DYNAMICS AND CONTROL OF PROCESS NETWORKS

M. Baldea [a,1], N. H. El-Farra [b] and B.E. Ydstie [c]

[a] Department of Chemical Engineering, The University of Texas at Austin, Austin, TX 78712

[b] Department of Chemical Engineering, University of California, Davis, Davis, CA

[c] Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA

Abstract

This paper discusses theoretical foundations for the modeling, analysis and control of chemical process networks that are tightly integrated through complex material, energy and information flows. The physical behavior of process networks is described using fundamental concepts from classical thermodynamics, while time-scale decomposition and singular perturbation theory provide the basis for exploring the network-level dynamic behavior that emerges as a result of tight inventory integration, and developing appropriate reduced-order models and a hierarchy of control systems for managing inventories and inventory flows. Finally, ideas from model-based networked control and Lyapunov theory are leveraged to develop an integrated control and communication strategy that manages the information flows between the network components and explicitly accounts for communication constraints.

Keywords

Complex Networks, Process Systems, Dissipative Systems Theory, Nonlinear Feedback Control, Time-scale decomposition.

Introduction

Large scale systems are created by connecting simple components together via material and information streams. The resulting networks integrate physical devices, computation and communication. They represent traffic flow, internet communication, chemical process plants, electrical grids, social, biological or financial systems (Ydstie, 2004).The common, underlying trait of all such systems is that each node has storage capacity and the ability to transform the stored entity, while the connections between the nodes provide means for transportation. The dynamic behavior of a network is usually quite different from any behavior which can be extracted from the individual sub-components or small groups of such. In fact, the network may learn and adapt simply by adjusting (controlling) the strength of the connections between the sub-systems. Its behavior may also exhibit surprising robustness in the sense that individual components may fail without significantly altering the performance of the entire system.

This paper focuses on a particular class of networks called chemical process networks. At the fundamental level, the dynamic behavior of process networks is characterized by inventory and information exchanges between units (the network flow). Inventory flow is driven by potential differences between the network nodes, and the network is at equilibrium when these driving forces are zero (classic examples include fluid flow driven by a pressure gradient and heat flow generated by a temperature gradient). Chemical process plants clearly belong to this category, as they are large-scale dynamical systems that involve complex, distributed arrangements of interconnected subsystems (Amaral and Ottino, 2004b,a; Jiang et al., 2007). The integration between the constituent subsystems through mass, energy and information flows and recycle gives rise to a specific, network-level dynamics, and the associated need to account for and accommodate this behavior in network-level control structures, and information exchange and communication strategies.

Control and supervision of networked process systems is a challenging problem that requires tight integration of computing, communication, and control into different levels of plant operations and information processes. The challenge in dealing with networked systems stems not only from the complex dynamic behavior of the component subsystems – due, for example, to nonlinear dynamics, uncertainty and constraints, which make the individual units difficult to control – but also from the interconnections which can create new, more complex dynamics, amplify instabilities and

[1] Corresponding author. Email: mbaldea@che.utexas.edu, Fax: (512) 471 7090.

potentially exacerbate disturbance and failure propagations across the entire network.

Over the past two decades, the fundamental and practical challenges associated with control of networked process systems have been the focus of significant research activities in the process control community and have motivated many research studies on the design of distributed and supervisory control schemes for process networks. Traditionally, the control of plants with geographically-distributed interconnected units has been studied within either the centralized or decentralized control frameworks. In the centralized setting, all measurements are collected and sent to a central unit for processing, and the resultant control commands are then sent back to the plant. While centralized control is known to provide the best performance – because it imposes the least constraints on the control structure – the computational and organizational complexity associated with centralized controllers often makes their implementation impractical. Also, the consequences of failures in a centralized controller can be detrimental to the entire plant. These considerations have motivated significant work on decentralized control. In this paradigm, the plant is decomposed into a number of simpler subsystems (typically based on functional and/or time-scale differences of the unit operations) with interconnections, and a number of local controllers are connected to each distributed subsystem with no signal transfer taking place between different local controllers. Decentralized control of multi-unit plants can reduce complexity in the controller design and implementation, and can also provide flexibility in dealing with local controller failures. However, since in this structure the interconnections between the constituent subsystems are totally neglected, the closed-loop performance of the plant may deteriorate, and in some cases stability may be lost. Significant research work has explored in depth the benefits and limitations of decentralized controllers as well as possible ways of overcoming some of their limitations (see, *e.g.,* Price et al., 1994; Sandell Jr et al., 1978; Siljak, 1991; Lunze, 1992; Sourlas and Manousiouthakis, 1995; Luyben et al., 1997; Cui and Jacobsen, 2002; Skogestad, 2004; Huang and Huang, 2004; Kariwala, 2007, and the references therein) . In recent times, there also has been significant and growing interest in studying plant-wide control problems within a diverse array of frameworks, including optimization-based distributed model predictive control (see, for example, (see, for example Katebi and Johnson, 1997; Camponogara et al., 2002; Venkat et al., 2005; Stewart et al., 2010; Maestre et al., 2011; Christofides et al., 2011), passivity-based control (see, for example, (see, for example Hangos et al., 1999; Garcia-Osorio and Ydstie, 2004; Jillson and Ydstie, 2007), agent-based systems (Tatara et al., 2005; Tetiker et al., 2008), and singular perturbation formulations (Kumar and Daoutidis, 2002; Baldea et al., 2006; Baldea and Daoutidis, 2007). In addition to these works, research has recently begun to integrate and address communication issues in the plant-wide control problem (e.g., resource constraints, real-time scheduling constraints, communication delays and disruptions, etc.), leading to the design of networked plant-wide control systems with explicitly-characterized stability and performance properties (Sun and El-Farra, 2008a,b, 2009, 2010a,b,c, 2011). These efforts are motivated by the increased reliance in the process industries on sensor and control systems that are accessed over shared wired or wireless communication networks instead of dedicated links (*e.g.,* Song et al., 2006), as well as the recent calls for expanding the traditional process control and operations paradigm in the direction of smart plant operations (*e.g.,* Ydstie, 2002; Christofides et al., 2007). A key component of this paradigm is the deployment and integration of networked sensors and actuators in process control systems to achieve tighter integration of process operations with real-time information and help realize objectives that cannot be met otherwise, including proactive fault-tolerance and real-time plant reconfiguration based on market demand changes.

