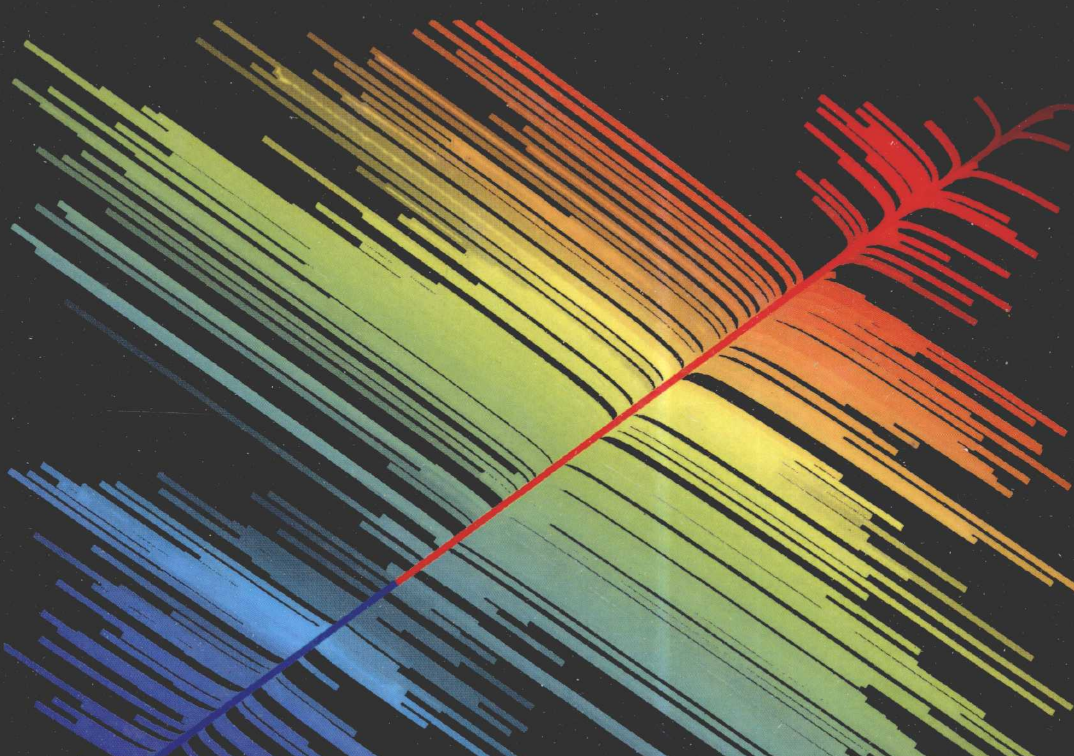
Dynamics and Nonlinear Control of Integrated Process Systems

Michael Baldea and Prodromos Daoutidis



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Dynamics and Nonlinear Control of Integrated Process Systems

Presenting a systematic model reduction and hierarchical controller design framework for broad classes of integrated process systems encountered in practice, this book first studies process systems with large material recycle and/or with small purge streams, followed by systems with energy integration. Step-by-step model reduction procedures are developed to derive nonlinear reduced models of the dynamics in each time scale. Hierarchical control architectures, consisting of coordinated levels of control action in different time scales, are proposed for each class of process systems considered in order to enforce stability, tracking performance, and disturbance rejection. Numerous process applications are discussed in detail to illustrate the application of the methods and their potential to improve process operations. Matlab codes are also presented to guide further application of the methods developed and facilitate practical implementations.

Michael Baldea is Assistant Professor in the Department of Chemical Engineering at The University of Texas at Austin. Prior to joining The University of Texas, he held industrial research positions with Praxair Technology Center in Tonawanda, NY and GE Global Research in Niskayuna, NY. He has received several research and service awards, including the Model Based Innovation Prize from Process Systems Enterprise and the Best Referee Award from the *Journal of Process Control*, and has co-authored over 60 papers and presentations.

Prodromos Daoutidis is Professor in the Department of Chemical Engineering and Materials Science at the University of Minnesota. He also held a position as Professor at the Aristotle University of Thessaloniki in 2004–2006. He is the recipient of several research and teaching awards and recognitions, including the NSF CAREER Award, the Model Based Innovation Prize from Process Systems Enterprise, the Ted Peterson Award of CAST, the George Taylor Career Development Award, the Mc'Knight Land Grant Professorship, the Ray D. Johnson/Mayon Plastics Professorship, and the Shell Chair at the University of Minnesota. He has also been a Humphrey Institute Policy Fellow. He has co-authored two books and 175 refereed papers.

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To our families

Preface

The chemical process industry is an intensely competitive environment, where cost reduction represents a critical factor towards increasing profit margins. Over the last few decades, an ever growing need to lower utility costs and energy consumption, and to improve raw material use, has spurred the development and implementation of increasingly integrated process designs that make extensive use of material recycling and energy recovery.

