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IFAC-PapersOnLine 49-7 (2016) 073–078

On the use of shape constraints for state estimation in reaction systems

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Abstract: State estimation techniques are used for improving the quality of measured signals and for reconstructing unmeasured quantities. In chemical reaction systems, nonlinear estimators are often used to improve the quality of estimated concentrations. These nonlinear estimators, which include the extended Kalman filter, the receding-horizon nonlinear Kalman filter and the moving-horizon estimator, use a state-space representation in terms of concentrations. An alternative to the representation of chemical reaction systems in terms of concentrations consists in representing these systems in terms of extents. This paper formulates the state estimation problem in terms of extents, which allows imposing *additional shape constraints* on the sign, monotonicity and concavity/convexity properties of extents. The addition of shape constraints often leads to significantly improved state estimates. A simulated example illustrates the formulation of the state estimation problem in terms of concentrations and extents, and the use of shape constraints.

Keywords: State estimation, receding-horizon nonlinear Kalman filter, vessel extents, shape constraints.

1. INTRODUCTION

Many processes in the (bio-)chemical industry utilize chemical reactions to convert feed materials into intermediate or final products. The quality of these products depends on the quality of the data used for monitoring, control and optimization. Measurements made during the course of a reaction are often limited in number and usually corrupted with noise. The field of state estimation focuses on both improving the accuracy of the measured signals and reconstructing unmeasured signals by enforcing their consistency with a given process model (Simon, 2006). For the static case, state estimation is referred to as data reconciliation (Narasimhan and Jordache, 1999).

The models of chemical reaction systems are most often derived from first principles and written as differential-algebraic equations (DAE), with concentrations, temperatures, pressures and possibly other quantities as state variables. These equations are nonlinear and highly coupled, since each state variable is influenced by multiple rate processes such as reactions, mass transfers, and flows. An alternative representation of reaction systems in terms of "vessel extents" has been proposed by Amrhein et al. (2010) and reformulated by Rodrigues et al. (2015). Vessel extents are to open reactors (reactors with inlet and outlet streams) what batch extents are to batch reactors. In the extent formulation, each state variable is influenced by a single rate process, which considerably simplifies the analysis. In turn, the original states (concentrations) can be represented as linear combinations of these vessel extents.

Several state estimators are available for nonlinear dynamic systems. Among these estimators, the most commonly used is probably the extended Kalman filter (EKF) (Jazwinski, 1970). EKF is recursive by nature and thus can easily be implemented in real time. The major drawback of EKF lies in its inability to handle bounds and algebraic constraints, which are common in the representation of chemical reaction systems. The moving-horizon estimator (MHE) constitutes an alternative that can handle constraints on the estimated states (Rao et al., 2001, 2003). A constrained optimization problem is formulated at each sampling time using a time window of past measurements. This allows incorporating shape constraints (such as sign, monotonicity and concavity/convexity) in the estimation problem for the given window. The drawback of the MHE method is the need to solve differential equations within the optimization loop, which can become a computational issue for real-time estimation.

The receding-horizon nonlinear Kalman filter (RNK) is another nonlinear state estimator. It is based on the prediction and update steps of the Kalman filter (Rengaswamy et al., 2013). In the update step, an optimization problem is solved using a time window of past measurements. The RNK method differs from the MHE methods in the sense that the optimization problem does not require solving differential equations, which considerably reduces the computational burden.

This paper formulates the state estimation problem in terms of vessel extents, which allows exploiting additional shape constraints associated with the extents. In certain cases, the shapes are known a priori, while for other cases,

10.1016/j.ifacol.2016.07.219

a data-driven approach can be used to formulate appropriate constraints. The objective of the paper is to compare state estimation in the (original) concentration domain with state estimation in terms of extents, in particular the advantage that results from being able to use additional shape constraints. Since the objective is not to compare the performance of various nonlinear estimators, the RNK method is chosen here for its computational simplicity.

This paper is organized as follows. Section 2 briefly reviews the representation of chemical reaction systems in terms of both numbers of moles and vessel extents. In Section 3, the shape properties of extents are discussed. Section 4 formulates the RNK in terms concentrations and extents. In Section 5, the performance of these two estimator formulations are compared via a case study, while Section 6 concludes the paper.