This paper seeks to develop a unified framework for the modeling, analysis and control of process networks whose component subsystems are tightly integrated through material, energy and information flows and recycle. These systems can be thought of in terms of a two-tier hierarchy, where in one tier the processing units exchange material and energy subject to physical laws and constraints, while in another tier the control systems exchange information through some communication medium subject to communication constraints. The developed framework brings together concepts and tools from classical thermodynamics, singular perturbations, and networked control. Classical thermodynamics provides the framework for developing a physically-based representation of process networks, while time-scale decomposition and singular perturbation theory provide the basis for exploring the impact of tight inventory integration on the network dynamics, and developing appropriate reduced-order control systems for managing the inventory flows. Finally, ideas from model-based networked control and Lyapunov theory are leveraged to develop an integrated control and communication strategy that manages the information flows between the network components in a way that takes communication constraints explicitly into account.

Structure and Connectivity in a Process Network

Figure 1 shows the architecture of a decentralized control system for a chemical plant. It consists of severals layers that allow operators and algorithms interact with the chemical process in real time. The interface layer converts measurements into signals that can be interpreted by the supervisory control and data acquisition (SCADA) system. SCADA performs low level control that adjust pumps, valves and other actuators in response to measurements. They contain programmable logic control systems to ensure safe and reliable operation, perform supervisory control tasks, send and receive data from the communication system through Fieldbus (IEC 61158) or similar communication protocols that allow a wide range of network communication topologies. PID controllers and to an increasing degree more advanced process control systems can be connected directly to Fieldbus or allow communication to Fieldbus devices through OPC as indicated in the figure. In a typical chemical process application there may be several thousand such devices and and algorithms connected into a dynamically changing network that integrates the physical process with communication and control devices of ever increasing complexity. How such networks can be designed, maintained and operated is at present an open problem and faults and poor performance often result when single devices or communication between devices fail. The objective of this paper is to discuss how such networks can be modeled and controlled usign ideas from nonlinear control theory and time-scale decomposition.

Chemical plants consist of a network of interconnected process units (Figure 2), which interact dynamically through material, energy and information streams. At the system level, such dynamic interactions contribute to the emergence of a complex, network-level behavior, that is present in addition to the dynamics of the individual units. At the local, unit level, the process interactions constitute disturbances which must be appropriately addressed in controller design. From a theoretical perspective, the analysis of process networks focuses on (interconnections of) open, finite-dimensional systems, with the dynamics of each sub-system j being described by a system of equations of the form:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \sum_{j=1}^{n} \mathbf{g}(\mathbf{x}, u_j,\ x_j) \tag{1}$$

where the drift $\mathbf{f}(\mathbf{x})$ denotes production, for example due to chemical reaction, $\mathbf{g}(\mathbf{x}, u_j, x_j)$ denotes flow between the sub-system and j other systems (each with state x_j); u_j denotes a vector of inputs (control signals) which adjust the input/output flow rates, thereby defining and determining the **interaction** of system j and other systems.

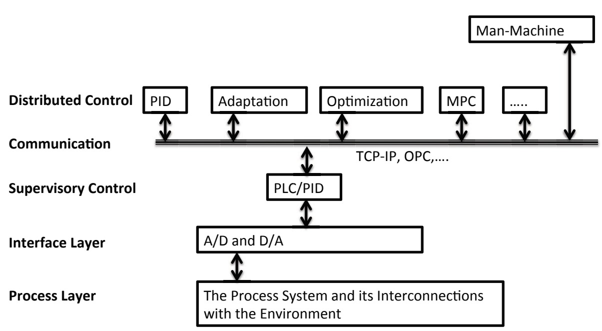

Figure 1: The architecture of a modern control system consists of several layers of hardware and software that integrates the process with control and optimization algorithms

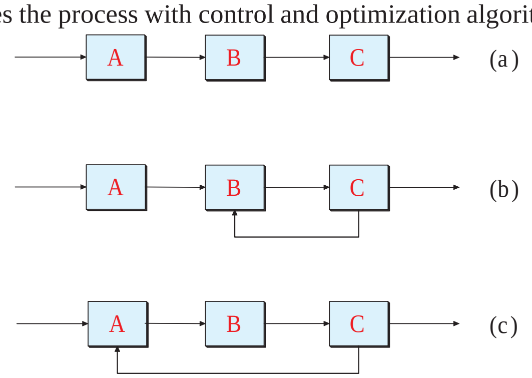

Figure 2: Connectivity structures in integrated process networks

As a consequence, in the case of process networks, the compensation of disturbances at the unit level involves not only obtaining measurements of *external* disturbances, but also obtaining state information from the units that are directly connected and/or in the physical proximity of the unit of interest. Naturally, a tradeoff exists between achievable control quality and the *extent* and *frequency* of information transfer (note that in modern plants, information exchange occurs over a data bus/network, whose bandwidth may be limited).

Controlling network nodes with a high degree of connectivity (*i.e.*, featuring more than a single input and a single output, such as node *B* in Figure 2 (b) or node *A* in Figure 2 (c)) will intuitively require more extensive information (*i.e.*, that data be acquired from several neighboring units), while the extent of information required for disturbance compensation in simple input/output nodes is more modest. Special consideration should be paid to the well established need to avoid ”recycling disturbances” when material or energy recycling loops are present in the process Seborg et al. (2010), and to acquiring the relevant disturbance information when recycling is unavoidable.

