$ is the rate vector, $\mathbf{k}$ is the model parameter vector (e.g., kinetic rate-constants, temperature, pressure), and $\mathbf{u}_{\mathrm{i}}$, and u_{o} are the input and output flow rates, respectively. A detailed description of CSTR systems is given in Section 2. In this three-part paper, we are interested in computing time-varying, component-wise bounds on the species concentrations $\mathbf{x}$, subject to system uncertainties and flow rate disturbances. The uncertain variables and unknown parameters are denoted by $\mathbf{u}$ for convenience. In the literature, this is commonly referred to as a reachable set computation problem. Given quantifiable bounds on uncertain system parameters/variables (e.g., lower and upper bounds), a reachable set for a CSTR system provides a rigorous estimate of how various uncertainties propagate through the system, and affect concentration profiles of individual species in time.

In this three-part paper, two bounding methods – direct and indirect-bounding methods – are proposed to compute interval enclosures for reachable sets of CSTR reaction systems. The proposed direct and indirect-bounding methods both use an invertible (or isomorphic) transformation to map the dynamics of CSTR

* Corresponding author.
E-mail addresses: tulsyan@mit.edu (A. Tulsyan), pib@mit.edu (P.I. Barton).

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reaction systems from the original state space into a transformed state space. Apart from the transformation being isomorphic, other prerequisites include the developed transformation leading to a relatively "simpler" and "sparser" system representation in transformed state space compared to the original state space. This paper, the first in the three-part paper, develops an isomorphic transformation to map sparsely a CSTR reaction system into the transformed state space. The proposed transformation is then used in the development of direct and indirect-bounding methods. The details of bounding methods and how they use the transformation are discussed in the second and third papers in this series (Tulsyan and Barton, 2017a,b).

The central idea used in this paper to obtain a sparse CSTR reaction system representation is based on decomposition of molar concentrations of species in a CSTR into multiple subspaces. This is done by constructing a transformation that decomposes the original state space into three specific complementary subspaces. The CSTR reaction system in the transformed state space is then represented by taking oblique projections of molar concentrations onto subspaces. Further, of the three subspaces constructed, only one pair is orthogonal, with the rest being non-orthogonal. Physically, the three subspaces describe the space of reaction variants, flow rate variants, and reaction and flow rate invariants for the CSTR reaction system. Finally, the linear structure of the proposed transformation allows for fast computation of dynamics in the transformed state space – which is essential in extending the use of proposed direct and indirect-bounding methods for real-time applications, such as monitoring (Tulsyan and Barton, 2016a) and optimization (Tulsyan and Barton, 2016b), where bounds need to be computed fairly quickly.

It is important to compare the transformation proposed in this paper with existing work. Note that representation of reaction systems in terms of variants and invariants has been extensively studied by several authors for the purpose of computing extent-of-reactions for different reactor configurations (Asbjørnsen and Field, 1970; Srinivasan et al., 1998; Bhatt et al., 2010). For example, a two-way decomposition of CSTR reaction systems into reaction variant and reaction invariant spaces was first derived by Asbjørnsen and Field (1970), Asbjørnsen (1972), Fjeld et al. (1974) for modeling and control of CSTR reaction systems. Similarly, a three-way decomposition into the spaces of reaction variants, flow rate variants, and reaction and flow rate invariants was first proposed by Srinivasan et al. (1998). Further, decomposition of CSTR reaction systems into variants and invariants is non-unique as different transformations and assumptions can lead to the same decomposition. For example, in Srinivasan et al. (1998), the authors developed a nonlinear transformation for CSTR systems to separate the effects of reactions and flow rates; and later, the same authors in Amrhein et al. (2010) redefined the transformation to make it linear. Recently, Rodrigues et al. (2015) also derived the results in Amrhein et al. (2010) using a different linear transformation under different assumptions. Transformations for batch systems have also been proposed (Scott and Barton, 2010).

Note that although the approach to compute a three-way decomposition of CSTR reaction systems proposed here yields results similar to Amrhein et al. (2010), the transformation, assumptions and motivation used herein are different. For example, the transformation in Amrhein et al. (2010) considers the following: (1) the column spaces spanned by $\mathbf{S}$ and $\mathbf{W}$ are independent with $[\mathbf{SW}]$ being a full-column rank matrix; (2) decomposition into orthogonal complementary subspaces; and (3) orthogonal projections onto subspaces. The transformation in Amrhein et al. (2010) further requires the reaction network to have non-zero initial concentrations to ensure that $[\mathbf{SWx_0}]$, where $\mathbf{x}_0$ is the initial concentrations of species in a CSTR, is a full-column rank matrix.

On the contrary, the transformation proposed in this paper requires a weaker assumption of $\mathbf{S}$ and $\mathbf{W}$ individually being full-column rank matrices. For CSTR reaction systems for which this assumption does not hold (e.g., reversible reaction networks, see Example 1), we provide results to ensure that the proposed transformation is still applicable to such systems. Moreover, the transformation developed in this paper is systematic and offers greater flexibility as it considers decomposition of the original state space into non-orthogonal complementary subspaces with oblique projections of molar concentrations of species.

It is instructive to highlight that while the transformation in Amrhein et al. (2010), Rodrigues et al. (2015) is well-suited for computing extent-of-reactions for CSTR reaction systems, the transformation in this paper is tailored for computing efficient interval enclosures for CSTR reaction systems. Note that it is possible to adapt the transformation in Amrhein et al. (2010), Rodrigues et al. (2015) to compute enclosures, the same way the proposed tranformation can be used to compute the extent-of-reactions. Nevertheless, since the focus of this paper is different from Amrhein et al. (2010), Rodrigues et al. (2015), the transformation developed here is therefore useful for computing tight interval enclosures for CSTR reaction systems and not extent-of-reactions. With this background information, the notation used in this paper is discussed next.

Notation. Lower-case and upper-case bold letters denote vectors and matrices, respectively. $\mathbf{v}^{\mathrm{T}}$ (or $\mathbf{M}^{\mathrm{T}}$) denotes the transpose of a vector (or matrix). $\mathbf{0}_{m\times n}$ and $\mathbf{1}_{m\times n}$ will denote $m \times n$ matrices of zeros and ones, respectively, and $\mathbf{I}_n$ an $n \times n$ identity matrix. For $\mathbf{A} \in \mathbb{R}^{m\times n}$, the rank of the matrix is denoted by Rank($\mathbf{A}$), column space as $\mathcal{C}(\mathbf{A}) = \{\mathbf{y} \in \mathbb{R}^m : \mathbf{y} = \mathbf{Ax} \text{ for some } \mathbf{x} \in \mathbb{R}^n\}$ and null space as $\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{Ax} = \mathbf{0}_{m\times 1}\}$. The dimension of $\mathcal{C}(\mathbf{A})$ is denoted by $\dim(\mathcal{C}(\mathbf{A}))$. For a finite, real matrix $\mathbf{A} \in \mathbb{R}^{m\times n}$, let $\mathbf{A}^+ \in \mathbb{R}^{n\times m}$ denote its Moore-Penrose inverse satisfying: (i) $\mathbf{AA}^+\mathbf{A} = \mathbf{A}$; (ii) $\mathbf{A}^+\mathbf{AA}^+ = \mathbf{A}^+$; (iii) $(\mathbf{AA}^+)^{\mathrm{T}} = \mathbf{AA}^+$; and (iv) $(\mathbf{A}^+\mathbf{A})^{\mathrm{T}} = \mathbf{A}^+\mathbf{A}$. Matrix $\mathbf{B} \in \mathbb{R}^{n\times m}$ is a $\{1,2\}$-inverse of $\mathbf{A}$ if it satisfies conditions (i) and (ii) Ben-Israel and Greville (2003). $\mathbb{R}_+$ denotes the set of non-negative reals. For $n \in \mathbb{N}$ and measurable set $T \subset \mathbb{R}$, the space of Lebesgue integrable functions $\mathbf{v} : T \to \mathbb{R}^n$ is denoted by $L^1(T,\mathbb{R}^n) \equiv \{(\mathbf{v} : T \to \mathbb{R}^n) : \int_T |v_i| < +\infty, \forall i\}$, such that $\mathbf{v} \in L^1(T,\mathbb{R}^n)$ implies $v_i \in L^1(T,\mathbb{R})$ for all i.

2. CSTR reaction model

Consider a schematic of the CSTR reaction system in Fig. 1. Let $n_x \in \mathbb{N}$ denote the number of species, $n_r \in \mathbb{N}$ the number of chemical reactions, $n_k \in \mathbb{N}$ the number of uncertain rate-constants and $n_p \in \mathbb{N}$ the number of input flow rates in a chemical kinetic system. For mathematical convenience, the CSTR is assumed to have one outlet; however, this need not be the case, in general. For given compact sets $D_k \subset \mathbb{R}^{n_k}, D_{u_i} \subset \mathbb{R}^{n_p}$ and $D_{u_o} \subset \mathbb{R}$, let $\mathbf{k}(t) \in D_k$ be the time-varying uncertain parameters (also includes time-invariant parameters), $\mathbf{u}_{\mathrm{i}}(t) \in D_{u_i}$ be the input flow rates and $u_{\mathrm{o}}(t) \in D_{u_o}$ denote the output flow rates. Defining $\mathbf{u}(t) \equiv (\mathbf{k}(t), \mathbf{u}_{\mathrm{i}}(t), u_{\mathrm{o}}(t)) \in U \equiv D_k \times D_{u_i} \times D_{u_o}$, let the set of time-varying inputs/parameters be denoted in a compact notation as

$$\mathcal{U} = \left\{\mathbf{u} \in L^1(T, \mathbb{R}^{n_k+n_p+1}) : \mathbf{u}(t) \in U, a.e.\, t \in T\right\},$$

where $T = [t_0, t_f] \subset \mathbb{R}$ is some time interval of interest. For a given set $D_x \subset \mathbb{R}^{n_x}$, let the set of possible initial concentrations of species in the CSTR at t_0 be $X_0 \subset D_x$. Let $\mathbf{S} \in \mathbb{R}^{n_x\times n_r}$ and $\mathbf{W} \in \mathbb{R}^{n_x\times n_p}$ be the stoichiometric and volumetric concentration matrices, respectively.

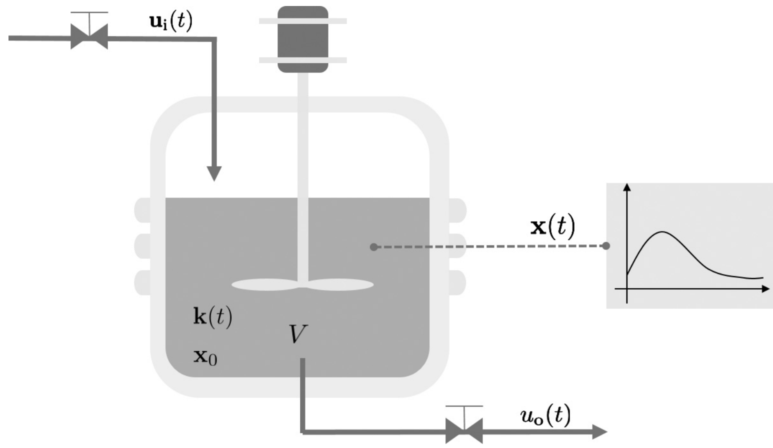

Fig. 1. A schematic of the CSTR reaction system considered in the paper. The CSTR of volume V includes n_p input flow rates, denoted by $\mathbf{u}_i$ and one outlet flow rate, denoted by u_o. The concentration of n_x species in the CSTR under n_r reactions is denoted by $\mathbf{x}(t)$, and initial concentration by $\mathbf{x}_0$. The n_k rate-constants are denoted by $\mathbf{k}(t)$.

