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Reduction of complex energy-integrated process networks using graph theory

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1. Introduction

Aggressive efforts in sustainability and improved energy efficiency in the process industries have led to the development of complex process designs with multiple energy integration loops. While these integrated systems have demonstrated significant economic benefits, they have had limited practical implementation owing to the difficulties in their operation and control. Specifically, these integrated networks exhibit complex, nonlinear, multi-time scale dynamics with strong interactions among process units (Jacobsen, 1999; Kumar and Daoutidis, 2002; Jogwar et al., 2009). These interactions limit the effectiveness of standard decentralized controllers. Fully centralized controllers, though possible to design, are impractical due to the large size of the plant model and are often ill-conditioned showing strong sensitivity to modeling errors (Larsson et al., 2003; Kiss et al., 2005; Kumar and Daoutidis, 2002).

Recently, network-level analysis approaches have been developed to address this problem in a systematic and generic manner. These approaches include:

• Passivity-based control (Ydstie, 2002; Hudson and Bao, 2012; Hioe et al., 2013; Dörfler et al., 2009) which involves determining the passivity/dissipativity of a process unit using thermodynamic

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ABSTRACT

This paper focuses on the analysis of complex (multi-loop) energy-integrated process networks. Simple (single-loop) energy-integrated networks (comprising of large energy recycle or throughput) with two-time scale dynamics are the building blocks for such complex networks. The modular structure of these complex networks lends them to a graph theoretic analysis, whereby weak and strong connections between process units arising from time scale separation are identified from structural information. Subsequently, a graph-theoretic framework for network analysis and control is developed, and connecting links are built to an equivalent analysis using singular perturbations. The proposed analysis framework is illustrated via application to a representative complex process network.

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properties, and analyzing the stability properties of the network based on the interconnections of these passive/dissipative components.

- Plantwide control which involves taking a holistic approach in terms of identifying control objectives, manipulated inputs and selecting a control structure for a network. Though some of the earlier contributions in this area were heuristics-based (Luyben et al., 1997; Stephanopoulos and Ng, 2000), recent works (Zhu et al., 2000; Skogestad, 2004) have added formalism to this approach.
- Distributed control (Venkat et al., 2008; Rawlings and Stewart, 2008; Liu et al., 2009) which places itself between the two extremes - decentralized and fully centralized control schemes. This approach involves designing controllers for subsystems (group of units) and allowing for information sharing (and possibly control/optimization objectives) among these controllers.
- Quasi-decentralized control (El-Farra et al., 2005; Sun and El-Farra, 2008; Baldea et al., 2013) which incorporates a local control system for each unit in a network along with a supervisory unit at the network level, and these local systems communicate with the supervisor as well as the other local systems through a shared communication medium.
- Hierarchical control (Scattolini, 2009; Kumar and Daoutidis, 2002; Jogwar et al., 2009) which aims at decomposing the control problem into different tiers, typically based on the corresponding time scales. The control objectives at a unit level are addressed by the lower tier whereas the objectives at the network level are addressed by the top tier.









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In previous work (Jogwar et al., 2010), we have identified two classes of energy-integrated networks, one characterized by the presence of large energy recycle (Fig. 1a) and the other characterized by the presence of large energy throughput (Fig. 1b), which are at the core of most energy-integrated networks. These networks show two-time scale dynamics and naturally lend themselves to a two-tiered control approach based on these time scales. Furthermore, we have shown that the underlying energy flow structure of a complex energy-integrated network consists of interconnections of these recycles and throughputs (Jogwar, 2011). For example, a network of distillation columns separating a five-component mixture (Fig. 2) has been shown to involve six recycles and three throughputs with energy flows of 3 different orders of magnitude (see Jogwar and Daoutidis (2010) for details). A reactor-heat exchanger network designed for naphtha reforming (Fig. 3) has also been shown to be composed of 9 recycles and 10 throughputs, with the various energy flows spanning three orders of magnitude (see logwar (2011) for details).

It can be reasonably argued that the multi-loop integrated structure of a complex process network has the potential to demonstrate multi-time scale dynamics, and the dynamic characteristics exhibited by the parent complex network can be inferred from the properties of its building blocks. Furthermore, the interconnection of (a large number of) these building blocks can result in interactions and dynamic phenomena being exhibited by these networks that are more intricate than can be anticipated by considering the mere association of these building blocks. The development of a model reduction and control framework for such complex networks, building upon the results obtained for simple networks is the main objective of this paper.

In Section 2, we develop a singular perturbations-based reduction framework for a generic complex energy-integrated process network. Singular perturbations have been used extensively for model reduction and control applications (O'Malley, 1991; Ladde and Siljak, 1983; Desoer and Shahruz, 1986; Khalil and Kokotovic, 1979; Kokotovic, 1981; Kokotovic et al., 1986; Dmitriev and Kurina, 2006). The key distinguishing feature of the systems considered is that they are (typically) in a non-standard singularly perturbed form. Such systems have received much less attention in the literature, especially in the case of multiple (more than two) time scales (Fenichel, 1979; Marino and Kokotovic, 1988; Kumar et al., 1998; Vora et al., 2006). The model reduction framework is subsequently exploited to develop a graph-based reduction framework which is the main contribution of this paper. In Section 3, we describe this graph-theoretic formulation to capture and automate the major reduction steps in the analysis of complex energy-integrated process networks. The advantages of the graph-based reduction framework over the model-based singular perturbations approach are also highlighted. The proposed methods are illustrated with the help of a complex process network. Preliminary results on this work were presented in Jogwar et al. (2011), Heo et al. (2012). Applications of the presented algorithm to complex energy-integrated systems have been described in Heo et al. (2014).