Intuitively, the *frequency* at which information exchange is *necessary* depends on the time constant(s) of the units involved (note that, as we will show below, the dynamics of individual process units are fast). On the other hand, the frequency at which information exchange is *possible or practical* will be inversely proportional to the degree of connectivity of the units. Assuming, for example, that the units use Model Predictive Control, limiting the communication frequency and the amount of data exchange will benefit the fast execution of the controller but may impede on its performance.

Furthermore, relying extensively on disturbance information in the design of a unit-level controller poses the risk of performance degradation or even loss of stability in the event of a communication failure.

Process Systems and Network Representations

Definition

In a chemical process network we can use the non-negative vector $\mathbf{x} = (U, V, N_1, \ldots N_{n_c})^T$ with $\mathbf{x} \in \mathbb{R}_+^{2+n_c}$, referred to as a system inventory, to represent the state. The non-negative of $\mathbf{x}$ confines the analysis of process systems to the subclass of positive dynamical systems (note that a practical consequence of this property is that mole- and mass-fractions sum to one). Inventories are additive so that, if system $\mathbb{S}$ consists of subsystems $\mathbb{S}_1$ and $\mathbb{S}_2$ and $\mathbf{x}_1$ and $\mathbf{x}_2$ are, respectively, the states of these systems, then we can write, $\mathbf{x} = \mathbf{x_1} + \mathbf{x_2}$, that is, the inventory of a system is the sum of the inventories of its subsystems. Note that additivity provides process systems with a linear vector space structure that is exploited extensively in thermodynamics and process control.

The inventory vector $\mathbf{x}$ constitutes the basis for the Gibbs classical state based theory of thermodynamics. In statistical mechanics, $\mathbf{x}$ is referred to as the micro-canonical ensemble and for a simple system it contains the measures of the energy inventory, volume and number of moles of n_c different chemical species. In a more general sense, the elements of the vector $\mathbf{x}$ can refer to any (extensive) variable that measures the inventory of a quantity, such as area, charge, momentum, number of items stored in a supply chain, cash deposits or liabilities Ydstie (2004). In chemical process modeling, enthalpy is often used instead of internal energy. Within the same context, it can be shown that there exists a special inventory $S \in \mathbb{R}_+$, called Entropy, which captures dissipation and stability by its tendency increase in isolated systems. In what follows, we will assume that entropy satisfies the Callen postulates Callen (Callen) i.e. $S(\mathbf{x})$ should be concave, homogeneous degree one and differentiable at least once.

Using the concepts above, we can define a vector of conjugate, intensive variables, as:

$$w^T = \frac{\partial S}{\partial \mathbf{x}} = \left(\frac{1}{T}, \frac{P}{T}, ..\frac{\mu_i}{T}\right)(2) \tag{2}$$

which can be used to compute the driving forces for flow between subsystems. Specifically, we can write the flow components of Eq. (1) as:

$$\mathbf{g}(\mathbf{x}, u_j, x_j) = \mathbf{g}_c(u) + L(w - w_j)(3) \tag{3}$$

where the first term corresponds to convective (non-dissipative) flow and the second term is dissipative. As ${\mathbf{g}_c}^T(w - w_j) = 0$ does not provide entropy production (due to mechanical reversibility), dissipation can be calculated as:

$$f_{Sj} = (w - w_j)^T L(w - w_j)$$

Note that the Second Law states that the entropy is non-negative, and, consequently, $f_S \geq 0$. This fact can also be seen from the fact that $L > 0$. Furthermore, the concavity of the entropy production function implies that process systems are dissipative.

The system dynamics in Eq. (1) can be augmented by associating a vector of measured output signals:

$$\mathbf{y} = \mathbf{h}(\mathbf{x}) \tag{4}$$

The measured variables $\mathbf{y}$ are typically intensive variables such as temperature, pressure, composition and voltage (which can be related to the state variables $\mathbf{x}$).

A Lyapunov Function for Process Systems

Together with the definition in Eq. (4), the formulation in Eq. (1) introduces a two-port representation of process systems. Figure 3 illustrates the two different classes of input and output signals of interest for a process system. The inventory flow variables $\mathbf{g}$ correspond to physical flows (heat, fluid, components and electrical current); these variables obey conservation laws, they can be positive or negative and their magnitude and direction are determined by potential differences. Inventory flows can be added and subtracted like inventories. On the other hand, u and y correspond to information flows and are not necessarily conserved. In effect, they are not homogeneous degree 1 functions and follow rules defined by block diagram algebra. The nonlinearity associated with the two-port nature of process networks is difficult to characterize in a generic way, which, in turn, is reflected in the difficulty to develop (and, in effect, the absence of) a general theory for nonlinear process control.

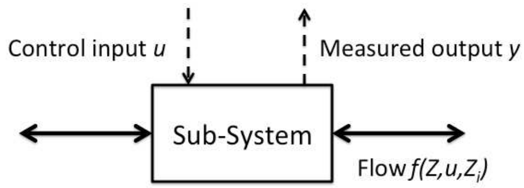

Figure 3: Two port representation of a process unit or sub-system

The concavity of the entropy function serves as a basis for defining a natural Lyapunov function V for a process unit:

$$V(\mathbf{x}, \mathbf{x}^*) = (w - w^*)^T(\mathbf{x} - \mathbf{x}^*) + \sum_{i=1}^{n_p}(x_i - x_i^*)^2 K_i \tag{5}$$

where * denotes variables at the stationary state, $K_i > 0$ and and n_p is the number of phases in the system. The first component of this function is related to the Gibbs tangent plane and it measures the distance between the intensive variables and their reference variables. The second component shows that we need to control as many inventories (extensive) variables as there are phases in the system. The construction allows us to conclude that:

$$V(\mathbf{x}, \mathbf{x}^*) > 0, \quad \text{if } \mathbf{x} \neq \mathbf{x}^*$$

and $V(\mathbf{x}, \mathbf{x}^*) = 0$ iff $\mathbf{x} = \mathbf{x}^*$. From statistical mechanics, it can be shown that S(Z) is twice differentiable, with a local curvature

$$M = \frac{\partial^2 S}{\partial \mathbf{x}_i \partial \mathbf{x}_j} \leq 0$$

The symmetric, non-positive matrix M contains parameters such as the heat capacity and the compressibility. A new differential system can then be defined by the coordinate transformation $dw = Md\mathbf{x}$ Integrating using Newton's theorem, we can express potential differences as a function of the states of different sub-systems, i.e.,

$$w - w_j = Q(\mathbf{x} - \mathbf{x}_j)$$

where

$$Q = \int_0^1 M(\mathbf{x} + (1 - \varepsilon)(\mathbf{x}_j - \mathbf{x})d\varepsilon$$