Definition 1. (Independent reactions and flow rates) The n_r reactions are linearly independent if the stoichiometric matrix $\mathbf{S}$ is full-column rank, i.e., $\text{Rank}(\mathbf{S}) = n_r$. The n_p inlet flow rates are linearly independent if the concentration matrix $\mathbf{W}$ is full-column rank, i.e., $\text{Rank}(\mathbf{W}) = n_p$.

The CSTR is an independent reaction system if it constitutes n_r independent reactions and n_p independent inlet flow rates. Finally, for a rate function $\mathbf{r} : D_k \times D_x \to \mathbb{R}^{n_r}$, the concentration profiles of species in a constant volume $V \in \mathbb{R}_+$ CSTR can be modeled as an initial value problem (IVP) given by

$$\dot{\mathbf{x}}(t,\mathbf{u}) = \mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{W}\mathbf{u}_i(t) - \frac{u_o(t)}{V}\mathbf{x}(t,\mathbf{u}), \tag{1}$$

with $\mathbf{x}(t_0,\mathbf{u}) \in X_0$. The solution to (1) is defined as a mapping $\mathbf{x} : T \times \mathcal{U} \to D_x$, such that for each $\mathbf{u} \in \mathcal{U}, \mathbf{x}(\cdot,\mathbf{u})$ is absolutely continuous and satisfies (1) a.e. on T. In this paper, we assume that for each $(\mathbf{u},\mathbf{x}_0) \in \mathcal{U} \times X_0$, a unique solution of (1) exists on the time horizon of interest.

Problem statement. Given a CSTR reaction system described by (1), compute an invertible transformation, $\tau : D_x \to D_z$, satisfying

$$\tau(\mathbf{x}(t,\mathbf{u})) = \mathbf{z}(t,\mathbf{u}),$$
$$\tau^{-1}(\mathbf{z}(t,\mathbf{u})) = \mathbf{x}(t,\mathbf{u}),$$

for all $(t,\mathbf{u}) \in T \times \mathcal{U}$, such that for some set $D_z \subset \mathbb{R}^{n_x}$, the dynamics of the mapping $\mathbf{z} : T \times \mathcal{U} \to D_z$ are "sparse" and $\mathbf{z}(\cdot,\mathbf{u})$ is absolutely continuous for each $\mathbf{u} \in \mathcal{U}$.

In the Problem Statement, the sparsity of the transformed system is to be understood in the following sense. In the original state space, the dynamics of molar concentrations in (1) is complex due to the presence of the $\mathbf{S}$ and $\mathbf{W}$ matrices. It is easy to see that premultiplying functions $\mathbf{r}$ and $\mathbf{u}_i$ with matrices $\mathbf{S}$ and $\mathbf{W}$, respectively, makes the state derivatives, $\dot{\mathbf{x}}$, in (1) a complex function of multiple nonlinear rate expressions $\mathbf{r}$ and input flow rates $\mathbf{u}_i$. Therefore the objective here is to introduce "sparsity" in the transformed system by eliminating the matrices $\mathbf{S}$ and $\mathbf{W}$ in (1). This is to be done through the design of an invertible transformation, τ, that maps (1) into a transformed state space described by $\mathbf{z}$. Here $\mathbf{z}$ represents the dynamics of the CSTR reaction system in the transformed state space. Graphically, the problem statement is illustrated in Fig. 2.

3. Generating sparse transformation

We propose an invertible transformation to map the CSTR reaction system described by (1) onto a transformed state space. Apart from the transformation being invertible, the transformation should also lead to a sparse representation of the system dynamics in transformed state space. The need for developing an invertible and sparse transformation is motivated by its application in computing tight and efficient interval enclosures for CSTR reaction system in (1) using direct and indirect-bounding methods. The details on how a sparse transformation aids in computing tight enclosures are not discussed here, but can be found in the second and third papers in this series (Tulsyan and Barton, 2017a,b).

One approach to obtain a sparse representation of the CSTR reaction system in the transformed state space is to design the transformation so that the matrices $\mathbf{S}$ and $\mathbf{W}$ are replaced with identity matrices that describe the dynamics in the transformed state space. This is the core idea explored in the remainder of this section and forms the basis for the transformation developed in this paper. Furthermore, to allow for fast simulation of the system in transformed state space, we restrict ourselves to the class of linear transformations. Before we proceed, several assumptions are necessary.

Assumption 1. The CSTR reaction system in (1) satisfies the following

1. $\text{Rank}(\mathbf{S}) = n_r$, and
2. $\text{Rank}(\mathbf{W}) = n_p$.

Assumptions 1(a) and (b) ensure that (1) is an independent reaction system (see Definition 1). Note that for certain important classes of reaction network systems, Assumptions 1(a) and (b) could be restrictive, as shown in the example below.

Example 1. Consider the following reversible reaction

$$\mathrm{A} \underset{k_2=3}{\overset{k_1=1}{\rightleftharpoons}} \mathrm{B}$$

in a CSTR of constant unit volume with 2 inlet flow streams $\mathbf{u}_i(t) = [u_{i,1}(t) u_{i,2}(t)]^{\mathrm{T}}$ and one outlet flow given as $u_o(t) = u_{i,1}(t) + u_{i,2}(t)$. $u_{i,1}(t)$ contains 1-molar concentration of complexes A and B, while $u_{i,2}(t)$ contains 2-molar concentration of A and B. The initial concentration of A and B in the reactor is 1 molar each. If the forward and backward rate laws are $k_1 x_A^2$ and $k_2 x_B$, respectively, then the dynamics can be modeled as

$$\dot{\mathbf{x}}(t,\mathbf{u}) = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_A^2 \\ 3x_B \end{bmatrix} + \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix} \mathbf{u}_i(t) - u_o(t)\mathbf{x}(t,\mathbf{u}),$$
$$\mathbf{x}(0) = \mathbf{1}_{2\times 1}.$$

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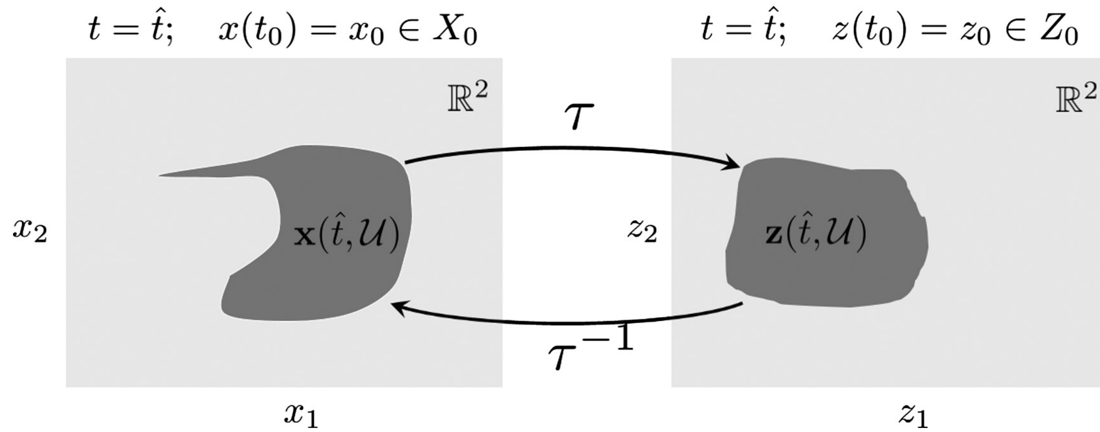

Fig. 2. An illustration of the problem addressed in this paper. The original solution set, denoted by $\mathbf{x}(\hat{t}, \mathcal{U})$, is transformed to the set $\mathbf{z}(\hat{t}, \mathcal{U})$ using an isomorphic transformation denoted generically by τ.

It is easy to see that Example 1 is not an independent reaction system as Assumptions 1(a) and (b) are violated with $\text{Rank}(\mathbf{S}) = 1 < 2 = n_r$ and $\text{Rank}(\mathbf{W}) = 1 < 2 = n_p$.

Example 1 gives an instance where Assumptions 1(a) and (b) are violated for a reversible kinetic system with dependent reactions and flow rates. In fact, Assumption 1 is violated by many other practical reaction networks. Fortunately, it is possible to rewrite the dynamics of a dependent reaction system in terms of an independent reaction system, as discussed in the next theorem.

Theorem 1. *Consider a dependent CSTR reaction system in (1) with* $\text{Rank}(\mathbf{S}) = n'_r < n_r$ *and* $\text{Rank}(\mathbf{W}) = n'_p < n_p$. *Let* $\mathbf{S}_1 \in \mathbb{R}^{n_x \times n'_r}$ *and* $\mathbf{W}_1 \in \mathbb{R}^{n_x \times n'_p}$ *be constructed by selecting* n'_r *and* n'_p *independent columns of* $\mathbf{S}$ *and* $\mathbf{W}$, *respectively, then (1) can also be written as*

$$\dot{\mathbf{x}}(t, \mathbf{u}') = \mathbf{S}_1 \mathbf{r}'(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u}')) + \frac{1}{V}\mathbf{W}_1 \mathbf{u}'_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{x}(t, \mathbf{u}'), \tag{2}$$

where:

$$\mathbf{r}'(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u}')) = [\mathbf{I}_{n'_r}\ \mathbf{A}_S]\mathbf{Q}_1 \mathbf{r}(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u}));$$
$$\mathbf{u}'_{\mathrm{i}}(t) = [\mathbf{I}_{n'_p}\ \mathbf{A}_W]\mathbf{Q}_2 \mathbf{u}_{\mathrm{i}}(t);$$

and $\mathbf{Q}_1 \in \mathbb{R}^{n_r \times n_r}$ *and* $\mathbf{Q}_2 \in \mathbb{R}^{n_p \times n_p}$ *are required permutation matrices to move the basis vectors of* $\mathbf{S}$ *and* $\mathbf{W}$ *to the first* n'_r *and* n'_p *columns of the matrices, respectively, and* $\mathbf{A}_S$ *and* $\mathbf{A}_W$ *are constant matrices of appropriate dimensions with* $\mathbf{x}(t_0, \mathbf{u}') \in X_0$.