The significant reduction in capital and operating costs associated with process integration does, however, come at the price of additional operational and control challenges. Research on the control of interconnected process systems and entire chemical plants has been driven both by developments in control and optimization theory, and by shifts in market demands and industry needs. Initial efforts focused on decentralized multi-loop control structures and on including plant-wide considerations in the tuning of PID controllers. The associated benefits dwindled, however, with the rise of modern, tightly integrated processes with strong dynamic coupling between the different process units. More recently, control systems developed within the linear model predictive control (MPC) paradigm have allowed centralized decision making and accounting for economic optimality under operating constraints. In the (petro)chemical industry, MPC remains the established means for regulatory control and plant operation around a given steady state.

The current economic environment is, however, highly dynamic. Economically optimal plant operations thus entail frequent switching among different operating conditions (i.e., different steady states), having different product grades and production rates. Adopting or adapting the existing fully centralized or completely decentralized control designs for enforcing such transitions is neither practical nor effective in the context of integrated processes, where the interactions between the process units become significant and unique dynamic features emerge.

Developed around an extensive body of recent research by the authors, this book provides a new paradigm for the effective control of tightly integrated process systems, by

- documenting rigorously the dynamic behavior that emerges at the plant level when tight integration through material recycling and energy recovery is employed
- presenting the means for deriving explicit and physically meaningful low-dimensional models of the dominant plant dynamics
- describing a hierarchical controller design framework that discerns and coordinates between regulatory control at the unit level and supervisory, plant-wide control, and enables the design of nonlinear controllers for enforcing plant-wide transitions
- illustrating the application of the theoretical concepts to several integrated processes found in the chemical and energy industries

The chapters strive to balance rigor and practicality. The systematic analysis of generic, prototypical processes that exemplify the process integration structures encountered in practice is emphasized together with the unique dynamic features and control challenges that they present. Illustrative examples and extensive case studies on specific problems support the theoretical developments and provide a practical vista. The text adopts a unique and quintessentially chemical engineering perspective by introducing the concept of a process-level dimensionless number to characterize process integration from both a process *design* and a process *control* point of view. We are hopeful that our approach will allow readers to rapidly master the underlying theory and develop extensions to other classes of problems. Implementation details (sample computer codes) are provided in order to further encourage the rapid deployment of practical applications.

The book targets graduate students and researchers interested in dynamics and control, as well as practitioners involved in advanced control in industry. It can serve as a reference text in an advanced process systems engineering or process control course and as a valuable resource for the researcher or practitioner. Written at a basic mathematical level (and largely self-contained from a mathematical point of view), the material assumes some familiarity with process modeling and an elementary background in nonlinear dynamical systems and control.

We are grateful to our colleagues at the Department of Chemical Engineering and Materials Science at Minnesota for maintaining an environment of scientific excellence and collegiality over the years. M.B. is also grateful to the fellow researchers at the Praxair Technology Center in Tonawanda, NY for creating an intellectually stimulating atmosphere. We owe special thanks to Ed Cussler for his advice and encouragement in the initial stages of the writing of this book, the staff at Cambridge University Press for their support and advice, and the National Science Foundation for the support it provided for the research that formed the basis for this book. We also owe a special note of appreciation to Aditya Kumar for his instrumental role in the initial phase of research on this subject, and to Sujit Jogwar, whose recent work further solidified the basic thesis and direction of the book.

This book is dedicated to my parents, with gratitude for their unconditional love and support, and to the memory of my grandparents, who fondly followed my childhood scientific pursuits.

M.B.

I dedicate this book to my wife Aphrodite for her uncompromising pursuit of beauty in all aspects of our life, and to my children Stylianos and Euphrosyne for the immeasurable joy and inspiration they bring.

P.D.

Contents

Part I

Preliminaries

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.

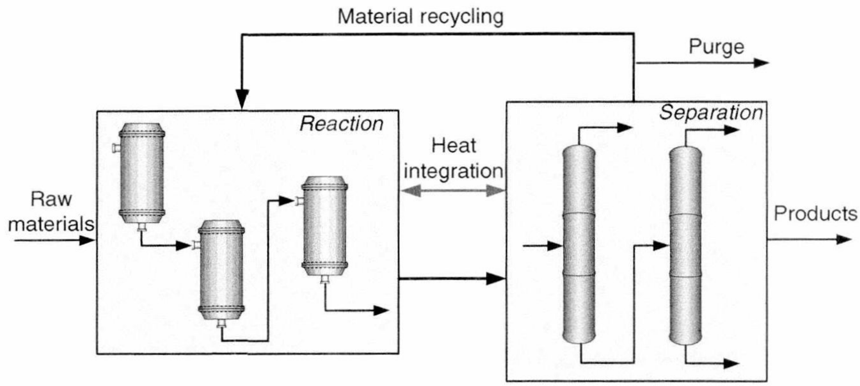

Figure 1.1 An integrated process system.

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