Part I

Preliminaries

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Excerpt
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1 Introduction

Integrated process systems, such as the one in Figure 1.1, consisting of multiple reaction and separation units, heat integrated and interconnected through material recycle streams, represent the rule rather than the exception in the modern process industries. The dynamics and control of such systems present distinct challenges: in addition to the nonlinear behavior of the individual units, the feedback interactions caused by the recycle connections typically give rise to a more complex, *overall* process dynamics. The use of design modifications, such as surge tanks and unit oversizing, and the choice of mild operating conditions, preventing the propagation of disturbances through the plant, initially allowed the problem of controlling chemical plants with material recycling to be dealt with at the unit level, using the "unit operations" approach (Umeda *et al.* 1978, Stephanopoulos 1983): control loops were designed for each unit, their tuning being subsequently adjusted to improve the operation of the entire plant. However, the shortage of raw materials, rising energy prices, and the need to lower capital costs have, over the past few decades, spurred the process industry's tendency to build "lean,"[1] integrated plants, relying heavily on material recycles and energy recovery.

Owing to dwindling fossil-fuel supplies (and the associated increase in the cost of energy), improving energy efficiency has become particulary important. Energy integration and recovery are key enablers to this end. Fundamentally, energy integration involves identifying the energy sources and sinks *within* a system and establishing the means for energy transfer between them,[2] thereby reducing the use of external energy sources and utility streams. Chemical reactors and distillation columns inherently contain such sources and sinks and clearly constitute prime targets for energy integration. Numerous energy-integrated process configurations have been proposed at the conceptual level: reactor-feed effluent heat exchanger systems, heat exchanger networks, heat-integrated and thermally coupled distillation columns, etc.

The design and optimization of energy integration schemes has been an active research area from the early days of process systems engineering. Initial efforts (Rathore *et al.* 1974, Sophos *et al.* 1978, Nishida *et al.* 1981) focused on the

[1] With little, if any, design margin (Stephanopoulos 1983).
[2] Assuming, of course, that such transfer is thermodynamically feasible.

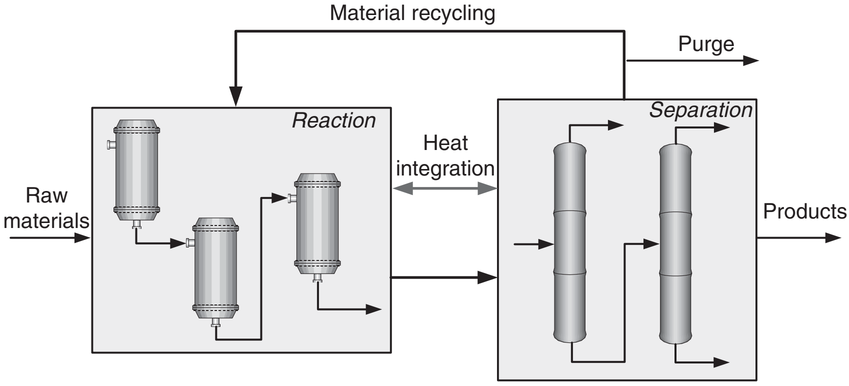

Figure 1.1 An integrated process system.

synthesis of energy-integrated processes using heuristics. Later, pinch analysis (Linnhoff and Hindmarsh 1983, Linnhoff *et al.* 1983) and bounding techniques for utility usage (Morari and Faith III 1980, Andrecovich and Westerberg 1985a, Mészáros and Fonyó 1986) were introduced, and they have since seen numerous successful applications in the synthesis of new energy integration systems as well as in plant retrofits. Mathematically rigorous formulations such as mixed-integer linear/nonlinear programming (Andrecovich and Westerberg 1985b, Floudas and Paules 1988, Yeomans and Grossmann 1999, Wei-Zhong and Xi-Gang 2009) and genetic algorithms (Wang *et al.* 1998, Yu *et al.* 2000, Wang *et al.* 2008) were subsequently developed to ensure the *optimality* of integrated processes. The significant reduction in capital and operating costs resulting from energy integration is now well documented (Muhrer *et al.* 1990, Yee *et al.* 1990, Annakou and Mizsey 1996, Reyes and Luyben 2000b, Westerberg 2004, El-Halwagi 2006, Diez *et al.* 2009).

As integrated process designs continued to gain acceptance owing to their improved economics, the process control community also became aware of the distinct challenges posed by the operation of such plants, and a number of research studies ensued.

An initial theoretical study (Gilliland *et al.* 1964) established that, for a simple plant model consisting of a continuous stirred-tank reactor (CSTR) and a distillation column, the material recycle stream increases the sensitivity to disturbances together with increasing the time constant of the overall plant over those of the individual units. Moreover, it was shown that in certain cases the plant can become unstable even if the reactor itself is stable.