It follows that the Lyapunov function of Eq. (5) in fact can be written as (local) quadratic function:

$$V(\mathbf{x}, \mathbf{x}^*) = -(w - w^*)^T Q(w - w^*) + \sum_{i=1}^{n_f}(\mathbf{x}_i - \mathbf{x}_i^*)^2 K_i \tag{6}$$

The negative sign follows from the non-positivity of M. This formulation provides a direct link between stability theory of thermodynamics and Lyapunov stability, and can be exploited in controller design, as we will see below.

Quasi Decentralized Networked Control

An approach that reconciles the need for frequently updating the state information of the neighbors of a unit in a network, and the limitations imposed by computation power and potential communication failures is quasi-decentralized control, QDC (Sun and El-Farra, 2008a). QDC refers to a distributed control strategy in which most signals used for control at the unit level are collected and processed locally, while certain signals (the total number of which is kept to a minimum) are transferred between the local units and controllers over a shared communication medium. This approach represents a compromise solution that aims to overcome the stability and performance limitations of decentralized control approaches while avoiding the complexity and lack of flexibility associated with implementing traditional centralized control structures. A key consideration in this strategy is to enforce the desired closed-loop stability and performance objectives of the plant with minimal information transfer between the component subsystems.

Consider a unit-wise description of a process system, consisting of n interconnected processing units, with a state-space representation that follows the generic description in Eq. (1):

$$\begin{aligned} \dot{\mathbf{x}}_1 &= \mathbf{f}_1(\mathbf{x}) + \mathbf{G}_1(\mathbf{x})\mathbf{u}_1 \\ \dot{\mathbf{x}}_2 &= \mathbf{f}_2(\mathbf{x}) + \mathbf{G}_2(\mathbf{x})\mathbf{u}_2 \\ &\vdots \\ \dot{\mathbf{x}}_n &= \mathbf{f}_n(\mathbf{x}) + \mathbf{G}_n(\mathbf{x})\mathbf{u}_n \end{aligned} \tag{7}$$

where $\mathbf{x}_i := [\mathbf{x}_i^{(1)} \ \mathbf{x}_i^{(2)} \ \cdots \ \mathbf{x}_i^{(p_i)}]^T \in \mathbb{R}^{p_i}$ denotes the vector of process state variables associated with the i-th processing unit, $\mathbf{x}^T$ denotes the transpose of a vector $\mathbf{x}$, $\mathbf{x} = [\mathbf{x}_1^T \ \mathbf{x}_2^T \ \cdots \ \mathbf{x}_n^T]^T$, $\mathbf{u}_i := [\mathbf{u}_i^{(1)} \ \mathbf{u}_i^{(2)} \ \cdots \ \mathbf{u}_i^{(q_i)}]^T \in \mathbb{R}^{q_i}$ denotes the vector of manipulated inputs associated with the i-th processing unit, and the functions $\mathbf{f}_i(\cdot)$ and $\mathbf{G}_i(\cdot)$ are sufficiently smooth nonlinear functions.

QDC Controller Design

The objective of QDC is *to design a distributed networked control strategy that stabilizes the individual units (and the overall plant) with minimal information flows between the component subsystems*, thereby reducing the susceptibility of the plant-wide control structure to communication disruptions.

A first step towards this goal is to ensure stability at the unit level, by synthesizing for each unit a feedback controller that enforces closed-loop stability in the absence of communication suspension (i.e., when the sensors of each unit transmit their data continuously to the control systems of the other plant units). To this end, we consider nonlinear feedback controllers of the general form:

$$\mathbf{u}_i = \mathbf{k}_i(\mathbf{x}), \ i = 1, 2, \cdots, n \tag{8}$$

where $\mathbf{k}_i(\cdot)$ is a nonlinear function chosen to ensure that the time-derivative of the Lyapunov function (5), –or of another suitable control Lyapunov function candidate V_i– of system i, along the trajectories of the i-th closed-loop subsystem satisfies a dissipation bound of the form:

$$\dot{V}_i = L_{f_i}V_i + L_{G_i}V_i k_i(\mathbf{x}) \leq -\alpha_i(\|x_i\|) < 0, \ \ i = 1, 2, \cdots, n \tag{9}$$

for some class $\mathcal{K}$ function $\alpha_i(\cdot)$, where $L_{\mathbf{f}}V$ denotes the Lie derivative of function V along the vector field $\mathbf{f}$.

The controller of Eq. (8) is thus designed to compensate for the effect of the interconnected subsystems on the states of the i-th unit. This allows for shaping the time-derivative of the Lyapunov function and obtaining an explicit characterization of the expected closed-loop behavior in terms of a time-varying bound that depends *only on the state of the local unit being controlled*. The stability properties of the individual plant units can therefore be assessed by monitoring their states locally without the need for state measurements from the rest of the plant. This controller-induced property facilitates the design and implementation of a dynamic strategy for managing the flow of information between the plant subsystems.