2. Analysis of complex energy-integrated networks

Let us consider a generic complex energy-integrated network, consisting of *N* units (indexed by *j*) and energy (enthalpy) flows, h_i , spanning *m* orders of magnitude (indexed by *i*). The energy flows of different order of magnitude are segregated from each other through the definition of small parameters ε_i , such that $\varepsilon_i \ll 1$ and $\varepsilon_{i+1}/\varepsilon_i \ll 1$ (with $\varepsilon_0 \approx 1$). Nominal steady state flows of each magnitude are used to define these small parameters such that $\varepsilon_i = h_{0,s}/h_{i,s}$, where subscript *s* denotes a steady state value. In energy-integrated systems, the small parameters ε_i represent the

ratios of liquid to vapor enthalpy (in the case of a combined boilercondenser configuration), small and large material flows (in the case of large reflux ratio) and/or the combination of these (in the case of heat pump operation for high purity separation).

For each unit, we consider the enthalpy change due to flow in/out from other units and external energy flows d_j (representing contributions from heat of reaction, compressor work, etc). These energy flows are scaled using the nominal steady state flows and the corresponding energy balance equations can be represented in the following form:

$$\frac{d\mathbf{H}}{dt} = \sum_{i=0}^{m-1} \frac{1}{\varepsilon_i} \mathbf{F}_i \mathbf{g}_i(\mathbf{H}, \mathbf{u}_i)$$
(1)

H is the vector of enthalpies of each of the *N* units in the network. **g**_i are vectors of dimension p_i corresponding to the contributions from the energy flows of order $O(1/\varepsilon_i)$. **F**_i (of dimension $N \times p_i$) represents the corresponding selector matrix such that $F_i(j, k)$ is 1 if the energy balance equation of the enthalpy H_j contains the term $g_i(k)$ and all the other elements of **F** are 0. **u**_i are scaled energy flow variables which can be used as potential manipulated inputs. Note that Eq. (1) results from an energy balance under the assumption that the contributions of kinetic and potential energy are very small compared to internal energy and can therefore be neglected, and the fact that at constant temperature and pressure, the rate of change of enthalpy and internal energy are the same.

Eq. (1) is a singularly perturbed system with multiple singular perturbation parameters in a non-standard form, potentially leading to energy dynamics evolving over m time scales (Vora et al., 2006). Due to the lack of explicit separation of the state variables according to the time scale they evolve in Eq. (1), a unit enthalpy may evolve in multiple time scales. To uncover this hierarchy of time scales of unit enthalpies, we successively use singular perturbations to derive approximate reduced order models of the dynamics in the different time scales, starting with the fastest (corresponding to the largest energy flows).

Defining a stretched time scale $\tau_{m-1} = t/\varepsilon_{m-1}$, the dynamic equations (1) become:

$$\frac{d\mathbf{H}}{d\tau_{m-1}} = \sum_{i=0}^{m-1} \frac{\varepsilon_{m-1}}{\varepsilon_i} \mathbf{F}_i \mathbf{g}_i(\mathbf{H}, \mathbf{u}_i)$$

In the limit $\varepsilon_{m-1} \rightarrow 0$, the description of the dynamics in the fastest time scale is given by:

$$\frac{d\mathbf{H}}{d\tau_{m-1}} = \mathbf{F}_{m-1}\mathbf{g}_{m-1}(\mathbf{H}, \mathbf{u}_{m-1})$$
(2)

as $\forall i \neq (m-1)$, $\varepsilon_{m-1}/\varepsilon_i \rightarrow 0$ as $\varepsilon_{m-1} \rightarrow 0$.

Note that all the enthalpies in a network may not be affected by the largest magnitude energy flows. This means \mathbf{F}_{m-1} does not necessarily have a full row rank. Premultiplying Eq. (2) by \mathbf{F}_{m-1}^{T} , we obtain the simplified description of the fast dynamics as:

$$\frac{d\mathbf{H}_{m-1}}{d\tau_{m-1}} = (\mathbf{F}_{m-1}^T \mathbf{F}_{m-1}) \hat{\mathbf{g}}_{m-1} (\mathbf{H}_{m-1}, \mathbf{u}_{m-1})$$
(3)

where $\mathbf{H}_{m-1} = \mathbf{F}_{m-1}^T \mathbf{H}$ represent the enthalpies evolving in this fast time scale and $\hat{\mathbf{g}}_{m-1}$ represents the \mathbf{g}_{m-1} vector in terms of \mathbf{H}_{m-1} .

$$\mathbf{g}_{m-1}(\mathbf{H}, \mathbf{u}_{m-1}) = \hat{\mathbf{g}}_{m-1}(\mathbf{H}_{m-1}, \mathbf{u}_{m-1})$$
(4)

Note that only the energy flows \mathbf{g}_{m-1} of order $\mathcal{O}(1/\varepsilon_{m-1})$ govern the dynamics in this time scale. This fast dynamics converges to a quasi-steady state given by the following constraints:

$$\mathbf{0} = (\mathbf{F}_{m-1}^T \mathbf{F}_{m-1}) \hat{\mathbf{g}}_{m-1} (\mathbf{H}_{m-1}, \mathbf{u}_{m-1})$$
(5)

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