Several papers have since focused on either reaction–separation–recycle processes (Verykios and Luyben 1978, Denn and Lavie 1982, Luyben 1993a, Scali and Ferrari 1999, Lakshminarayanan *et al.* 2004) or individual multi-stage processes (Kapoor *et al.* 1986) and have shown that recycle streams can "slow down" the overall process dynamics (described by a small number of time constants) compared with the dynamics of the individual units, and may even lead to the recycle loop being unstable. An analogy was drawn (Denn and Lavie 1982) between the recycle system and a closed-loop system with positive feedback, thus concluding that the presence of a recycle stream may increase the overall response time of the plant and may increase the steady-state gain by a significant amount. The effect of the recycle on the zero dynamics was studied (Jacobsen 1999), and it was demonstrated that the feedback effect of the recycle stream can induce a non-minimum-phase behavior even for the transfer function of single units. Most of the aforementioned analyses were based on simplified transfer function models and linear analysis tools. More recently, a number of studies (Morud and Skogestad 1994, Mizsey and Kalmar 1996, Bildea *et al.* 2000, Pushpavanam and Kienle 2001, Kiss *et al.* 2002, Larsson *et al.* 2003, Kiss *et al.* 2005, Vasudevan and Rangaiah 2009) have indicated that, even in simple, prototype models of reactor–separator systems, the recycle stream can lead to strongly nonlinear overall dynamics, manifested in the form of multiple steady states, limit cycles or even chaotic behavior (Jacobsen and Berezowski 1998). The above results indicate that recycle streams are responsible for the complex behavior of process systems, and place the control of recycle loops at the heart of the plant-wide control problem.

The necessity to develop systematic procedures for coordinating distributed (i.e., unit-level) and plant-wide control objectives and strategies was thus acknowledged, and several studies have been dedicated to this purpose. Dynamic process control (DPC) (Buckley 1964) was the first control strategy to divide the control actions for a process plant (with or without recycle streams) into two categories: material-balance control (necessary for the management of the plant's operation in the presence of *low-frequency* (slow) changes, such as production flow rate), and product-quality control (for countering the effects of *high-frequency* (fast) disturbances acting at the unit level). Although it was a pioneering effort at the time, DPC is not effective in modern, tightly integrated plants, where the strong coupling induced by mass and energy recycling leads to the propagation of disturbances across the frequency spectrum through multiple process units.

Later on, the complexities introduced by process integration were fully acknowledged by researchers in the field, and motivated a series of studies on the effect of the material recycle streams on the design, controllability, and control structure selection for specific reaction/separation processes.

Luyben (1993a) provided valuable insights into the characteristics of recycle systems and their design, control, and economics, and illustrated the challenges caused by the feedback interactions in such systems, within a multi-loop linear control framework. Also, in the context of steady-state operation, it was shown (Luyben 1994) that the steady-state recycle flow rate is very sensitive to disturbances in feed flow rate and feed composition and that, when certain control configurations are used, the recycle flow rate increases considerably facing feed flow rate disturbances. This behavior was termed "the snowball effect."

The publication of an actual industrial plant-wide control problem, the Tennessee Eastman challenge process (Downs and Vogel 1993) generated several valuable studies on the control of recycle processes, both within a linear control framework (McAvoy and Ye 1994, Banerjee and Arkun 1995, Lyman and Georgakis 1995, Ricker 1996, Wu and Yu 1997, Larsson *et al.* 2001, Wang and McAvoy 2001, Tian and Hoo 2005) and within a nonlinear (Ricker and Lee 1995) control framework.

The control challenges posed by the feedback interactions induced by the recycle were also illustrated in studies carried out on other problems, such as supercritical fluid extraction (Ramchandran *et al.* 1992) and recycle reactors (Kanadibhotla and Riggs 1995, Antoniades and Christofides 2001).

The above results have revealed that process integration severely limits the effectiveness of the traditional, unit-operations approach, with fully decentralized controllers for individual process units, which assumes that the combination of these controllers (possibly with some adjustments) would constitute an effective control scheme for the overall plant. The strong coupling between the control loops in different process units in an integrated process system was thus recognized early on (Foss 1973) as a major issue that must be addressed in a plant-wide control setting, and several generic strategies to this end have been proposed.