The implementation of each control law in Eq. (8) requires the availability of state measurements from both the local subsystem being controlled and the units that are connected to it. To reduce the transfer of information between the local control systems as much as possible without sacrificing stability, a set of dynamic models of the interconnected plant units is embedded within the local control system of each unit to provide it with an estimate of the evolution of the states of its neighboring units when measurements are not available. The use of models allows the sensors of the neighboring units to collect and send their data less frequently since the model can provide an approximation of the plant's dynamics. Feedback from one unit to another is performed by updating the state of each model using the actual states of the corresponding unit provided by its sensors at discrete time instances. Figure 4 illustrates the implementation of this model-based control architecture for a unit (Unit 2) whose dynamics are influenced by both an upstream and a downstream unit (Units 1 and 3, respectively). By providing estimates of the states of units 1 and 3 when measurements are unavailable, the embedded models also increase the robustness of local control systems with respect to disturbances from upstream and downstream, as well as to unexpected communication outages that may disrupt the flow of information through the network.

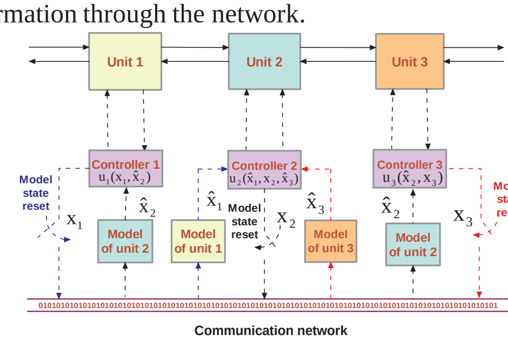

Figure 4: A networked control architecture featuring models of neighboring units, which can act as state observers to increase the robustness of the local control system to disturbances and communication outages

The implementation of the local model-based control law for each unit proceeds as follows:

$$
\begin{aligned}
u_i(t) &= k_i(\widehat{\underline{\mathbf{x}}}^i, x_i(t)),\ i=1,2,\cdots,n \\
\dot{\hat{x}}^i_j(t) &= \widehat{f}_j(\widehat{\underline{\mathbf{x}}}^i, x_i(t)) + \widehat{G}_j(\widehat{\underline{\mathbf{x}}}^i, x_i(t))\hat{u}^i_j(t) \\
\hat{u}^i_j(t) &= k_j(\widehat{\underline{\mathbf{x}}}^i, x_i(t)),\ t\in(t^i_k, t^i_{k+1}) \\
\widehat{x}^i_j(t^i_k) &= x_j(t^i_k),\ \ j=1,\cdots,n,\ ,j\neq i,\ k=0,1,2,\cdots
\end{aligned} \tag{10}
$$

where $\widehat{x}^i_j$ is an estimate of x_j, used by the local control system of the i-th unit, $\widehat{\underline{\mathbf{x}}}^i$ is a vector containing the estimates of the states of the plant units except the i-th unit, i.e., $\widehat{\underline{\mathbf{x}}}^i = [\widehat{x}^{iT}_1,\cdots,\widehat{x}^{iT}_{i-1},\widehat{x}^{iT}_{i+1},\cdots,\widehat{x}^{iT}_n]^T$, $\widehat{f}_j(\cdot)$ and $\widehat{G}_j(\cdot)$ are nonlinear functions that model the dynamics of the j-th unit, and t^i_k denotes the k-th time instance that the states of the models embedded in i-th control system are updated using the state measurements transmitted from the rest of the plant.

Information Update and Communication Policies

The frequency at which the i-th control system (Eq. 10) receives measurements from the other units through the network to update the corresponding model estimates is determined by the update period $h^i_k := t^i_{k+1} - t^i_k$ (*i.e.,* the reciprocal of the communication rate). The update period is an important measure of the extent of information transfer, and can be calculated statically or dynamically.

Using a static communication policy (*i.e.,* the update period is constant and the same for all the units, $t^i_{k+1} - t^i_k := h,\ k=1,2,\cdots,n$) presents the advantage that the minimum allowable communication rate can be calculated off-line prior to plant operation (Sun and El-Farra, 2009). However, a constant communication rate may not always be the best choice, especially in cases when plant operations are subject to unpredictable and time-varying external disturbances.

In this case, a dynamic communication policy that allows the local control system to determine and adjust the necessary communication rate on-line (i.e., during plant operation) based on the state of the plant becomes desirable (Sun and El-Farra, 2010c). The Lyapunov stability constraint derived in Eq. (9) can be used as a guide for establishing and suspending communication. Specifically, consider the plant of Eq. (7) for which each Lyapunov function,V_i, $i=1,\cdots,n$, satisfies Eq. (9) when state measurements are exchanged continuously between the plant units. Consider also the i-th plant unit subject to the model-based networked controller of Eq. (10). Then, an update law of the form:

$$
\widehat{x}^i_j(t^i_k) = x_j(t^i_k),\ \forall\ j\neq i,\ \text{where}\ \dot{V}_i(x_i(t^{i-}_k))\ \geq 0 \tag{11}
$$

where $x_i(t^{i-}_k) = \lim_{t\to t^{i-}_k} x_i(t)$, ensures that $\dot{V}_i(x_i(t^i_k)) < 0$.