Proof. Under the given hypotheses, matrices $\mathbf{S}$ and $\mathbf{W}$ can be decomposed as $\mathbf{S} = [\mathbf{S}_1\ \mathbf{S}_2]\mathbf{Q}_1$ and $\mathbf{W} = [\mathbf{W}_1\ \mathbf{W}_2]\mathbf{Q}_2$, where $\mathbf{S}_2 \in \mathbb{R}^{n_x \times (n_r - n'_r)}$ and $\mathbf{W}_2 \in \mathbb{R}^{n_x \times (n_p - n'_p)}$ represent the dependent columns of $\mathbf{S}$ and $\mathbf{W}$, respectively. Substituting this decomposition of $\mathbf{S}$ and $\mathbf{W}$ into (1) yields

$$\dot{\mathbf{x}}(t, \mathbf{u}) = [\mathbf{S}_1 \mathbf{S}_2]\mathbf{Q}_1 \mathbf{r}(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u})) + \frac{1}{V}[\mathbf{W}_1\ \mathbf{W}_2]\mathbf{Q}_2 \mathbf{u}_{\mathrm{i}}(t) - \frac{1}{V}u_{\mathrm{o}}(t)\mathbf{x}(t, \mathbf{u}). \tag{3}$$

Let $\mathbf{A}_S$ and $\mathbf{A}_W$ satisfy $\mathbf{S}_2 = \mathbf{S}_1 \mathbf{A}_S$ and $\mathbf{W}_2 = \mathbf{W}_1 \mathbf{A}_W$, respectively. Note that $\mathbf{A}_S$ and $\mathbf{A}_W$ always exist for every given matrix pair $\mathbf{S}_1$ and $\mathbf{W}_1$ because $\mathbf{S}_1$ and $\mathbf{W}_1$ form basis vectors for $\mathcal{C}(\mathbf{S})$ and $\mathcal{C}(\mathbf{W})$, respectively. Substituting $\mathbf{S}_2 = \mathbf{S}_1 \mathbf{A}_S$ and $\mathbf{W}_2 = \mathbf{W}_1 \mathbf{A}_W$ into (3) gives

$$\begin{aligned} \dot{\mathbf{x}}(t, \mathbf{u}) =& [\mathbf{S}_1 \mathbf{S}_1 \mathbf{A}_S]\mathbf{Q}_1 \mathbf{r}(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u})) \\ & + \frac{1}{V}[\mathbf{W}_1 \mathbf{W}_1 \mathbf{A}_W]\mathbf{Q}_2 \mathbf{u}_{\mathrm{i}}(t) - \frac{1}{V}u_{\mathrm{o}}(t)\mathbf{x}(t, \mathbf{u}), \\ =& \mathbf{S}_1 [\mathbf{I}_{n'_r} \mathbf{A}_S]\mathbf{Q}_1 \mathbf{r}(\mathbf{k}(t), \mathbf{x}(t, \mathbf{u})) \\ & + \frac{1}{V}\mathbf{W}_1 [\mathbf{I}_{n'_p} \mathbf{A}_W]\mathbf{Q}_2 \mathbf{u}_{\mathrm{i}}(t) - \frac{1}{V}u_{\mathrm{o}}(t)\mathbf{x}(t, \mathbf{u}). \end{aligned} \tag{4}$$

Defining $\mathbf{r}' \equiv [\mathbf{I}_{n'_r} \mathbf{A}_S]\mathbf{Q}_1 \mathbf{r}$ and $\mathbf{u}'_{\mathrm{i}} \equiv [\mathbf{I}_{n'_p}\ \mathbf{A}_W]\mathbf{Q}_2 \mathbf{u}_{\mathrm{i}}$, and substituting them into (4) yields the desired result. □

Theorem 1 shows how the dynamics of a dependent CSTR reaction system can be represented in terms of an independent reaction system. Mathematically, under the hypotheses of Theorem 1, IVPs (1) and (2) are equivalent. An instance of Theorem 1 on Example 1 is shown next.

Example 2. Consider the dependent reaction system in Example 1. The ranks of $\mathbf{S}$ and $\mathbf{W}$ indicate there is only one independent reaction and one independent flow rate. Using Theorem 1, Example 1 can be represented as an independent reaction system with dynamics described as

$$\dot{\mathbf{x}}(t, \mathbf{u}) = \begin{bmatrix} -1 \\ 1 \end{bmatrix}(x_{\mathrm{A}}^2 - 3x_{\mathrm{B}}) + \begin{bmatrix} 1 \\ 1 \end{bmatrix}(u_{\mathrm{i},1}(t) + 2u_{\mathrm{i},2}(t)) - u_{\mathrm{o}}(t)\mathbf{x}(t, \mathbf{u}),$$
$$\mathbf{x}(0, \mathbf{u}) = \mathbf{1}_{2\times 1},$$

where $r' \equiv (x_{\mathrm{A}} - 3x_{\mathrm{B}})$ and $u'_{\mathrm{i}} \equiv u_{\mathrm{i},1} + 2u_{\mathrm{i},2}$ are the new rate function and input flow rate, respectively. Mathematically, Examples 1 and 2 are equivalent; however, while Example 1 violates Assumption 1, Example 2 does not. In fact without any prior information, Example 2 can be mistaken for an irreversible reaction system of type $\mathrm{A} \rightarrow \mathrm{B}$, which is different from the chemistry described by Example 1. Nevertheless, since we only require the IVPs in (1) and (2) to be mathematically equivalent for the transformation developed in this paper to be valid, we do not concern ourselves with any misleading inference that might be drawn from the IVP (2) regarding the underlying chemistry of the reaction network under consideration.

Finally, Theorem 1 provides a procedure to rewrite a dependent CSTR reaction network in terms of an independent reaction network, as required by Assumption 1. In the remainder of this paper we will assume Assumption 1 holds for the CSTR reaction system in (1) unless stated otherwise. With Assumption 1 in place, next we briefly discuss the notion of projection onto subspaces along complementary subspaces, which is central to the construction of the sparse transformations developed in this paper.

Definition 2. Let M and N be complementary subspaces of $\mathbb{R}^p$ then $\mathcal{P}_{M,N} : \mathbb{R}^p \rightarrow \mathbb{R}^p$ is the unique linear projector onto M along N if for every $\mathbf{y} \in \mathbb{R}^p$, we can write

$$\mathbf{y} = \mathcal{P}_{M,N}\mathbf{y} + (\mathbf{I}_p - \mathcal{P}_{M,N})\mathbf{y},$$

where $\mathcal{P}_{M,N}\mathbf{y} \in M$ and $(\mathbf{I}_p - \mathcal{P}_{M,N})\mathbf{y} \in N$, or write

$$\mathbf{y} = \mathcal{P}_{M,N}\mathbf{y}$$

if and only if $\mathbf{y} \in M$.

Definition 2 does not require the complementary subspaces to be orthogonal. An illustration of Definition 2 is given in Fig. 3; and an instance of Definition 2 for a pair of orthogonal subspaces generated by a matrix is illustrated in the example below.

Example 3. For matrix $\mathbf{A} \in \mathbb{R}^{p\times q}$, $\mathcal{C}(\mathbf{A})$ and $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ are orthogonal complementary subspaces in $\mathbb{R}^p$, so that

$$\mathbf{y} = \mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})}\mathbf{y} + (\mathbf{I}_p - \mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})})\mathbf{y}$$

holds for every $\mathbf{y} \in \mathbb{R}^p$. Further, for every $\mathbf{y} \in \mathcal{N}(\mathbf{A}^{\mathrm{T}})$, $\mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})}\mathbf{y} = \mathbf{0}_{p\times 1}$. A similar relationship can also be described for all $\mathbf{y} \in \mathcal{C}(\mathbf{A})$.

In Example 3, $\mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})}\mathbf{y}$ describes the projection of $\mathbf{y}$ onto $\mathcal{C}(\mathbf{A})$ along $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$. Further, since $\mathcal{C}(\mathbf{A})$ and $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ are orthogonal, the projection is also orthogonal. If the subspaces in Definition 2 are generated by matrices, then the linear projectors can be computed as shown below.

Lemma 1. *If $\mathbf{A} \in \mathbb{R}^{p\times q}$ and $\mathbf{B} \in \mathbb{R}^{q\times p}$ are $\{1,2\}$-inverses of each other, such that $\mathbf{ABA} = \mathbf{A}$ and $\mathbf{BAB} = \mathbf{B}$, then the pairs $\mathcal{C}(\mathbf{B}),\mathcal{N}(\mathbf{A})$ and $\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{B})$ are both complementary and $\mathbf{BA} = \mathcal{P}_{\mathcal{C}(B),\mathcal{N}(A)}$ and $\mathbf{AB} = \mathcal{P}_{\mathcal{C}(A),\mathcal{N}(B)}$.*

Proof. See Corollary 7, Section 4 Ch. 2 in Ben-Israel and Greville (2003). □

Lemma 1 describes an oblique projection if the underlying subspaces are not orthogonal; however, if the underlying subspaces are orthogonal, as in Example 3, the projections are also indeed orthogonal and the required linear projectors are computed as given in the following corollary.

Corollary 1. *For a given matrix $\mathbf{A} \in \mathbb{R}^{p\times q}$, let $\mathbf{A}^+ \in \mathbb{R}^{q\times p}$ denote its Moore-Penrose inverse, then the orthogonal projection of $\mathbf{x} \in \mathbb{R}^p$ onto $\mathcal{C}(\mathbf{A})$ is $\mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})} = \mathbf{AA}^+$ and projection onto $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ is $\mathcal{P}_{\mathcal{N}(\mathbf{A}^{\mathrm{T}}),\mathcal{C}(\mathbf{A})} = (\mathbf{I}_p - \mathbf{AA}^+)$.*

Proof. See Ex. 1, Section 1 Ch. 3 in Stewart and Sun (1990). □

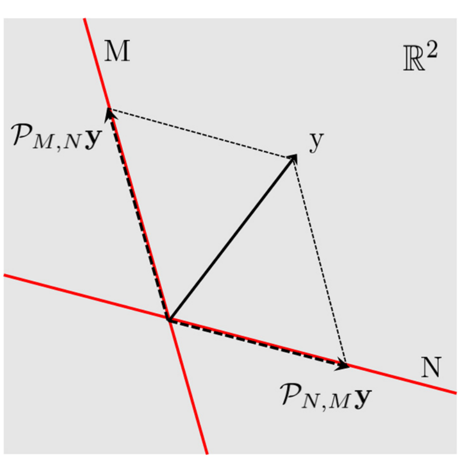

Fig. 3. An illustration of the projection defined in Definition 2. Here M and N, denoted by the solid red lines, form a pair of non-orthogonal complementary subspaces in $\mathbb{R}^2$. The solid black arrow is any vector $\mathbf{y} \in \mathbb{R}^2$. The dashed black arrow on subspace N is the vector $\mathcal{P}_{N,M}\mathbf{y}$, which is the oblique projection of $\mathbf{y}$ onto N along the subspace M. Similarly, the dashed black arrow on subspace M is the vector $\mathcal{P}_{M,N}\mathbf{y}$, which is the projection of $\mathbf{y}$ onto M along N.