Drawing on the ideas of Buckley (1964), Price and Georgakis (1993) provided guidelines for designing inventory-control structures that are consistent with the main mass and energy flows of the process, surmising that the best performance is achieved when some empirically selected control loops are tightly tuned and the others have loose tuning. Banerjee and Arkun (1995) presented a procedure for screening possible control configurations for a plant, using linearized models for assessing the robustness of the control loops, without specifically accounting for the presence of mass or energy recycles. Georgakis (1986) suggested the use of empirically identified extensive fast and slow variables for the synthesis of controllers for a process. In Ng and Stephanopoulos (1996), a hierarchical procedure for plant-wide controller synthesis is proposed, recommending a multiple-time-horizon control structure, with the longest horizon being that of the plant itself. Luyben *et al.* (1997) presented a tiered, heuristic controller design procedure for process systems that addresses both energy management and inventory and product purity control. A multi-step heuristic design procedure was also introduced in Larsson and Skogestad (2000), advocating a top-down plant analysis for identifying control objectives, followed by a bottom-up controller implementation. A set of criteria for designing and assessing the performance of plant-wide controllers has been proposed in Vasudevan and Rangaiah (2010).

In a different vein, Kothare *et al.* (2000) formally defined the concept of partial control on the basis of the practical premise that, in some cases, complex chemical processes can be reasonably well controlled by controlling only a small subset of the process variables, using an equally small number of "dominant" manipulated variables. An analysis method for identifying the dominant variables of a process was proposed in Tyreus (1999).

Using the concept of passivity, Farschman *et al.* (1998), Ydstie (2002), Jillson and Ydstie (2007), Bao and Lee (2007), Rojas *et al.* (2009) introduced a formal framework for stability analysis and stabilization of process systems using decentralized control, subject to thermodynamic and equipment constraints. Within this context, the passivity/dissipativity properties of individual units in a process are established using thermodynamic arguments, and existing results for the interconnections of passive/dissipative systems (*e.g.*, Desoer and Vidyasagar 2009) are used to determine the closed-loop stability properties of the overall process. Within this framework, the stabilization of the process dynamics is achieved via decentralized inventory controllers.

Following the ideas of Morari *et al.* (1980), Skogestad (2000, 2004), and Downs and Skogestad (2009) proposed an algorithm for determining a "self-optimizing" plant-wide control structure, consisting of identifying a set of controlled variables that, when kept at constant setpoints, indirectly lead to near-optimal operation with respect to a given economic objective. The proposed approach relies on steady-state optimization and thus additional simulation steps are needed in order to select the control structure with the best dynamic performance.

A hierarchical decision procedure for formulating control structures on the basis of the minimization of economic penalties, while also accounting for the process dynamics, was also proposed in Zheng et al. (1999), following Douglas's hierarchical method for conceptual process design (Douglas 1988). However, the formulated control structures often require that additional surge capacities be provided/installed in the process in order to achieve reasonable dynamic performance, and may therefore increase the capital cost of the plant.

McAvoy (1999) advanced the use of optimization calculations at the controller design stage, proposing the synthesis of plant-wide control structures that ensure minimal actuator movements. The initial work relying on steady-state models (McAvoy 1999) was recast into a controller synthesis procedure based on linear dynamic plant models (Chen and McAvoy 2003, Chen *et al.* 2004), whereby the performance of the generated plant-wide control structures was evaluated through dynamic simulations.

The plant-wide control techniques referenced above are generally based on the use of linear, multi-loop, decentralized control structures. Model predictive control (MPC) constitutes a different class of control techniques, consisting of determining the manipulated inputs of a process by minimizing an objective function capturing either the deviation between the process states and the corresponding setpoints (Prett and Garcia 1988) or an economic objective (Edgar 2004, Diehl *et al.* 2011), possibly under the physical constraints associated with the plant operation, over a receding time horizon. MPC can be applied to plant-wide control problems, having multivariable control and constraint-handling capabilities. However, calculating the manipulated inputs involves the solution of an often computationally expensive optimization problem (owing to the use of high-dimensional plant models in the problem formulation) at each time step, and, although they are numerous (Qin and Badgwell 2003), successful practical implementations have been confined to the realm of plants with *slow dynamics*, such as oil refineries.

A more recent direction relies on the use of *distributed* model-based control strategies as an alternative to centralized controllers (based on the full plant model) for large, integrated systems. Local controller design has been approached both via MPC techniques (see, e.g., Zhu *et al.* 2000, Zhu and Henson 2002, Venkat *et al.* 2006, 2008, Rawlings and Stewart 2008, Liu *et al.* 2008, 2009, Scattolini 2009, Stewart *et al.* 2010) and as an agent-based problem (e.g., Tatara *et al.* 2007, Tetiker *et al.* 2008). Typically, the analysis and implementation of distributed architectures considers the plant as a set of interconnected subsystems, with each subsystem being assumed to have a controller that exchanges (some of the) subsystem state information with the controllers of all the other subsystems. Within the distributed MPC framework, it has been shown that predictive control applications are possible for large plants with *fast dynamics*, since closed-loop stability is assured at all times by formulating the optimization problem to be feasible at every iteration.