The implementation of this policy thus requires that each local control system monitor the evolution of the corresponding Lyapunov function to determine when the models' states must be updated and communication re-established. Specifically, if V_i begins to increase at any time, the sensor suites of the neighboring units are prompted to send their data over the network to update their corresponding disturbance models embedded in the i-th unit and re-set the model estimation errors to zero. Communication from the rest of the plant to the i-th unit is then suspended for as long as the Lyapunov function V_i continues to decay. In this way, only units that require attention (i.e., those on the verge of instability) receive measurement updates, while the rest do not. This targeted update strategy is more robust to unpredictable disturbances (compared with a static policy with a constant update period) and allows the plant to respond quickly in an adaptive fashion to a unit that requires immediate attention. In addition to stability considerations, performance specifications can also be incorporated into the communication policy by appropriate modification of the update law. For example, an update law of the form:

$$
\begin{aligned}
\widehat{x}^i_j(t^i_k) &= x_j(t^i_k), \\
\dot{V}_i(x_i(t^{i-}_k)) &\geq -(1-\beta)\alpha_i(\|x_i(t^{i-}_k)\|)
\end{aligned} \tag{12}
$$

where$\beta\in(0,1)$, ensures that not only does V_i decay monotonically along the trajectories of the i-th networked closed-loop subsystem, but also that it does so at a certain minimum rate (which is a fraction of the rate prescribed for the non-networked plant). By examining the above communication logic, it can be seen that an update law with $\beta\neq 1$ imposes a stronger restriction on the growth of the model estimation error than the stability-based logic of Eq. (11), in the sense that it limits the extent to which model estimation errors (resulting from communication suspensions) can slow down the non-networked closed-loop response. This in turn implies –quite intuitively– that accommodating the additional performance requirements comes at the expense of an increase in the rate at which the i-th control system needs to receive measurement and disturbance updates from the rest of the plant.

The arguments above have dealt with the *frequency* of information exchange between the units. The *extent* of data exchange between units is driven by the number of models that need to be incorporated in each control system, which, in turn depends on the structure of the plant and the connectivity of the units.

Consider again the network structures in Figure 1. For example, in the presence of weak integration (*e.g.,* a low inventory recycle flow), the integrated process network in Figure 2 reduces to a simple cascade (series) connection of units. Since in this case unit 1 receives no input from the other units, the number of models embedded in its control system is zero. Unit 2 receives input from unit 1, so a model of unit 1 needs to be included in the local control system of unit 2. If any interactions exist between units 2 and 3 (*e.g.,* through the influence of the downstream pressure on the mass flow between the two units), Unit 2 should also incorporate a model of Unit 3. Unit 3 receives two inputs - one directly from unit 2 and another indirectly from unit 1 (which feeds into unit 2) - and therefore requires two models: one to estimate the behavior of unit 2 and another to estimate the behavior of unit 1.

If computational load becomes an issue (e.g., when N is large), it is possible replace some or all of the models with simpler zero-order hold models of the form:

$\dot{\hat{x}}^i_j(t) = 0,\ t\in[t^i_k, t^i_{k+1})$

This corresponds to the case in which each control system holds the last available measurement from a given unit until the next one is made available at the update time. It should be noted, however, that while this strategy helps reduce the number of models that need to be solved, it may increase the communication requirements between the component subsystems relative to that associated with the model-based scheme. In general, it is expected that the estimate generated by a physically-based model outperforms the estimate generated by a zero-order hold strategy (unless the plant-model mismatch is significant).

Process Networks Networks with Tight Integration

Let us consider a generic integrated network of chemical process systems, such as the one in Figure 2 c), consisting of N process in series. We use the terms "integrated" and "integration" to denote the presence of a recycle connection R, intended to transfer inventory from the last unit to the first, as illustrated in Figure 5.

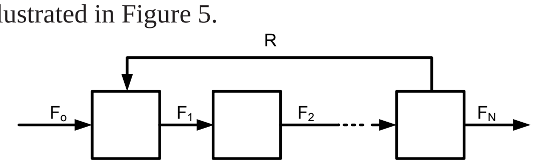

Figure 5: Generic integrated process system, featuring N units and an inventory recycle connection

The mathematical model describing the evolution of an inventory (e.g., material, energy) of this system can be written (Kumar and Daoutidis, 2002; Baldea and Daoutidis, 2007) as:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \sum_{j=0,N} g_j(\mathbf{x})u_j + Rc\sum_{j=1}^{N-1} k_j g_j(\mathbf{x})u_j + Rcg_R(\mathbf{x})u_r \quad (13)$$

where $u_j = (F_j/F_{j,s})$ represent (possibly manipulated) dimensionless variables that correspond to the inventory flows, $k_j = F_{j,s}/F_{R,s}, j = 1 \ldots N$, and $g_j(\mathbf{x})$ and $g_R(\mathbf{x})$ are vector functions of appropriate dimensions. The subscript s denotes steady state values. The model explicitly identifies the terms that involve the process port flows ($j = 0,N$), the internal inventory flows ($j = 1,\ldots,N-1$) and the recycle flow ($j = R$). In order to investigate the impact on the presence and magnitude of inventory recycling on the process dynamics, Eq. (13) also makes use of the recycle number Rc, a process-wide dimensionless number expressed as the ratio of the (steady state) rate at which inventory is recycled to the rate at which inventory is introduced in the process through the inlet port:

$$Rc = \frac{R_s}{F_{os}} \quad (14)$$

This perspective allows us to delineate two limiting case:

- $Rc \ll 1$, i.e., the flow rate of the recycle stream is small compared to the flow rate of fresh feed. Intuitively, in this case the dynamics of the process network in Figure 5 will not differ significantly from the dynamic behavior of a cascade of Nprocess units in series as in Figure 1 a).
- $Rc \gg 1$, which corresponds to significant inventory recycling. Intuitively, in this case the contribution of the last two (internal inventory flow and inventory recycle) terms in Eq. (13) to the evolution of the states $\mathbf{x}$ is significantly higher than the contribution of the first two, and we can expect that the dynamic behavior of the process represent a significant departure from that of a cascade system.