Note that while Definition 2 and Lemma 1 allow for oblique projections onto non-orthogonal complementary subspaces, Example 3 and Corollary 1 strictly describe orthogonal projections onto orthogonal complementary subspaces generated by matrices. From Lemma 1 and Corollary 1, an oblique and orthogonal projection of a vector onto the column space of $\mathbf{A}$ can be calculated using a $\{1,2\}$-inverse and Moore-Penrose inverse of $\mathbf{A}$, respectively. It is important to highlight that for a non-square matrix $\mathbf{A}$, while the choice of its $\{1,2\}$-inverse is non-unique, its Moore-Penrose inverse is always unique (Ben-Israel and Greville, 2003). In fact, the Moore-Penrose inverse is an element of the set $\{1,2\}$-inverse matrices. In practice, given a matrix $\mathbf{A}$, the Moore-Penrose inverse, denoted by $\mathbf{A}^+$, can be computed in `MATLAB` using the routine `pinv`. If $\mathbf{A}$ is full-column rank then $\mathbf{A}^+ = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}$, such that in Corollary 1, $\mathcal{P}_{\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})} = \mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}$ and $\mathcal{P}_{\mathcal{N}(\mathbf{A}^{\mathrm{T}}),\mathcal{C}(\mathbf{A})} = (\mathbf{I}_p - \mathbf{A}(\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}})$. Finally, note that in Corollary 1, since $\mathcal{C}(\mathbf{A}),\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ forms a pair of orthogonal complementary subspaces of $\mathbb{R}^p$ the orthogonal projection onto $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ is defined by the projector $\mathcal{P}_{\mathcal{N}(\mathbf{A}^{\mathrm{T}}),\mathcal{C}(\mathbf{A})} = (\mathbf{I}_p - \mathbf{AA}^+)$, where $\mathbf{AA}^+$ is the projector for orthogonal projection onto $\mathcal{C}(\mathbf{A})$. Now if the columns of a full-column rank matrix, say $\mathbf{P}$, for example, span $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ then the projection onto $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ is also defined by the projector $\mathcal{P}_{\mathcal{N}(\mathbf{A}^{\mathrm{T}}),\mathcal{C}(\mathbf{A})} = \mathbf{P}(\mathbf{P}^{\mathrm{T}}\mathbf{P})^{-1}\mathbf{P}^{\mathrm{T}}$. From Definition 2, since the projection onto $\mathcal{N}(\mathbf{A}^{\mathrm{T}})$ along $\mathcal{C}(\mathbf{A})$ is unique, we have

$$\mathcal{P}_{\mathcal{N}(\mathbf{A}^{\mathrm{T}}),\mathcal{C}(\mathbf{A})} = \mathbf{P}(\mathbf{P}^{\mathrm{T}}\mathbf{P})^{-1}\mathbf{P}^{\mathrm{T}} = (\mathbf{I}_p - \mathbf{AA}^+). \tag{5}$$

Eq. (5) is an important relationship, and will be frequently used in the remainder of this section. With this background, the transformation for the CSTR reaction system is discussed next.

Lemma 2. *Consider the CSTR reaction system in (1). Given $\mathbf{S}$, let $\mathbf{S}^+ \in \mathbb{R}^{n_r\times n_x}$ be its Moore-Penrose inverse and let $\mathbf{N} \in \mathbb{R}^{n_x\times(n_x-n_r)}$ be a basis for $\mathcal{N}(\mathbf{S}^{\mathrm{T}}) \subset \mathbb{R}^{n_x}$ then there exists a unique solution to the IVP*

$$\dot{\mathbf{n}}_1(t,\mathbf{u}) = \frac{1}{V}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_1(t,\mathbf{u}), \tag{6a}$$

$$\begin{aligned}\dot{\mathbf{n}}_2(t,\mathbf{u}) = {} & \mathbf{r}(\mathbf{k}(t),\mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{n}_1(t,\mathbf{u})) \\ & + \frac{1}{V}\mathbf{S}^+\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_2(t,\mathbf{u}),\end{aligned} \tag{6b}$$

satisfying the conditions

$$\mathbf{n}(t,\mathbf{u}) \equiv \begin{bmatrix}\mathbf{n}_1(t,\mathbf{u})\\ \mathbf{n}_2(t,\mathbf{u})\end{bmatrix} = \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^+\end{bmatrix}\mathbf{x}(t,\mathbf{u}), \tag{7a}$$

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{n}_1(t,\mathbf{u}), \tag{7b}$$

for all $(t,\mathbf{u},\mathbf{x}_0) \in T \times \mathcal{U} \times X_0$.

Proof. Let $\mathbf{x} \in \mathbb{R}^{n_x}$ be the unique solution of the CSTR reaction system in (1). From Example 3, $\mathbf{x}$ is the sum of its projections onto orthogonal complementary subspaces, such that

$$\mathbf{x}(t,\mathbf{u}) = \mathcal{P}_{\mathcal{C}(\mathbf{S}),\mathcal{N}(\mathbf{S}^{\mathrm{T}})}\mathbf{x}(t,\mathbf{u}) + \mathcal{P}_{\mathcal{N}(\mathbf{S}^{\mathrm{T}}),\mathcal{C}(\mathbf{S})}\mathbf{x}(t,\mathbf{u}).$$

Assuming $\dim(\mathcal{N}(\mathbf{S}^{\mathrm{T}})) \geqslant 1$, the columns of $\mathbf{N}$ and $\mathbf{S}$ form basis vectors for the subspaces $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ and $\mathcal{C}(\mathbf{S})$, respectively (from hypothesis, and Assumption 1(a) that $\mathbf{S}$ is full-column rank), such that

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}(\mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}\mathbf{S}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u}),$$

for all $\mathbf{x}(t,\mathbf{u}) \in \mathbb{R}^{n_x}$. For full-column rank $\mathbf{S}$, the Moore-Penrose inverse of $\mathbf{S}$ is given by $\mathbf{S}^+ = (\mathbf{S}^{\mathrm{T}}\mathbf{S})^{-1}\mathbf{S}^{\mathrm{T}}$. Therefore,

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{S}^{+}\mathbf{x}(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u}). \tag{8}$$

Defining $\mathbf{n}(t,\mathbf{u}) \equiv [\mathbf{N}(\mathbf{S}^{+})^{\mathrm{T}}]^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$ and writing (8) in terms of $\mathbf{n}(t,\mathbf{u})$ gives

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{n}_1(t,\mathbf{u}). \tag{9}$$

Differentiating $\mathbf{n}(t,\mathbf{u}) = [\mathbf{N}(\mathbf{S}^{+})^{\mathrm{T}}]^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$, and substituting $\dot{\mathbf{x}}(t,\mathbf{u})$ with (1) yields

$$\begin{aligned}\begin{bmatrix}\dot{\mathbf{n}}_1(t,\mathbf{u})\\ \dot{\mathbf{n}}_2(t,\mathbf{u})\end{bmatrix} &= \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\dot{\mathbf{x}}(t,\mathbf{u}),\\ &= \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\left(\mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{x}(t,\mathbf{u})\right).\end{aligned} \tag{10}$$

Substituting the conditions $\mathbf{N}^{\mathrm{T}}\mathbf{S} = \mathbf{0}_{(n_x-n_r)\times n_r}, \mathbf{S}^{+}\mathbf{S} = \mathbf{I}_{n_r}$ and $\mathbf{n}(t,\mathbf{u}) \equiv [\mathbf{N}(\mathbf{S}^{+})^{\mathrm{T}}]^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$ in (10) give

$$\begin{bmatrix}\dot{\mathbf{n}}_1(t,\mathbf{u})\\ \dot{\mathbf{n}}_2(t,\mathbf{u})\end{bmatrix} = \begin{bmatrix}\frac{1}{V}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_1(t,\mathbf{u})\\ \mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{S}^{+}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_2(t,\mathbf{u})\end{bmatrix}.$$

Now replacing $\mathbf{x}$ in (11) with (9) yields (6a) and (6b). Thus the IVP (6a) and (6b) thus has at least one solution satisfying (7a) and (7b). Let $\mathbf{m}(t,\mathbf{u})$ be another solution of (6a) and (6b) and define $\mathbf{q}(t,\mathbf{u}) \equiv \mathbf{S}\mathbf{m}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{m}_1(t,\mathbf{u})$. Differentiating $\mathbf{q}(t,\mathbf{u})$ yields

$$\begin{aligned}\dot{\mathbf{q}}(t,\mathbf{u}) =& \mathbf{S}\dot{\mathbf{m}}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\dot{\mathbf{m}}_1(t,\mathbf{u}),\\ =& \mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{S}\mathbf{m}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{m}_1(t,\mathbf{u}))\\ &+ \left(\mathbf{S}\mathbf{S}^{+} + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\right)\frac{1}{V}\mathbf{W}\mathbf{u}(t)\\ &- \frac{u_{\mathrm{o}}(t)}{V}\left(\mathbf{S}\mathbf{m}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{m}_1(t,\mathbf{u})\right),\\ =& \mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{q}(t,\mathbf{u})) + \frac{1}{V}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{q}(t,\mathbf{u}),\end{aligned}$$

for all $(t,\mathbf{u}) \in T \times \mathcal{U}$. The last equality results from (8). Therefore, the uniqueness assumption on (1) implies $\mathbf{q}(t,\mathbf{u}) = \mathbf{x}(t,\mathbf{u})$ for all $(t,\mathbf{u}) \in T \times \mathcal{U}$. We have $\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{m}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{m}_1(t,\mathbf{u})$, which can also be written as

$$\begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\mathbf{S}\mathbf{m}_2(t,\mathbf{u}) + \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{m}_1(t,\mathbf{u}) = \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\mathbf{x}(t,\mathbf{u}). \tag{11}$$

Substituting the conditions:

$$\begin{bmatrix}\mathbf{N}^{\mathrm{T}}\mathbf{S}\\ \mathbf{S}^{+}\mathbf{S}\end{bmatrix} = \begin{bmatrix}\mathbf{0}_{(n_x-n_r)\times n_r}\\ \mathbf{I}_{n_r}\end{bmatrix};\ \text{and}$$
$$\begin{bmatrix}\mathbf{N}^{\mathrm{T}}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\\ \mathbf{S}^{+}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\end{bmatrix} = \begin{bmatrix}\mathbf{I}_{(n_x-n_r)}\\ \mathbf{0}_{n_r\times(n_x-n_r)}\end{bmatrix}.$$

into (11) yields

$$\begin{bmatrix}\mathbf{m}_1(t,\mathbf{u})\\ \mathbf{m}_2(t,\mathbf{u})\end{bmatrix} = \begin{bmatrix}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\mathbf{x}(t,\mathbf{u}),$$

which implies $\mathbf{m}(t,\mathbf{u}) = \mathbf{n}(t,\mathbf{u})$ for all $(t,\mathbf{u},\mathbf{x}_0) \in T \times \mathcal{U} \times X_0$. Thus the solution of (6a) and (6b) is unique. □

Eq. (7b) is the orthogonal projection of $\mathbf{x}$ onto a pair of subspaces of $\mathbb{R}^{n_x}$ defined by $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ (see Fig. 4). The projections of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ are given by $\mathbf{S}\mathbf{S}^{+}\mathbf{x}$ and $\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{x}$, respectively. Since $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ are orthogonal, the projections in (7b) satisfy $[\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{n}_1]^{\mathrm{T}}\mathbf{S}\mathbf{n}_2 = [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{x}]^{\mathrm{T}}\mathbf{S}\mathbf{S}^{+}\mathbf{x} = \mathbf{0}_{n_x}$. In reaction theory, the subspaces $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ are generically referred to as the reaction variant and invariant subspaces, respectively.

