

Hamiltonian Feedback Design for Mass Action Law Chemical Reaction Networks

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Abstract: A special polynomial state feedback structure is proposed for open chemical reaction networks obeying the mass action law (MAL-CRNs) that stabilizes them for any of their admissible positive set of parameters. The proposed feedback makes the closed-loop system a reversible CRN that enables a generalized Hamiltonian description assuming that their number of reversible reactions is less or equal that the number of species. The design is based on solving a mixed integer linear optimization problem (MILP).

A simple example is used to illustrate the basic concepts and the design method.

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1. INTRODUCTION

Process systems are often highly nonlinear with a wide range of nonlinear phenomena that make their dynamic analysis and control a challenging task. At the same time, they have a characteristic nonlinear structure that is determined by the laws of thermodynamics, that opens the possibility to apply physically inspired special approaches (e.g. Lagrangian or Hamiltonian methods [19], [11]) for their dynamic analysis and controller design.

The major sources of the nonlinearity in process systems are the chemical reactions. A separate special positive nonlinear system class, the chemical reaction networks (CRN) with mass action law (MAL) kinetics is suitable to characterize their nonlinear dynamic behavior. It has been shown that the MAL CRN system class is a wide class, that is often used to model complex biological mechanisms [18], or even models of application fields far from chemistry such as mechanical or electrical systems [22]. The increasing interest for this field is shown by numerous surveys and tutorials in different journals [25], [5], [2].

Motivated by the fact that MAL CRNs exhibit all the qualitative dynamic behavior patterns (e.g. oscillations, chaotic behavior, stable and unstable equilibrium points) that a lumped process system with smooth nonlinearities may show, the possibility of deriving a MAL CRN representation i.e. a model in MAL CRN form for them has been proposed recently [15].

The idea of constructing a Hamiltonian description of process systems is not new [13], but it has become popular

in recent years (see e.g. [21], [16]). However, no feasible way of constructing a Hamiltonian description of a general lumped process system has been found so far, but only for some special cases (e.g. isothermal, one balance volume, constant mass holdup etc). For the special case of reversible chemical reaction networks it was shown [20] that they admit a generalized Hamiltonian description if the number of reversible reactions is less or equal than the number of species in the system. Very recently, a port-Hamiltonian description of close complex balanced chemical reaction networks have also been proposed [24].

The aim of this paper is to propose a method for kinetic nonlinear feedback design to the simplest case of a lumped process system that enables to have a generalized Hamiltonian structure for the closed-loop system. The basic idea is similar to the one applied earlier to general polynomial systems (see e.g. [17]), namely to use a specially designed polynomial feedback to the open loop system that makes the closed loop system to have a desired property, a generalized Hamiltonian structure in our case.

2. BASIC NOTIONS

Consider a specially opened chemical reaction network, where the reactions are taking place in a perfectly stirred (lumped) reactor with the possibility of feeding in some of the pure components (species). This corresponds to the fed-batch operation case in the terminology of process systems engineering.

Then the dynamic model is in the form of a set of ordinary differential equations (possibly equipped with algebraic equations, but we assume that these can be substituted into the balance equations). In order to have the simplest

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possible case, the following **general assumptions** are made:

- (1) constant temperature, i.e. no energy balance equations are considered,
- (2) constant pressure (in-compressible fluid phases),
- (3) the presence of an inert solvent with great excess such that the reactor has constant overall volume despite of the feed,
- (4) chemical reactions obey the mass action law (MAL),
- (5) constant physico-chemical properties.

This way we assume that the system is open with an inflow of pure species, where the number of species is n . Then we can describe the open-loop system by the following variables and parameters:

- the specie mass flow rates of component (or specie) A_s denoted by $v_{I,s}$, $s = 1, \dots, n$ (measured in kg/s), that are the manipulable inlet variables,
- the concentration (measured in $\frac{mol}{m^3}$) of component (or specie) A_s that is denoted by x_s , $s = 1, \dots, n$.
- the reaction rate constants denoted by $k_{\ell,l}$, where the pair ℓ, l is the identifier of the reaction.

2.1 Dynamic model equations

Under the general assumptions above, the model equations originate from the component mass balances for the considered balance volume. These dynamic balances are of the following general form for lumped balance volumes [14]:

$$\left\{ \begin{array}{l} \text{rate of} \\ \text{change} \end{array} \right\} = \left\{ \begin{array}{l} \text{in-} \\ \text{flow} \end{array} \right\} \pm \left\{ \begin{array}{l} \text{source} \\ \text{sink} \end{array} \right\} \quad (1)$$

The first term on the right-hand side of the above equation corresponds to the inbound convection term, while in the source or sink terms may correspond to various other mechanisms. For the sake of simplicity we only assume to have chemical reactions obeying the mass action law.