Given the current trend towards ever tighter integration of chemical plants through material recycling and energy recovery, the case where Rc is a large number is of elevated interest. It will constitute the focus of the developments below. To this end, let us rewrite the model in Eq. (13) in a more general form as:

$$\dot{\mathbf{x}} = f(\mathbf{x}) + \mathbf{G}^s(\mathbf{x})\mathbf{u}^s + \frac{1}{\varepsilon}\mathbf{G}^l(\mathbf{x})\mathbf{u}^l \quad (15)$$

where, as above, $\mathbf{x}$ is the vector of unit inventories, $\mathbf{u}^s \in \mathbb{R}^{m^s}$ is the vector of scaled input variables that correspond to the small input/output of inventory from the process, $\mathbf{u}^l \in \mathbb{R}^{m^l}$ is the vector of scaled input variables that correspond to the large internal inventory flows (including inventory recycling), $\varepsilon = 1/Rc$ and $\mathbf{G}^s(\mathbf{x})$ and $\mathbf{G}^l(\mathbf{x})$ are matrices of appropriate dimensions. The model in Eq. (15) is a nonstandard singularly perturbed system of equations Kumar and Daoutidis (1999); its dynamics thus have the potential to exhibit a multiple time scale behavior. The rational approach for addressing the control of such systems involves the properly coordinated synthesis of separate fast and slow controllers so that overall stability, output tracking and disturbance rejection performance can be achieved. The design of such controllers is carried out using separate reduced-order models that describe the dynamics in the fast and slow time scales. These issues are addressed below.

Reduced Order Modeling

We define a fast, "stretched" time scale $\tau = t/\varepsilon$. Rewriting Eq. (15) in this time scale and considering the limit case $\varepsilon \to 0$ (which physically corresponds to an infinitely high recycle number or, equivalently, an infinitely high inventory recycle rate), we obtain a description of the fast dynamics of the process:

$$\frac{d\mathbf{x}}{d\tau} = \mathbf{G}^l(\mathbf{x})\mathbf{u}^l \quad (16)$$

Note that the above model only involves the (large) flowrates $\mathbf{u}^l$ of the inventory recycle and internal inventory streams, and does not involve the (smaller) flowrates $\mathbf{u}^s$ of input and output of inventory to and, respectively, from the process. Examining Eq. (13), it is intuitive that the internal inventory flows do not affect the total inventory in the process, and that the total inventory is affected only by the flow rates $\mathbf{u}^s$ of the input/output streams. In other words, Eq. (16) effectively describes the dynamics of the individual unit inventories in the recycle loop and does not capture the overall (process-level) changes in inventory. We can use this observation to further infer that:

- The differential equations in Eq. (16) are not linearly independent. By consequence, the steady state condition $0 = \mathbf{G}^l(\mathbf{x})\mathbf{u}^l$for the fast dynamics in Eq. (16) does not specify a set of isolated equilibrium points, but rather a low-dimensional equilibrium subspace (manifold), in which a slow component of the system dynamics evolves. The slow component of the process dynamics is associated with the evolution of the total inventory of the process.

- Based on physical considerations, at most $C+1$ equations (where C is the number of chemical components) are required to completely capture the overall and component-wise material balance, and the overall energy balance of the process. Thus, we can expect that the dimension of the system of equations describing the slow dynamics of the process system to be at most $C+1$, and the equilibrium manifold of the fast dynamics to be at most $C+1$-dimensional.

In order to obtain the description of the slow dynamics, we will assume that it is possible to isolate a set of $n-(C+1)$ linearly independent constraints corresponding to the fast dynamics, i.e., that the matrix $\mathbf{G}^l(\mathbf{x})$ can be decomposed as:

$$\mathbf{G}^l(\mathbf{x}) = \mathbf{B}(\mathbf{x})\bar{\mathbf{G}}^l(\mathbf{x}) \tag{17}$$

with $\mathbf{B}(\mathbf{x}) \in \mathbb{R}^{n\times(n-(C+1))}$ being a full column rank matrix and the matrix $\bar{\mathbf{G}}^l(\mathbf{x}) \in \mathbb{R}^{(n-(C+1))\times m^l}$ having linearly independent rows.

Multiplying Eq. (15) by ε and considering the limit of an infinitely high recycle flow rate (i.e., $\varepsilon \to 0$) in the original time scale t, we obtain the linearly independent constraints $\bar{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l = 0$ which correspond to the quasi-steady state of the fast dynamics and must be satisfied in the slow time scale. Also in the limit as $\varepsilon \to 0$, the terms $(\bar{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l)/\varepsilon$ which correspond to the differences of large flow rates present in the inventory equations of every process unit, become indeterminate. Defining $\mathbf{z} = \lim_{\varepsilon\to 0} \frac{\bar{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l}{\varepsilon}$ as the vector of these finite, but unknown terms, the system in Eq. (15) becomes:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) + \mathbf{G}^s(\mathbf{x})\mathbf{u}^s + \mathbf{B}(\mathbf{x})\mathbf{z} \\ 0 &= \bar{\mathbf{G}}^l(\mathbf{x})\mathbf{u}^l \end{aligned} \tag{18}$$

which represents a Differential Algebraic Equation model of the slow dynamics of the process, induced by the presence of significant inventory recycling.

Hierarchical Control of Integrated Processes

The two-time scale behavior of the inventory of integrated processes suggests the use of a hierarchical control structure with two tiers of control action: i) distributed control, addressing control objectives for individual process units in the fast time scale and, ii) supervisory control, addressing control objectives for the overall process in the slow time scale To this end, let us complete the description of Eq. (18) with a vector of output variables $\mathbf{y} = \mathbf{h}(\mathbf{x}) = [\mathbf{y}^l\,\mathbf{y}^s]^T$. $\mathbf{y}$ extends the definition of the output vector in (4) to the level of the integrated process network, where $\mathbf{y}^l$ denote the subset of the output variables that are associated with control objectives for the individual process units (typically involving the control of local inventories) and $\mathbf{y}^s$ those that are associated with control objectives for the overall network, *e.g.*, production rate, total inventory and product quality.