The IVP in Lemma 2 is desirable because: (a) states $\mathbf{n}_1$ and $\mathbf{n}_2$ are independently described in $\mathbb{R}^{n_x-n_r}$ and $\mathbb{R}^{n_r}$, respectively; and (b) the rate function $\mathbf{r}$ appears in only n_r equations. The sparsity in the IVP (6a) and (6b) is achieved since $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$ are orthogonal, with columns of $\mathbf{N}$ spanning the subspace $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$. Thus defining $\mathbf{n}_1 \equiv \mathbf{N}^{\mathrm{T}}\mathbf{x}$ removes $\mathbf{S}\mathbf{r}$ in (6a). Similarly, defining $\mathbf{n}_2 \equiv \mathbf{S}^{+}\mathbf{x}$ replaces $\mathbf{S}\mathbf{r}$ with $\mathbf{r}$ in (6b). The dynamics of the CSTR reaction system in the reaction invariant and variant vector spaces is thus completely defined by the transformed states $\mathbf{n}_1$ and $\mathbf{n}_2$, respectively. It is instructive to highlight that although $\mathbf{n}_1$ and $\mathbf{n}_2$ individually evolve in a reduced dimensional space, the IVP (6a) and (6b) is still in $\mathbb{R}^{n_x}$, i.e., there is no dimension reduction in the transformed state space. The IVP in Lemma 2 is called a two-way decomposition which splits (1) into the space of reaction invariants and variants.

While (7a) transforms the system from the original to transformed state space, (7b) lifts it back onto the original state space. This invertible relation establishes the isomorphic property of the transformations (7a) and (7b) in Lemma 2, as required.

Note that although (6a) and (6b) provides a relatively sparse representation of (1) – with $\mathbf{r}$ removed from (6a) and stoichiometric matrix $\mathbf{S}$ replaced with $\mathbf{I}_{n_r}$ in (6b) – the structure is still dense. This is because $\mathbf{N}^{\mathrm{T}}\mathbf{W}$ and $\mathbf{S}^{+}\mathbf{W}$ in (6a) and (6b) can be dense and contribute to the complexity of CSTR reaction system in the transformed state space. The next lemma introduces additional sparsity in the reaction invariant space by projecting $\mathbf{n}_1$ onto orthogonal subspaces of $\mathbb{R}^{n_x-n_r}$.

Lemma 3. *Consider the CSTR reaction system in (1) and Lemma 2 under the following hypotheses*

(a) $\mathrm{Rank}(\mathbf{N}^{\mathrm{T}}\mathbf{W}) = n_p$,
(b) $n_x > n_r + n_p$.

If $\mathbf{M}^{+} \in \mathbb{R}^{n_p\times(n_x-n_r)}$ *is the Moore-Penrose inverse of* $\mathbf{N}^{\mathrm{T}}\mathbf{W}$ *and* $\mathbf{F} \in \mathbb{R}^{(n_x-n_r)\times(n_x-n_r-n_p)}$ *be a basis for* $\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})$, *then there exists a unique solution to the IVP*

$$\dot{\mathbf{z}}_1(t,\mathbf{u}) = -\frac{u_{\mathrm{o}}(t)}{V}\mathbf{z}_1(t,\mathbf{u}), \tag{12a}$$

$$\dot{\mathbf{z}}_2(t,\mathbf{u}) = \frac{1}{V}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{z}_2(t,\mathbf{u}), \tag{12b}$$

$$\begin{aligned}\dot{\mathbf{n}}_2(t,\mathbf{u}) = \mathbf{r}\Big(&\mathbf{k}(t),\mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u})\Big) + \frac{1}{V}\mathbf{S}^{+}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_2(t,\mathbf{u}),\end{aligned} \tag{12c}$$

satisfying the conditions

$$\begin{bmatrix}\mathbf{z}_1(t,\mathbf{u})\\ \mathbf{z}_2(t,\mathbf{u})\\ \mathbf{n}_2(t,\mathbf{u})\end{bmatrix} = \begin{bmatrix}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\\ \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\\ \mathbf{S}^{+}\end{bmatrix}\mathbf{x}(t,\mathbf{u}), \tag{13a}$$

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) =& \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}(\mathbf{N}^{\mathrm{T}}\mathbf{W})\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}),\end{aligned} \tag{13b}$$

for all $(t,\mathbf{u},\mathbf{x}_0) \in T \times \mathcal{U} \times X_0$.

Proof. Let $\mathbf{x} \in \mathbb{R}^{n_x}$ and $\mathbf{n} \in \mathbb{R}^{n_x}$ denote the unique solutions of the CSTR system in (1) and (6a) and (6b), respectively. The uniqueness of $\mathbf{x}$ and $\mathbf{n}$ are ensured by the uniqueness assumption on Model (1)

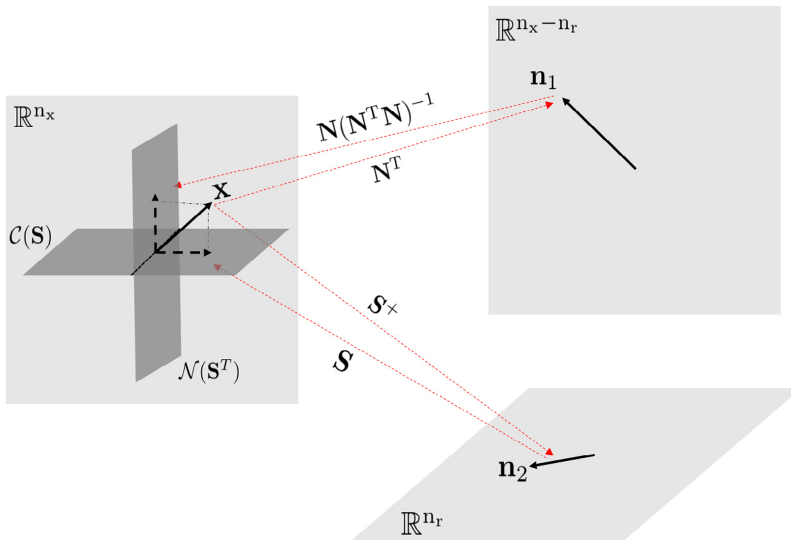

Fig. 4. A schematic of Lemma 2 showing projection of CSTR dynamics, $\mathbf{x}$, onto two orthogonal complementary subspaces defined by $\mathcal{C}(\mathbf{S})$ and $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$. The corresponding projectors are given by $\mathcal{P}_{\mathcal{C}(\mathbf{S}),\mathcal{N}(\mathbf{S}^{\mathrm{T}})} = \mathbf{S}\mathbf{S}^{+}$ and $\mathcal{P}_{\mathcal{N}(\mathbf{S}^{\mathrm{T}}),\mathcal{C}(\mathbf{S})} = \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}$, respectively. The state $\mathbf{n}$ describes the dynamics of the CSTR reaction system in the transformed state space. In this figure, while the solid black-arrow indicates a vector in space, black-dashed arrow shows its orthogonal projections. The red-dashed arrow indicates how spaces are connected, and the text over it describes the transformation required to transform between spaces.

and Lemma 2, respectively. Using the relation between $\mathbf{x}$ and $\mathbf{n}$ in (7a), define

$$\begin{bmatrix} \mathbf{z}_1(t,\mathbf{u}) \\ \mathbf{z}_2(t,\mathbf{u}) \\ \mathbf{n}_2(t,\mathbf{u}) \end{bmatrix} \equiv \begin{bmatrix} \mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}} \\ \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}} \\ \mathbf{S}^{+} \end{bmatrix} \mathbf{x}(t,\mathbf{u}) = \begin{bmatrix} \mathbf{F}^{\mathrm{T}}\mathbf{n}_1(t,\mathbf{u}) \\ \mathbf{M}^{+}\mathbf{n}_1(t,\mathbf{u}) \\ \mathbf{S}^{+}\mathbf{x}(t,\mathbf{u}) \end{bmatrix}. \tag{14}$$

For $\mathbf{N}^{\mathrm{T}}\mathbf{W} \in \mathbb{R}^{(n_x-n_r)\times n_p}$, the pair $\mathcal{C}(\mathbf{N}^{\mathrm{T}}\mathbf{W}), \mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})$ forms a pair of orthogonal complementary subspaces of $\mathbb{R}^{n_x-n_r}$. Thus any $\mathbf{n}_1 \in \mathbb{R}^{n_x-n_r}$ can be decomposed as

$$\mathbf{n}_1(t,\mathbf{u}) = \mathcal{P}_{\mathcal{C}(\mathbf{N}^{\mathrm{T}}\mathbf{W}),\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})}\mathbf{n}_1(t,\mathbf{u}) + \mathcal{P}_{\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N}),\mathcal{C}(\mathbf{N}^{\mathrm{T}}\mathbf{W})}\mathbf{n}_1(t,\mathbf{u}). \tag{15}$$

Recall that $\mathbf{N}^{\mathrm{T}}\mathbf{W}$ is full-column rank from hypothesis (a) and $\mathbf{F}$ exists from hypothesis (b), which implies that $\dim(\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})) \geqslant 1$, and is also full-column rank by construction. Thus the projectors in (15) can be written as

$$\begin{aligned} \mathbf{n}_1(t,\mathbf{u}) = {} & (\mathbf{N}^{\mathrm{T}}\mathbf{W})[(\mathbf{N}^{\mathrm{T}}\mathbf{W})^{\mathrm{T}}(\mathbf{N}^{\mathrm{T}}\mathbf{W})]^{-1}(\mathbf{N}^{\mathrm{T}}\mathbf{W})^{\mathrm{T}}\mathbf{n}_1(t,\mathbf{u}) \\ & + \mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{n}_1(t,\mathbf{u}). \end{aligned} \tag{16}$$

For a full-column rank matrix $\mathbf{N}^{\mathrm{T}}\mathbf{W}$, its Moore Penrose inverse, $\mathbf{M}^{+}$, is given by $\mathbf{M}^{+} = [(\mathbf{N}^{\mathrm{T}}\mathbf{W})^{\mathrm{T}}(\mathbf{N}^{\mathrm{T}}\mathbf{W})]^{-1}(\mathbf{N}^{\mathrm{T}}\mathbf{W})^{\mathrm{T}}$. Thus substituting $\mathbf{M}^{+}$ into (16) yields

$$\begin{aligned} \mathbf{n}_1(t,\mathbf{u}) &= (\mathbf{N}^{\mathrm{T}}\mathbf{W})\mathbf{M}^{+}\mathbf{n}_1(t,\mathbf{u}) + \mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{n}_1(t,\mathbf{u}), \\ &= (\mathbf{N}^{\mathrm{T}}\mathbf{W})\mathbf{z}_2(t,\mathbf{u}) + \mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}). \end{aligned} \tag{17}$$