2. SYSTEM REPRESENTATION

In this section, chemical reaction systems are first modeled in terms of numbers of moles and then in terms of extents.

2.1 Numbers of moles

Consider a homogeneous reaction system involving S species, R independent reactions, p inlet streams, and one outlet stream. A dynamic model in terms of the numbers of moles can be written as

$$\dot{\mathbf{n}}(t) = \mathbf{N}^{\mathrm{T}}\mathbf{r}_v(t) + \mathbf{W}_{in}\mathbf{u}_{in}(t) - \omega(t)\mathbf{n}(t), \quad \mathbf{n}(0) = \mathbf{n}_0, \quad (1)$$

where $\mathbf{n}$ is the S-dimensional vector of numbers of moles, $\mathbf{r}_v := V\,\mathbf{r}$ with V the volume and $\mathbf{r}$ the R-dimensional vector of reaction rates, $\mathbf{u}_{in}$ is the p-dimensional vector of inlet mass flowrates, $\omega := \frac{u_{out}}{m}$ is the inverse residence time with the mass m and the outlet mass flowrate u_{out}, $\mathbf{N}$ is the $R \times S$ stoichiometric matrix, $\mathbf{W}_{in} = \mathbf{M}_w^{-1}\check{\mathbf{W}}_{in}$ is the $S \times p$ matrix of inlet compositions, with $\mathbf{M}_w$ the S-dimensional diagonal matrix of molecular weights and $\check{\mathbf{W}}_{in} = [\check{\mathbf{w}}_{in}^1 \cdots \check{\mathbf{w}}_{in}^p]$ with $\check{\mathbf{w}}_{in}^j$ the S-dimensional vector of weight fractions of the jth inlet flow, and $\mathbf{n}_0$ is the S-dimensional vector of initial conditions. Note that the mass m can be computed from the numbers of moles $\mathbf{n}$ as $m(t) = \mathbf{1}_S^{\mathrm{T}}\mathbf{M}_w\,\mathbf{n}(t)$ or through integration of the continuity equation upon knowledge of the inlet and outlet streams: $\dot{m}(t) = \mathbf{1}_p^{\mathrm{T}}\mathbf{u}_{in}(t) - u_{out}(t)$, $m(0) = m_0$.

The concentrations are computed from the numbers of moles as $\mathbf{c}(t) = \frac{\mathbf{n}(t)}{V(t)}$ and the reaction rates $\mathbf{r}(t)$ are typically nonlinear functions of $\mathbf{c}(t)$.

The S-dimensional representation given in Eq. (1) often contains redundancies, as the system evolves in time only due to the R independent reactions, the p independent inlets and the outlet stream. Hence, for a reactor with outlet, there exists $q := S - (R + p + 1)$ invariants, which are identically equal to zero, such that,

$$\mathbf{P}^{+}\mathbf{n}(t) = \mathbf{0}_q, \quad (2)$$

where the $S \times q$ matrix $\mathbf{P}$ describes the q-dimensional null space of the matrix $[\mathbf{N}^{\mathrm{T}}\ \mathbf{W}_{in}\ \mathbf{n}_0]$, and $\mathbf{P}^{+}$ is the pseudo-inverse of $\mathbf{P}$. The invariant relationships given in Eq. (2) can be used to rewrite Eq. (1) in terms of $d := R + p + 1$ independent species. The dynamic model can then be rewritten as:

$$\dot{\mathbf{n}}_1(t) = \mathbf{N}_1^{\mathrm{T}}\mathbf{r}_v(t) + \mathbf{W}_{in,1}\mathbf{u}_{in}(t) - \omega(t)\mathbf{n}_1(t), \quad \mathbf{n}_1(0) = \mathbf{n}_{01} \quad (3a)$$

$$\mathbf{n}_2(t) = -\mathbf{P}_2\,\mathbf{P}_1^{+}\,\mathbf{n}_1(t), \quad (3b)$$