The above time scale decomposition provides a transparent framework for the selection of manipulated inputs that can be used for control in the two time scales. Specifically, it establishes that the output variables $\mathbf{y}^l$ need to be controlled in the fast time scale, using the large flow rates$\mathbf{u}^l$, while the control of the variables $\mathbf{y}^s$ is to be considered in the slow time scale, using the variables $\mathbf{u}^s$. Moreover, the reduced-order approximate models for the fast dynamics (Eq. (16)) and slow dynamics (the state-space realization of Eq. (18)) can serve as a basis for the synthesis of well-conditioned (nonlinear) controllers in each time scale. Note that, due to the dependence of the algebraic constraints in Eq. (18) on the inputs $\mathbf{u}^l$, the fast controller design must precede the design of the slow controller.

As stated in the previous section of this paper, the design of the unit-level controllers can be addressed as a collection of decentralized, networked control problems using *e.g.*, the Lyapunov-based controllers in Eq. (8). The supervisory controller is typically a nonlinear, multivariable optimization-based construct that addresses plant-wide control objectives, such as inventory and product quality control, as well as energy management by modifying the setpoints and control objectives of the decentralized controllers.

It can be shown (Baldea et al., 2010) that, provided that the fast controllers are designed to exponentially stabilize the fast dynamics, the stability of the overall network is determined by the stability of the supervisory control system in the slow time scale. From this perspective, the composite control approach delineated above affords the control engineer a significant amount of design flexibility. The availability of a reduced-order model (i.e., a state-space realization of Eq. (18)) of the slow dynamics that is non-stiff and well-conditioned means that any of the available inversion- or optimization-based controller design methods (Kravaris and Kantor, 1990; Mayne et al., 2000; Zavala and Biegler, 2009) can be used to design a stabilizing supervisory control system for the slow dynamics, guaranteeing at the same time stability at the process level. The composite control approach delineated above is also beneficial from an implementation point of view: the reduced dimensions and improved conditioning (reduced stiffness) of the supervisory controller (compared to a controller based on the original model (15) will result in reduced online calculation times and less sensitivity to noise and disturbances.

Information Transfer and Communication Policies at the Process Network Level

Relying on a reduced-order model for supervisory controller synthesis presents the benefit of reducing the information transfer requirements at the level of the entire process network. Following the developments above, the supervisory controller designed based on the reduced-order model of the slow process dynamics guarantees stability at the network level, provided that i) the quasi-decentralized controllers ensure exponential stability of the fast dynamics and, ii) there are no communication failures between the process and the supervisory controller. Note that the latter provision allows for a continuous updating of any model that is used in computing the controller output.

The ideas developed above can serve as a basis for understanding the role of communication constraints and potential communication failures on stability at the level of the process network.

To this end, we will resort to a generalization of the Tellegen theorem (Jillson and Ydstie, 2007) to extend Eq. (6) and derive a Lyapunov function for a process network with multiple nodes. This approach uses the fact that the intensive variables are unique (which follows from the concavity of the entropy function) to show that we have:

$$\sum_{nodes} w^T \left(\frac{d\mathbf{x}}{dt} - \mathbf{f} \right) = \sum_{ports} w^T \mathbf{g} - \sum_{flows} (w_i - w_j)^T (\mathbf{g}_i - \mathbf{g}_j) \quad (19)$$

The expression above gives the entropy balance for the network since:

$$\frac{dS}{dt} = \sum_{nodes} w^T \frac{d\mathbf{x}}{dt} \quad (20)$$

and the entropy can serves compute a network Lyapunov function at the process network level, with

$$\begin{aligned} \frac{dV_{network}}{dt} &= \sum_{ports} \bar{w}^T \bar{\mathbf{g}} + \sum_{nodes} \bar{w}^T \bar{\mathbf{f}} - \sum_{flows} (\bar{w}_i - \bar{w}_j)^T (\bar{\mathbf{g}}_i - \bar{\mathbf{g}}_j) \quad (21) \\ &+ \sum_{nodes} \sum_{phases} K_j \bar{\mathbf{x}}_j \frac{d\bar{\mathbf{x}}_j}{dt} \end{aligned}$$

and the function:

$$V_{network} = \sum_{nodes} V_i \geq 0 \quad (22)$$

is defined by summing the Lyapunov functions (5) of each each node (process unit).

An adaptive communication policy at the process network level can subsequently be defined using the same ideas applied at the level of a process unit. A similar Lyapunov stability constraint as the one derived in Eq. (9) can be established at the level of the network, using the Lyapunov function (22), *i.e.,*

$$\dot{V}_{network} = \leq -\alpha(\|\mathbf{x}\|) < 0 \quad (23)$$

$\dot{V}_{network}$ can subsequently be used as a guide for defining the minimum update requirements of the model built in the supervisory controller and, consequently, the network level communication needs. For example, an update law of the form:

$$\widehat{\mathbf{x}}(t_k) = \mathbf{x}(t_k), \text{ when } \dot{V}(\widehat{\mathbf{x}}(t_k^-)) \geq 0 \quad (24)$$

can be considered.

Based on the considerations outlined in the previous section, the dynamics of the network Lyapunov function (22) are much slower than the evolution of the corresponding unit-level functions (5), and the network-level update frequency that results from applying the update law (24) is significantly slower than the unit-level update frequency defined by (11).

Conclusions and Outlook

The increasing need to improve operational efficiency and lower energy and utility consumption have given rise to a new class of chemical plants - the process network - featuring tight integration between individual units (process systems) through material, energy and information flows. Integration gives rise to strong dynamic interactions, causing an overall, network-level dynamics to emerge.

The complexity of this behavior, and its impact on process control, requires a paradigm shift in our analysis tools. Uniting concepts from classical thermodynamics, singular perturbation theory, Lyapunov stability and networked control into a broadly applicable framework for the analysis and control of integrated process networks, the paper presented a novel avenue for addressing the aforementioned challenges. We have advocated the use of a hierarchical networked approach, consisting of a set of quasi-decentralized controllers at the unit level, and a supervisory controller which addresses control objectives at the level of the process network, and argued that the proposed structure represents a powerful tool for ensuring stability and performance for complex process networks.

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