The last equality is from the relation $\mathbf{z}_1(t,\mathbf{u}) = \mathbf{F}^{\mathrm{T}}\mathbf{n}_1(t,\mathbf{u})$ and $\mathbf{z}_2(t,\mathbf{u}) = \mathbf{M}^{+}\mathbf{n}_1(t,\mathbf{u})$ defined in (14). Finally, (17) gives the decomposition of $\mathbf{n}_1 \in \mathbb{R}^{n_x-n_r}$ into $\mathbf{z}_1 \in \mathbb{R}^{n_x-n_r-n_p}$ and $\mathbf{z}_2 \in \mathbb{R}^{n_p}$. Now since (7b) describes the decomposition of $\mathbf{x}$ in terms of $\mathbf{n}$, substituting (17) into (7b) yields

$$\begin{aligned} \mathbf{x}(t,\mathbf{u}) = {} & \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{n}_1(t,\mathbf{u}), \\ = {} & \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}(\mathbf{N}^{\mathrm{T}}\mathbf{W})\mathbf{z}_2(t,\mathbf{u}) \\ & + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}), \end{aligned} \tag{18}$$

which is the same as Eq. (13b). Differentiating (14) and substituting the conditions $\mathbf{F}^{\mathrm{T}}(\mathbf{N}^{\mathrm{T}}\mathbf{W}) = \mathbf{0}_{(n_x-n_r-n_p)\times n_p}, \mathbf{M}^{+}(\mathbf{N}^{\mathrm{T}}\mathbf{W}) = \mathbf{I}_{n_p}$ along with $\mathbf{N}^{\mathrm{T}}\mathbf{S} = \mathbf{0}_{(n_x-n_r)\times n_r}$ and $\mathbf{S}^{+}\mathbf{S} = \mathbf{I}_{n_r}$ from Lemma 2, we get

$$\begin{aligned} \begin{bmatrix} \dot{\mathbf{z}}_1(t,\mathbf{u}) \\ \dot{\mathbf{z}}_2(t,\mathbf{u}) \\ \dot{\mathbf{n}}_2(t,\mathbf{u}) \end{bmatrix} &= \begin{bmatrix} \mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}} \\ \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}} \\ \mathbf{S}^{+} \end{bmatrix} \dot{\mathbf{x}}(t,\mathbf{u}) \\ &= \begin{bmatrix} \mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}} \\ \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}} \\ \mathbf{S}^{+} \end{bmatrix} \left(\mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{x}(t,\mathbf{u}) \right), \\ &= \begin{bmatrix} -\frac{u_{\mathrm{o}}(t)}{V}\mathbf{z}_1(t,\mathbf{u}) \\ \frac{1}{V}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{z}_2(t,\mathbf{u}) \\ \mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u})) + \frac{1}{V}\mathbf{S}^{+}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_{\mathrm{o}}(t)}{V}\mathbf{n}_2(t,\mathbf{u}) \end{bmatrix}. \end{aligned} \tag{19}$$

Thus substituting (18) into (19) yields (12a), (12b), (12c). This guarantees the existence of at least one solution to the IVP (12a), (12b), (12c) satisfying (13a) and (13b). Finally, the uniqueness proof is similar to the proof given in Lemma 2, and is not included here for the sake of brevity. □

Lemma 3 considers projection of state $\mathbf{n}_1 \in \mathbb{R}^{n_x-n_r}$ onto the subspaces $\mathcal{C}(\mathbf{N}^{\mathrm{T}}\mathbf{W})$ and $\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})$ (see Fig. 5 for illustration). Now for the pair of orthogonal complementary subspaces $\mathcal{C}(\mathbf{N}^{\mathrm{T}}\mathbf{W}), \mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})$, the columns of $\mathbf{F}$ span the subspace $\mathcal{N}(\mathbf{W}^{\mathrm{T}}\mathbf{N})$. Thus defining $\mathbf{z}_1 \equiv \mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ removes the influence of inlet flow rates in (12a). Similarly, defining $\mathbf{z}_2 \equiv \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ turns $\mathbf{W}\mathbf{u}_{\mathrm{i}}$ into $\mathbf{u}_{\mathrm{i}}$ in (12b).

Physically, if $\mathbf{n}_1$ describes the dynamics of the CSTR reaction system in the reaction invariant space, $\mathbf{z}_1$ and $\mathbf{z}_2$ describe the system dynamics in the reaction and flow rate invariant space and flow rate variant space, respectively. Note that $\mathbf{n}_2$ in (12c) still describes the dynamics in the reaction variant space, similar to Lemma 2, except that it is completely expressed in terms of $\mathbf{z}_1, \mathbf{z}_2$ and $\mathbf{n}_2$.

Eq. (13b) describes the decomposition of $\mathbf{x}$ into the sum of its projections onto three underlying subspaces - $\mathcal{C}(\mathbf{S})$, $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W})$ and $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$, see Appendix A. Further, Appendix A proves that while the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ is

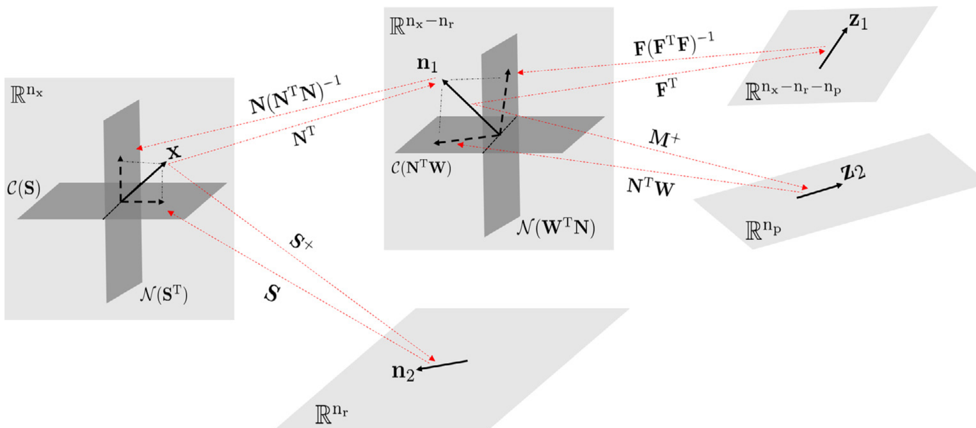

Fig. 5. A schematic showing the transformation in Lemma 3 splitting the reaction invariant space described by $\mathbf{n}_1$ into reaction and flow rate invariant space and flow rate variant space. The decomposition is done by projecting $\mathbf{n}_1$ onto the subspaces $\mathcal{C}(\mathbf{N}^T\mathbf{W})$ and $\mathcal{N}(\mathbf{W}^T\mathbf{N})$ using the projectors $\mathcal{P}_{\mathcal{N}(\mathbf{W}^T\mathbf{N}),\mathcal{C}(\mathbf{N}^T\mathbf{W})} = \mathbf{F}(\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T$ and $\mathcal{P}_{\mathcal{C}(\mathbf{C}^T\mathbf{W}),\mathcal{N}(\mathbf{W}^T\mathbf{N})} = \mathbf{N}^T\mathbf{W}\mathbf{M}^+$. The dynamics of the CSTR system in the reaction and flow rate invariant space and flow rate variant space are described by $\mathbf{z}_1$ and $\mathbf{z}_2$, respectively. In this figure, while the solid black-arrow indicates a vector in space, black-dashed arrow shows its orthogonal projections. The red-dashed arrow indicates how spaces are connected, and the text over it describes the transformation required to transform between spaces.

orthogonal, as in Lemma 2, the projection of $\mathbf{x}$ onto subspaces $\mathcal{C}(\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{N}^T\mathbf{W})$ and $\mathcal{C}(\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F})$ are oblique and along $\mathcal{N}(\mathbf{M}^+\mathbf{N}^T)$ and $\mathcal{N}((\mathbf{F}^T\mathbf{F})^{-1}\mathbf{F}^T\mathbf{N}^T)$, respectively. Thus in contrast to Lemma 2, where $\mathbf{x}$ is decomposed into two orthogonal projections, Lemma 3 decomposes $\mathbf{x}$ into 1 orthogonal and 2 oblique projections. From (13b), we also get the relation $[\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^T\mathbf{F})^{-1}\mathbf{z}_1]^T\mathbf{S}\mathbf{n}_2 = \mathbf{0}_{n_x}$ This suggests that in (13b) only $\mathcal{C}(\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F})$ is orthogonal to the subspace $\mathcal{C}(\mathbf{S})$.

Remark 1. In Lemma 3, the hypothesis (a) may not hold for all CSTR reaction systems. In such situations, Theorem 1 can be applied to the IVP in Lemma 2 such that the resulting system satisfies hypothesis (a).

The pair of Eqs. (13a) and (13b) establishes the isomorphic property of the transformation, as required in this paper. Note that the CSTR reaction system in the transformed state space described by Lemmas 2 and 3 are independent of each other and can thus be independently simulated. In terms of sparsity, the IVP (12a), (12b), (12c) is sparser than IVP (6a) and (6b). This is because IVP (12a) and (12b) does not involve computations involving the matrix $\mathbf{N}^T\mathbf{W}$. Finally, note that although the CSTR reaction system in Eqs. (12a) and (12b) is sparsely represented in the reaction invariant space, it is still possible to introduce additional sparsity in the reaction variant space by removing matrix $\mathbf{S}^+\mathbf{W}$ from (12c).

Theorem 2. *Consider the CSTR reaction system in (1) and Lemma 3. If the matrices* $\mathbf{N}$ *and* $\mathbf{S}^+$ *are defined as in Lemma 2, and* $\mathbf{F}$ *and* $\mathbf{M}^+$ *as given in Lemma 3 then there exists a unique solution to the IVP*

$$\dot{\mathbf{z}}_1(t,\mathbf{u}) = -\frac{u_o(t)}{V}\mathbf{z}_1(t,\mathbf{u}), \tag{20a}$$

$$\dot{\mathbf{z}}_2(t,\mathbf{u}) = \frac{1}{V}\mathbf{u}_i(t) - \frac{u_o(t)}{V}\mathbf{z}_2(t,\mathbf{u}), \tag{20b}$$

$$\dot{\mathbf{z}}_3(t,\mathbf{u}) = \mathbf{r}\left(\mathbf{k}(t), \mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^T\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u})\right) - \frac{u_o(t)}{V}\mathbf{z}_3(t,\mathbf{u}), \tag{20c}$$

satisfying the conditions

$$\mathbf{z}(t,\mathbf{u}) \equiv \begin{bmatrix} \mathbf{z}_1(t,\mathbf{u}) \\ \mathbf{z}_2(t,\mathbf{u}) \\ \mathbf{z}_3(t,\mathbf{u}) \end{bmatrix} = \begin{bmatrix} \mathbf{F}^T\mathbf{N}^T \\ \mathbf{M}^+\mathbf{N}^T \\ \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^T) \end{bmatrix}\mathbf{x}(t,\mathbf{u}), \tag{21a}$$

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^T\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}), \tag{21b}$$

for all $(t,\mathbf{u},\mathbf{x}_0) \in T \times \mathcal{U} \times X_0$.