The challenge posed by establishing and maintaining communication between distributed controllers has also stimulated research in the area of networked process control (El-Farra *et al.* 2005, Mhaskar *et al.* 2007, Sun and El-Farra 2008, 2010). The central issue of maintaining closed-loop stability in the presence of bandwidth constraints and limitations in transmitter battery longevity is typically addressed by a judicious distribution of computation and communication burdens between local/distributed control systems and a centralized supervisory controller.

In general, MPC implementations (including those cited above) rely on the use of data-driven linear plant models for computing the optimal plant inputs. However, chemical processes are inherently nonlinear, and these models lose accuracy when economic circumstances call for operating the process under conditions that differ significantly from the operating region in which model identification was carried out. The implementation of MPC to processes with nonlinearities (nonlinear MPC, NMPC) remains one of the most difficult problems associated with plant-wide MPC applications: because NMPC relies on using a nonlinear dynamic model, a nonlinear optimization problem must be solved at each time step in order to calculate the optimal plant inputs, and the computation time scales very unfavorably with the dimension of the plant model. To date, NMPC implementations for integrated processes (e.g., Ricker and Lee 1995, Zhu and Henson 2002) have made extensive use of modeling and controller simplifications in order to reduce computational complexity.

Many of the aforementioned heuristic decentralized control synthesis approaches rely on engineering judgement rather than rigorous analysis. On the other hand, the implementation of advanced, model-based, control strategies for process systems is hindered by the often overwhelming size and complexity of their dynamic models. The results cited above indicate that the design of fully centralized controllers on the basis of entire process models is impractical, such controllers being almost invariably ill-conditioned, difficult to tune, expensive to implement and maintain, and sensitive to measurement errors and noise. Thus, the need to find a rational and transparent paradigm for synthesizing process-wide model-based nonlinear control structures has emerged as (and remains) a key issue in modern process control. This need is also an integral part of the ongoing smart manufacturing initiative of twenty-first-century industry (Christofides *et al.* 2007, Edgar and Davis 2009).

A salient feature of integrated process systems is their *multiple-time-scale behavior*, owing to physical and chemical phenomena that occur at vastly different rates, a feature that translates into their dynamic models being described by stiff systems of differential equations. Stiffness represents in effect one of the main hindrances to the implementation of plant-wide model-based control techniques. It is at the origin of the ill conditioning of linear and nonlinear inversion-based and optimization-based controller designs, and greatly increases the difficulty of obtaining a numerical solution for optimal control problems.[3]

Although repeatedly acknowledged (directly or unwittingly) in plant-wide control studies (Buckley 1964, Georgakis 1986, Price and Georgakis 1993, Ng and Stephanopoulos 1996, Wang and McAvoy 2001, Lakshminarayanan *et al.* 2004), the issue of time-scale multiplicity at the plant level has not been accounted for in a mathematically rigorous way until recently (Kumar and Daoutidis 2002, Baldea and Daoutidis 2007, Jogwar *et al.* 2009). The goal of this text is thus to explain the origin of time-scale multiplicity at the process level, and to elucidate its impact on the development of systematic, hierarchical controller design procedures for the control of integrated process systems featuring material recycling and/or energy recovery. To this end, we will make use of generic, prototype systems that are representative for the design and operation of broad classes of integrated processes. Moreover, we will introduce a novel set of *process-level dimensionless numbers* that capture the salient *steady-state* design features of the processes under consideration, and establish a connection between these design features and process *dynamics and control*. Our goal is therefore to develop fundamental, rather than heuristic, results that are widely applicable in process systems engineering and beyond our discipline. Evidently, we illustrate the use of these results through numerous examples as well as an extensive case study at the end of each chapter.

The book is organized as follows. Chapter 2 provides an introduction to the mathematical description of multiple-time-scale systems and to singular

[3] The term *ill conditioning* refers to the condition number of the linearized model of a plant, defined as $\gamma = \lambda_{\max}/\lambda_{\min}$, with λ being the eigenvalues of the model. For large values of γ, the plant dynamics will span more time scales (its time constants being defined as the reciprocals of the eigenvalues), and the larger γ is, the more ill-conditioned (stiff) the plant is considered to be. By way of consequence, model-based controllers that are designed on the basis of inverting the (linear or nonlinear) plant model will be ill-conditioned as well. Ill-conditioned controllers tend to amplify disturbances and modeling errors, and even induce closed-loop instability.

perturbation theory used in their analysis. Chapter 3 discusses the design, dynamics and control of integrated process systems with significant material recycle streams. Chapter 4 focuses on processes with *small* purge streams (an important and common feature in chemical plants). Chapter 5 provides a modeling and model reduction framework for process systems featuring purge streams *and* large material recycle streams. The impact of energy recovery on process dynamics and control is analyzed in Chapter 6, while Chapter 7 concentrates on the dynamic behavior of process systems with high energy throughput.