It is important to note that the convective component mass inflow rate $v_{I,s}$ corresponds to the concentration inflow $x_{I,s} = \frac{v_{I,s}}{V}$ for the chemical specie A_s , where the volume of the reactor is V .

2.2 Chemical reaction networks and the reaction graph

A CRN obeying the mass action law is a closed system where chemical species A_s , $s = 1, \dots, n$ take part in r chemical reactions. The concentrations of the species denoted by x_s , ($s = 1, \dots, n$) form the state vector x . The *elementary reaction steps* have the following form:



where α_{sj} is the so-called *stoichiometric coefficient* of component A_s in reaction $C_j \rightarrow C_l$, and β_{sl} is the stoichiometric coefficient of the product A_s . The linear combinations of the species in Eq. (2), namely $C_j = \sum_{s=1}^n \alpha_{sj} A_s$ and $C_l = \sum_{s=1}^n \beta_{sl} A_s$ are called the *complexes* and are denoted by C_1, C_2, \dots, C_m . Reactions may share complexes in complex reaction schemes, therefore m is generally not equal to the number of reactions. Moreover, reactions are assumed to be irreversible in classical reaction kinetic systems, therefore the *stoichiometric coefficients are always nonnegative integers*.

The *reaction rates* of the individual reactions $C_j \rightarrow C_l$ can be described as

$$\rho_{jl}(x) = k_{j,l} \prod_{s=1}^n x_s^{\alpha_{sj}} \quad (3)$$

where $k_{j,l} > 0$ is the *reaction rate coefficient* of the reaction, and x_s is the concentration of specie A_s .

In our computations, the following form will be used for the description of the dynamics of CRNs obeying the mass action law [8]:

$$\dot{x} = M \cdot \varphi(x) = Y \cdot A_k \cdot \varphi(x) \quad (4)$$

where $\alpha_{sj} = Y_{sj}$, $Y \in \mathbb{R}^{n \times m}$ stores the stoichiometric composition of the complexes, $A_k \in \mathbb{R}^{m \times m}$ contains information about the structure of the reaction network, and $\varphi : \mathbb{R}^n \mapsto \mathbb{R}^m$ is a monomial-type vector mapping given by

$$\varphi_j(x) = \prod_{s=1}^n x_s^{\alpha_{sj}}, \quad j = 1, \dots, m \quad (5)$$

A_k is a column conservation matrix (i.e. the sum of the elements in each column is zero), called the *Kirchhoff matrix* of the CRN, defined as

$$[A_k]_{lj} = \begin{cases} - \sum_{\substack{\ell=1 \\ \ell \neq j}}^m k_{l,\ell}, & \text{if } l = j \\ k_{j,l}, & \text{if } l \neq j \end{cases} \quad (6)$$

where $[A_k]_{lj}$ denotes the lj th element of the matrix A_k . It is important to note that the pair (Y, A_k) uniquely characterizes a particular CRN with its structure and parameters.

To handle the exchange of materials between the environment and the reaction network, the so-called "zero-complex" can be introduced and used which is a special complex where all stoichiometric coefficients are zero i.e., it is represented by a zero column vector in the Y matrix [8]. Note, however, that the presence of the zero complex may imply the openness of the reaction kinetic system.

Similarly to [8] and many other authors, the following weighted directed graph (called **reaction graph**) is assigned to the reaction network (2). The directed graph $D = (V_d, E_d)$ of a reaction network consists of a finite nonempty set V_d of vertices and a finite set E_d of ordered pairs of distinct vertices called directed edges. The vertices correspond to the complexes, i.e. $V_d = \{C_1, C_2, \dots, C_m\}$, while the directed edges represent the reactions, i.e. $(C_l, C_j) \in E_d$ if complex C_l is transformed to C_j in the reaction network. The reaction rate coefficients $k_{l,j}$ for $j = 1, \dots, m$ in (3) are assigned as positive weights to the corresponding directed edges in the graph.

An example of a reaction graph is seen in Fig. 1.

For each reaction $C_i \rightarrow C_j$ corresponds a **reaction vector**:

$$e_k = [Y]_{\cdot,j} - [Y]_{\cdot,i}, \quad k = 1, \dots, r, \quad (7)$$

where $[Y]_{\cdot,i}$ denotes the i th column of Y and r is the number of reactions. The set of reaction vectors is equivalent to the column vectors of $Y \cdot B_G$ where B_G is the incidence matrix of the reaction graph.

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