Proof. Let $\mathbf{x} \in \mathbb{R}^{n_x}$ be the unique solution of the CSTR reaction system in (1). Let $\mathbf{z}_1, \mathbf{z}_2$ and $\mathbf{n}_2$ be the unique solution of the IVP in Lemma 3. The uniqueness of these solutions is established by the uniqueness assumption on Eq. (1) and Lemma 3. Note that $\mathbf{z}_1, \mathbf{z}_2$ obtained by solving (12a) and (12b) are the same as the solution obtained by solving (20a) and (20b). This is because the IVPs in (12a) and (12b) and (20a) and (20b) are identical. Thus from Lemma 3, the conditions $\mathbf{z}_1(t,\mathbf{u}) = \mathbf{F}^T\mathbf{N}^T\mathbf{x}(t,\mathbf{u})$ and $\mathbf{z}_2(t,\mathbf{u}) = \mathbf{M}^+\mathbf{N}^T\mathbf{x}(t,\mathbf{u})$ also hold true under the hypotheses of Theorem 2.

Since $\mathcal{C}(\mathbf{S}), \mathcal{N}(\mathbf{S}^T)$ forms a pair of orthogonal complementary subspaces of $\mathbb{R}^{n_x}$, for orthogonal projection onto $\mathcal{N}(\mathbf{S}^T)$, the projector can be defined as $(\mathbf{I}_{n_x} - \mathbf{S}\mathbf{S}^+)$, where $\mathbf{S}\mathbf{S}^+$ is the projector for orthogonal projection onto $\mathcal{C}(\mathbf{S})$. Since the columns of the full-column rank matrix, $\mathbf{N}$, span $\mathcal{N}(\mathbf{S}^T)$, the projection onto $\mathcal{N}(\mathbf{S}^T)$ is also defined by the projector $\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{N}^T$. From Definition 2, since the projection onto $\mathcal{N}(\mathbf{S}^T)$ along $\mathcal{C}(\mathbf{S})$ is unique, we have

$$\mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{N}^T = (\mathbf{I}_{n_x} - \mathbf{S}\mathbf{S}^+). \tag{22}$$

From Lemma 3, using (13b), $\mathbf{x}(t,\mathbf{u}) \in \mathbb{R}^{n_x}$ can be written in terms of $\mathbf{z}_1, \mathbf{z}_2$ and $\mathbf{n}_2$ as follows

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) = {} & \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + (\mathbf{I}_{n_x} - \mathbf{S}\mathbf{S}^+)\mathbf{W}\mathbf{z}_2(t,\mathbf{u}) \\ & + \mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^T\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}),\end{aligned} \tag{23}$$

where (23) uses the result in (22). Substituting $\mathbf{n}_2(t,\mathbf{u}) = \mathbf{S}^+\mathbf{x}(t,\mathbf{u})$ from (13a) into (23) yields

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) &= \mathbf{S}\mathbf{S}^+\mathbf{x}(t,\mathbf{u}) + (\mathbf{I}_{n_x} - \mathbf{S}\mathbf{S}^+)\mathbf{W}\mathbf{z}_2(t,\mathbf{u}) \\ &\quad + \mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}\left(\mathbf{F}^T\mathbf{F}\right)^{-1}\mathbf{z}_1(t,\mathbf{u}), \\ &= \mathbf{S}\mathbf{S}^+(\mathbf{x}(t,\mathbf{u}) - \mathbf{W}\mathbf{z}_2(t,\mathbf{u})) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) \\ &\quad + \mathbf{N}(\mathbf{N}^T\mathbf{N})^{-1}\mathbf{F}\left(\mathbf{F}^T\mathbf{F}\right)^{-1}\mathbf{z}_1(t,\mathbf{u}).\end{aligned} \tag{24}$$

Substituting $\mathbf{z}_2(t,\mathbf{u}) = \mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$ only into the first term in (24) gives

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) =& \mathbf{S}\mathbf{S}^+\left(\mathbf{x}(t,\mathbf{u}) - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})\right) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}),\\ =& \mathbf{S}\mathbf{S}^+\left(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\right)\mathbf{x}(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}).\end{aligned} \tag{25}$$

Now define

$$\mathbf{z}_3(t,\mathbf{u}) \equiv \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\mathbf{x}(t,\mathbf{u}). \tag{26}$$

Substituting $\mathbf{z}_3(t,\mathbf{u})$ defined in (26) into (25) gives

$$\mathbf{x}(t,\mathbf{u}) = \mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}), \tag{27}$$

which is the same as (21b). Now differentiating $\mathbf{z}_1(t,\mathbf{u}) = \mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$ and $\mathbf{z}_2 = \mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})$ gives (20a) and (20b), respectively (see Lemma 3); and differentiating (26) yields

$$\begin{aligned}\dot{\mathbf{z}}_3(t,\mathbf{u}) =& \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\dot{\mathbf{x}}(t,\mathbf{u}),\\ =& \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\mathbf{S}\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u}))\\ &+ \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\frac{1}{V}\mathbf{W}\mathbf{u}_{\mathrm{i}}(t)\\ &- \frac{u_0(t)}{V}\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\mathbf{x}(t,\mathbf{u}),\\ =& (\mathbf{S}^+\mathbf{S} - \mathbf{S}^+\mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{S})\mathbf{r}(\mathbf{k}(t),\mathbf{x}(t,\mathbf{u}))\\ &+ (\mathbf{S}^+\mathbf{W} - \mathbf{S}^+\mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{W})\frac{1}{V}\mathbf{u}_{\mathrm{i}}(t)\\ &- \frac{u_0(t)}{V}\mathbf{z}_3(t,\mathbf{u}).\end{aligned} \tag{28}$$

Substituting (27) into (28) yields

$$\begin{aligned}\dot{\mathbf{z}}_3(t,\mathbf{u}) =& (\mathbf{S}^+\mathbf{S} - \mathbf{S}^+\mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{S})\mathbf{r}(\mathbf{k}(t),\mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}))\\ &+ (\mathbf{S}^+\mathbf{W} - \mathbf{S}^+\mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{W})\frac{1}{V}\mathbf{u}_{\mathrm{i}}(t) - \frac{u_0(t)}{V}\mathbf{z}_3(t,\mathbf{u}).\end{aligned} \tag{29}$$

Recall that since the columns of $\mathbf{N}$ form a basis for $\mathcal{N}(\mathbf{S}^{\mathrm{T}})$, and $\mathbf{S}^+$ and $\mathbf{M}^+$ are Moore-Penrose inverses of $\mathbf{S}$ and $\mathbf{N}^{\mathrm{T}}\mathbf{W}$, respectively, we have $\mathbf{N}^{\mathrm{T}}\mathbf{S} = \mathbf{0}_{(n_x-n_r)\times n_r}, \mathbf{S}^+\mathbf{S} = \mathbf{I}_{n_r}$, and $\mathbf{M}^+\mathbf{N}^{\mathrm{T}}\mathbf{W} = \mathbf{I}_{n_p}$. Substituting these conditions into (29) yields

$$\begin{aligned}\dot{\mathbf{z}}_3(t,\mathbf{u}) =& \mathbf{r}\left(\mathbf{k}(t),\mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1} \times \mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u})\right)\\ &- \frac{u_0(t)}{V}\mathbf{z}_3(t,\mathbf{u}).\end{aligned} \tag{30}$$

This guarantees the existence of at least one solution to the IVP (20a), (20b), (20c). Again, the uniqueness of the solution can be proved as given in Lemma 2. □

Theorem 2 redefines the dynamics of the CSTR system in the reaction variant space by modifying (12c) in Lemma 3. In (12c), $\mathbf{S}^+\mathbf{W}\mathbf{u}_{\mathrm{i}}(t)$ is potentially non-zero since $\mathbf{W}\mathbf{u}_{\mathrm{i}}(t)$ is not necessarily an element of the null-space of $\mathbf{S}^+$, i.e., $\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) \notin \mathcal{N}(\mathbf{S}^+)$. Theorem 2 addresses this by replacing the Moore-Penrose inverse, $\mathbf{S}^+$ with a $\{1,2\}$-inverse, $\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})$, such that $\mathbf{W}\mathbf{u}_{\mathrm{i}}(t)$ is now an element of $\mathcal{N}(\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}))$. Appendix B shows that $\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})$ and $\mathbf{S}$ are indeed $\{1,2\}$-inverses of each other, and $\mathbf{W}\mathbf{u}_{\mathrm{i}}(t) \in \mathcal{N}(\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}))$. Thus defining $\mathbf{z}_3 \equiv \mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}})\mathbf{x}$ removes the influence of flow rates in (12c) with new reaction variant space dynamics described by (20c). As in Lemma 3, the states $\mathbf{z}_1, \mathbf{z}_2$ in (20a) and (20b) continue to model the dynamics of the CSTR system in the reaction invariant space. An illustration of Theorem 2 is given in Fig. 6.

Eq. (21b) describes the solution to the CSTR reaction system, $\mathbf{x}$, as a sum of its projections onto 3 subspaces of $\mathbb{R}^{n_x}$ – $\mathcal{C}(\mathbf{S}); \mathcal{C}(\mathbf{W})$; and $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$. This claim is supported by the proof given in Appendix C. Appendix C further shows that unlike Lemmas 2 and 3, the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ in Theorem 2 is not orthogonal, but oblique along $\mathcal{N}(\mathbf{S}^+(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}))$. Further, the projections of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{W})$ and $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$ are also oblique, and along $\mathcal{N}(\mathbf{M}^+\mathbf{N}^{\mathrm{T}})$ and $\mathcal{N}((\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}})$, respectively. Thus (21b) describes $\mathbf{x}$ uniquely in terms of oblique projections onto underlying subspaces of $\mathbb{R}^{n_x}$. Finally, notice that of the three subspaces onto which $\mathbf{x}$ is projected in (21b) only $\mathcal{C}(\mathbf{S})$ is orthogonal to $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$, such that $[\mathbf{S}\mathbf{z}_3]^{\mathrm{T}}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}\mathbf{z}_1 = \mathbf{0}_{n_x}$. In (20a), (20b), (20c), $\mathbf{z}_1$ models the influence of the initial condition in the reaction and flow rate invariant space; $\mathbf{z}_2$ models the influence of flow rates in the flow rate variant space; and $\mathbf{z}_3$ models the influence of reaction in the reaction variant space.

Compared to Lemmas 2 and 3, the choice of oblique projections onto subspaces of $\mathbb{R}^{n_x}$ in Theorem 2 yields the sparsest representation of the dynamics of the CSTR reaction system in the transformed state space. Finally, the IVP in Theorem 2 is decoupled

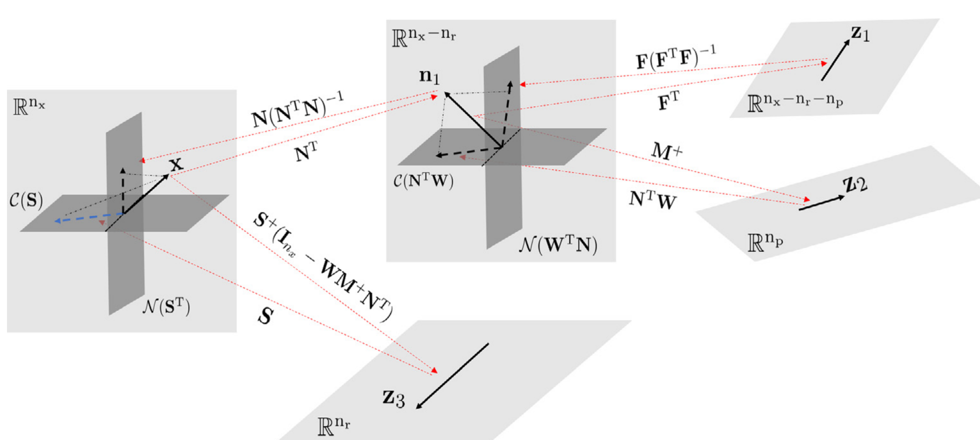

Fig. 6. Theorem 2 refines the reaction variant space described by (12c) in Lemma 3 by removing the influence of flow rates. This is done by choosing an oblique projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ along $\mathcal{N}(\mathbf{S}^+[\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^+\mathbf{N}^{\mathrm{T}}])$. With the new projection, the dynamics of the CSTR system in the modified reaction variant space is described by $\mathbf{z}_3$. In this figure, while the solid black-arrow indicates a vector in space, black-dashed arrow shows its orthogonal projection and dashed blue-arrow its oblique projection. The red-dashed arrow indicates how spaces are connected, and the text over it describes the transformation required to transform between spaces.