where $\mathbf{n}_1$ is the d-dimensional vector of independent species, $\mathbf{n}_2$ the q-dimensional vector of dependent species, $\mathbf{N}_1$ is the $R \times d$ subset of the stoichiometric matrix, $\mathbf{W}_{in,1}$ the $d \times p$ subset of inlet compositions, $\mathbf{n}_{01}$ the d-dimensional vector of initial conditions, $\mathbf{P}_2$ is the $q \times q$ subset of $\mathbf{P}$ corresponding to the dependent species and $\mathbf{P}_1$ the $d \times q$ subset of $\mathbf{P}$ corresponding to the independent species. Note that the set of independent species are chosen such that rank of the matrix $[\mathbf{N}_1^{\mathrm{T}}\ \mathbf{W}_{in,1}\ \mathbf{n}_{01}] = d$.

2.2 Vessel extents

The reaction system (3a) can be expressed in terms of vessel extents by using the linear transformation (Rodrigues et al., 2015) [1]

$$\mathbf{x}(t) = \mathbf{T}_1\,\mathbf{n}_1(t) = \left[\mathbf{N}_1^{\mathrm{T}}\ \ \mathbf{W}_{in,1}\ \ \mathbf{n}_{01}\right]^{-1}\mathbf{n}_1(t). \quad (4)$$

The transformed system reads:

$$\dot{\mathbf{x}}_r(t) = \mathbf{r}_v(t) - \omega(t)\,\mathbf{x}_r(t), \qquad \mathbf{x}_r(0) = \mathbf{0}_R \quad (5a)$$

$$\dot{\mathbf{x}}_{in}(t) = \mathbf{u}_{in}(t) - \omega(t)\,\mathbf{x}_{in}(t), \qquad \mathbf{x}_{in}(0) = \mathbf{0}_p \quad (5b)$$

$$\dot{x}_{ic}(t) = -\omega(t)\,x_{ic}(t), \qquad x_{ic}(0) = 1, \quad (5c)$$

with the reconstruction equations:

$$\mathbf{n}_1(t) = \mathbf{N}_1^{\mathrm{T}}\,\mathbf{x}_r(t) + \mathbf{W}_{in,1}\mathbf{x}_{in}(t) + \mathbf{n}_{01}\,x_{ic}(t) \quad (6a)$$

$$\mathbf{n}_2(t) = \mathbf{N}_2^{\mathrm{T}}\,\mathbf{x}_r(t) + \mathbf{W}_{in,2}\mathbf{x}_{in}(t) + \mathbf{n}_{02}\,x_{ic}(t). \quad (6b)$$

The vessel extent of reaction $x_{r,i}(t)$ expresses the amount of material produced or consumed by the ith reaction that is still in the reactor at time t, the negative term on the right-hand side accounting for what has left the reactor. Similarly, the vessel extent of inlet expresses the amount of material loaded by the jth inlet that is still in the reactor at time t. Finally, $x_{ic}(t)$ indicates the fraction of the initial conditions that is still in the reactor at time t. The various extents can be grouped in the extent vector $\mathbf{x} := [\mathbf{x}_r^{\mathrm{T}}\ \ \mathbf{x}_{in}^{\mathrm{T}}\ \ x_{ic}]^{\mathrm{T}}$. Note that Eqs (6a) and (6b) can be written together as:

$$\mathbf{n}(t) = \mathbf{N}^{\mathrm{T}}\,\mathbf{x}_r(t) + \mathbf{W}_{in}\mathbf{x}_{in}(t) + \mathbf{n}_0\,x_{ic}(t). \quad (7)$$

3. STATE CONSTRAINTS

Constraints on state estimates can be formulated based on either the numbers of moles or the extents. Furthermore, these constraints are either known a priori because they are generally valid or they can be inferred from measured data. Section 3.1 introduces constraints on the numbers of moles and on the extents based on prior knowledge. Section 3.2 introduces a procedure for estimating shape constraints on the numbers of moles and on the extents based on measurements.

[1] The $(S \times S)$-dimensional transformation matrix in Rodrigues et al. (2015) reads $\mathbf{T} := \left[\mathbf{N}^{\mathrm{T}}\ \ \mathbf{W}_{in}\ \ \mathbf{n}_0\ \ \mathbf{P}\right]^{-1}$. Here $\mathbf{T}_1$ is a submatrix of dimension $d \times d$.