



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



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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

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

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}_i and u_o are the input and output flow rates, respectively. A detailed description of CSTR systems is given

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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

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 $[\mathbf{S}\mathbf{W}]$ 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 $[\mathbf{S}\mathbf{W}\mathbf{x}_0]$, 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 transformation 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}^T (or \mathbf{M}^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 $\text{Rank}(\mathbf{A})$, column space as $\mathcal{C}(\mathbf{A}) = \{\mathbf{y} \in \mathbb{R}^m : \mathbf{y} = \mathbf{A}\mathbf{x} \text{ for some } \mathbf{x} \in \mathbb{R}^n\}$ and null space as $\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}\mathbf{x} = \mathbf{0}_{m \times 1}\}$. 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) $\mathbf{A}\mathbf{A}^+\mathbf{A} = \mathbf{A}$; (ii) $\mathbf{A}^+\mathbf{A}\mathbf{A}^+ = \mathbf{A}^+$; (iii) $(\mathbf{A}\mathbf{A}^+)^T = \mathbf{A}\mathbf{A}^+$; and (iv) $(\mathbf{A}^+\mathbf{A})^T = \mathbf{A}^+\mathbf{A}$. 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 $\mathbf{v} : T \rightarrow \mathbb{R}^n$ is denoted by $L^1(T, \mathbb{R}^n) \equiv \{\{\mathbf{v} : T \rightarrow \mathbb{R}^n\} : \int_T |\mathbf{v}_i| < +\infty, \forall i\}$, 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), $\mathbf{u}_i(t) \in D_{u_i}$ be the input flow rates and $u_o(t) \in D_{u_o}$ denote the output flow rates. Defining $\mathbf{u}(t) \equiv (\mathbf{k}(t), \mathbf{u}_i(t), u_o(t)) \in U \equiv D_k \times D_{u_i} \times D_{u_o}$, let the set of time-varying inputs/parameters be denoted in a compact notation as

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

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.

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