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from the IVPs in Lemma 2 and Lemma 3, and therefore can also be independently simulated. Note that Theorem 2 does not make any explicit assumptions on the rate law $\mathbf{r}$ or the input flow rate profile $\mathbf{u}_i$. Thus Theorem 2 is general, and applicable to a wide-class of CSTR systems described by (1) and operating under different flow conditions.

4. Conclusions

A new linear transformation is presented in this paper to obtain a sparse representation of CSTR reaction systems in a transformed state space. The proposed transformation creates sparsity by obliquely projecting molar concentration vectors describing a CSTR onto three special non-orthogonal complementary subspaces defined in the original state space. Physically, the subspaces corresponds to the space of reaction variants, flow rate variants, and reaction and flow rate invariants. Further, the developed transformation is invertible, thereby allowing to obtain system representations in both original and transformed state space. The motivation for developing an invertible, sparse, and linear transformation in this paper is to be able to compute tight interval enclosures for CSTR reaction systems using direct and indirect-bounding methods proposed in the second and third papers in this series (Tulsyan and Barton, 2017a,b).

Acknowledgments

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Appendix A. Projections in Lemma 3

Consider (13b) written completely in terms of $\mathbf{x}$, we get

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) =& \mathbf{S}\mathbf{n}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{z}_2(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u}),\\ =& \mathbf{S}\mathbf{S}^{+}\mathbf{x}(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u}).\end{aligned} \tag{A.1}$$

The state $\mathbf{x}$ in (A.1) is described as the sum of three terms. We show that these terms correspond to the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S}), \mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W})$ and $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$, respectively. Further, while $\mathbf{x}$ has an orthogonal projection onto $\mathcal{C}(\mathbf{S})$, the projection onto $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W})$ is along $\mathcal{N}(\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$ and projection onto $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$ is along $\mathcal{N}((\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}})$. We prove this claim next.

1. Since $\mathbf{S}^{+}$ is a Moore-Penrose inverse of $\mathbf{S}$, from Corollary 1, $\mathbf{S}\mathbf{S}^{+}\mathbf{x}$ describes the orthogonal projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$.
2. To show $\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ describes the projection of $\mathbf{x}$ onto the subspace $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W})$ along $\mathcal{N}(\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$, from Lemma 1, we only need to prove that $\mathbf{A}_1 \equiv \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}$ and $\mathbf{B}_1 \equiv \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}$ are $\{1,2\}$-inverses of each other. We prove this next.
   (a) To show $\mathbf{A}_1\mathbf{B}_1\mathbf{A}_1 = \mathbf{A}_1$:
   $$\begin{aligned}\mathbf{A}_1\mathbf{B}_1\mathbf{A}_1 &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}][\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}],\\ &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}][\mathbf{M}^{+}][\mathbf{N}^{\mathrm{T}}\mathbf{W}],\\ &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}] = \mathbf{A}_1.\end{aligned}$$
   (b) To show $\mathbf{B}_1\mathbf{A}_1\mathbf{B}_1 = \mathbf{B}_1$:
   $$\begin{aligned}\mathbf{B}_1\mathbf{A}_1\mathbf{B}_1 &= [\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}][\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{N}^{\mathrm{T}}\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}],\\ &= [\mathbf{M}^{+}][\mathbf{N}^{\mathrm{T}}\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}],\\ &= [\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}] = \mathbf{B}_1.\end{aligned}$$
   In (a) and (b), we use the fact that $\mathbf{N}^{\mathrm{T}}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1} = \mathbf{I}_{(n_x-n_r)}$ and $\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{W} = \mathbf{I}_{n_p}$. This proves that $\mathbf{A}_1, \mathbf{B}_1$ are $\{1,2\}$-inverses of each other.
3. Similarly, to show that $\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ describes the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$ along $\mathcal{N}((\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}})$, we only need to show that $\mathbf{A}_2 \equiv \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}$ and $\mathbf{B}_2 \equiv (\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}$ are $\{1,2\}$-inverses of each other. We prove this next.
   (a) To show $\mathbf{A}_2\mathbf{B}_2\mathbf{A}_2 = \mathbf{A}_2$:
   $$\begin{aligned}\mathbf{A}_2\mathbf{B}_2\mathbf{A}_2 &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}][(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}][\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}],\\ &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}][(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}][\mathbf{F}],\\ &= [\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}] = \mathbf{A}_2.\end{aligned}$$
   (b) To show $\mathbf{B}_2\mathbf{A}_2\mathbf{B}_2 = \mathbf{B}_2$:
   $$\begin{aligned}\mathbf{B}_2\mathbf{A}_2\mathbf{B}_2 &= [(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}][\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}][(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}],\\ &= [(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}][\mathbf{F}][(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}],\\ &= [(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}][\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}] = \mathbf{B}_2.\end{aligned}$$
   In (a) and (b), we use the fact that $\mathbf{N}^{\mathrm{T}}\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1} = \mathbf{I}_{(n_x-n_r)}$ and $(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{F} = \mathbf{I}_{(n_x-n_r-n_p)}$. This proves that $\mathbf{A}_2, \mathbf{B}_2$ are $\{1,2\}$-inverses of each other.

This completes the proof. □

Appendix B. $\{1,2\}$-inverse of S

We claim that $\mathbf{A}_3 \equiv \mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$ and $\mathbf{S}$ are $\{1,2\}$-inverses of each other. To prove this, we need to show that $\mathbf{A}_3$ and $\mathbf{S}$ satisfy (a) $\mathbf{A}_3\mathbf{S}\mathbf{A}_3 = \mathbf{A}_3$ and (b) $\mathbf{S}\mathbf{A}_3\mathbf{S} = \mathbf{S}$.

1. To show $\mathbf{A}_3\mathbf{S}\mathbf{A}_3 = \mathbf{A}_3$:
   $$\begin{aligned}\mathbf{A}_3\mathbf{S}\mathbf{A}_3 &= [\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})][\mathbf{S}][\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})],\\ &= [\mathbf{S}^{+}(\mathbf{S} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{S})][\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})],\\ &= [\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})] = \mathbf{A}_3.\end{aligned}$$
2. To show $\mathbf{S}\mathbf{A}_3\mathbf{S} = \mathbf{S}$:
   $$\begin{aligned}\mathbf{S}\mathbf{A}_3\mathbf{S} &= [\mathbf{S}][\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})][\mathbf{S}],\\ &= [\mathbf{S}][\mathbf{S}^{+}(\mathbf{S} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{S})],\\ &= \mathbf{S}.\end{aligned}$$

Here we use the fact that $\mathbf{N}^{\mathrm{T}}\mathbf{S} = \mathbf{0}_{(n_x-n_r)\times n_r}$ and $\mathbf{S}^{+}\mathbf{S} = \mathbf{I}_{n_r}$. This proves that $\mathbf{A}_3$ and $\mathbf{S}$ are $\{1,2\}$-inverses. □

Appendix C. Projections in Theorem 2

Consider (21b) written completely in terms of $\mathbf{x}$, we get

$$\begin{aligned}\mathbf{x}(t,\mathbf{u}) =& \mathbf{S}\mathbf{z}_3(t,\mathbf{u}) + \mathbf{W}\mathbf{z}_2(t,\mathbf{u}) + \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{z}_1(t,\mathbf{u})),\\ =& \mathbf{S}\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})\mathbf{x}(t,\mathbf{u}) + \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})\\ &+ \mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}(t,\mathbf{u})).\end{aligned} \tag{C.1}$$

The state $\mathbf{x}$ in (C.1) is described as the sum of three terms. We show that the terms correspond to the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S}), \mathcal{C}(\mathbf{W})$ and

$\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$, respectively. We also show in (C.1), the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ is along $\mathcal{N}(\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}))$, and projections onto $\mathcal{C}(\mathbf{W})$ and $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$ are along $\mathcal{N}(\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$ and $\mathcal{N}((\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}})$, respectively. We prove this claim.

1. To show that $\mathbf{S}\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})\mathbf{x}$ is the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{S})$ along $\mathcal{N}(\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}))$, from Lemma 1, we only need to prove that $\mathbf{S}$ and $\mathbf{S}^{+}(\mathbf{I}_{n_x} - \mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$ are $\{1,2\}$-inverses of each other. See Appendix B for proof.
2. To show that $\mathbf{W}\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ is the projection of $\mathbf{x}$ onto the subspace $\mathcal{C}(\mathbf{W})$ along $\mathcal{N}(\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}})$, from Lemma 1, we only need to prove that $\mathbf{A}_4 \equiv \mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}$ and $\mathbf{W}$ are $\{1,2\}$-inverses of each other. We prove this next.
   (a) To show $\mathbf{A}_4\mathbf{W}\mathbf{A}_4 = \mathbf{A}_4$:
   $$\begin{aligned}\mathbf{A}_4\mathbf{W}\mathbf{A}_4 &= [\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}][\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}],\\ &= [\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}],\\ &= [\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}] = \mathbf{A}_4.\end{aligned}$$
   (b) To show $\mathbf{W}\mathbf{A}_4\mathbf{W} = \mathbf{W}$:
   $$\begin{aligned}\mathbf{W}\mathbf{A}_4\mathbf{W} &= [\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}][\mathbf{W}],\\ &= [\mathbf{W}][\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{W}],\\ &= \mathbf{W}.\end{aligned}$$
   In (a) and (b), we use the fact that $\mathbf{M}^{+}\mathbf{N}^{\mathrm{T}}\mathbf{W} = \mathbf{I}_{n_p}$. This proves that $\mathbf{A}_4$ and $\mathbf{W}$ are $\{1,2\}$-inverses.
3. To show that $\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}\mathbf{x}$ is the projection of $\mathbf{x}$ onto $\mathcal{C}(\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F})$ along the subspace $\mathcal{N}((\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}})$, from Lemma 1, we need to prove $\mathbf{N}(\mathbf{N}^{\mathrm{T}}\mathbf{N})^{-1}\mathbf{F}$ and $(\mathbf{F}^{\mathrm{T}}\mathbf{F})^{-1}\mathbf{F}^{\mathrm{T}}\mathbf{N}^{\mathrm{T}}$ are $\{1,2\}$-inverses. This result is proved in Appendix A.3

This completes the proof. □

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