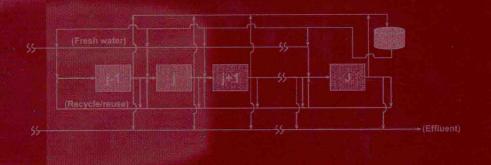
Thokozani Majozi



Batch Chemical Process Integration

Analysis, Synthesis and Optimization



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ISBN 978-90-481-2587-6 e-ISBN 978-90-481-2588-3 DOI 10.1007/978-90-481-2588-3 Springer Dordrecht Heidelberg London New York

Library of Congress Control Number: 2009939334

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Printed on acid-free paper

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Foreword

Over the past three decades, process integration has evolved as a holistic approach to design and operation which emphasizes the unity of the tackled systems. The overwhelming majority of research publications and textbooks in the field have focused on continuous systems. This has been the case for two main reasons. First, until recently, most of the sizable process industries have been designed to operate in a near steady-state and continuous mode. This is changing given the need to produce a number of specialty chemical to address variable market needs, the increasing level of flexibility, and the emergence of new industrial sectors (e.g., biorefineries) that favor batch operations. Second, process integration techniques for unsteady-state operations are more challenging than those for steady-state operations. As such, contributions to the field of batch process integration have come from a limited number of researchers. Such contributions have invoked advanced concepts in process design, operation, and scheduling, network synthesis and analysis, and some graphical but largely mathematical programming techniques. Hence, these contributions have been read and utilized by a select few experts. There has been a clear literature gap. Therefore, it was with great delight that I learned about Prof. Thokozani Majozi's project to overcome this literature gap by introducing this textbook that addresses batch chemical process integration. Having followed Prof. Majozi's exciting work in the field, I was convinced that the product will be superb. Indeed, now that the book is complete and that I had the privilege of reviewing it in full, I am thrilled that such an outstanding contribution is now available to researchers, students, and practicing engineers. The book is very well written and gradually introduces key concepts in batch process integration including the necessary background in mathematical programming, network representation, and operational concepts. The book also emphasizes the conceptual framework behind many of the mathematical formulations and focuses on the insights that drive the design, operation, and scheduling strategies. The book is loaded with examples that streamline the concepts and facilitate the learning process. There is a nice spectrum of applications ranging from basic manufacturing to waste reduction (primarily water management and wastewater minimization) to viii Foreword

heat integration. This is a much-needed and highly-valued book that will open the door for many readers to learn the fundamentals and application of batch process integration.

Dallas, TX

Mahmoud El-Halwagi

Preface

Research in batch processes only received heightened interest in the last 2 to 3 decades. Most of the work in published chemical engineering literature tends to focus on continuous processes at steady state. This occurrence dovetails with the evolution of the chemical industry as well as the dynamics of the global markets since the dawn of industrial revolution. From the late nineteenth to the mid-twentieth centuries, global markets were characterised by reasonable stability and crafted on bulk demand and mass production which favoured continuous processes. Demand for small volume high value added products constituted a very small fraction in that era. This pattern, however, began to change drastically in the latter part of the last century, with major markets displaying high levels of volatility that required processes amenable to sudden changes. Batch processes are ideally suited for this situation. Consequently, research in batch process scheduling began in earnest from the mid to the late 1970s. Scheduling, which is aimed at capturing the essence of time, is the cornerstone of all batch related activities, including *Process Integration*.

Process integration was developed and rose to prominence during the energy crisis of the 1970s in the form of Pinch Technology. The latter proved to be the breakthrough in energy optimization and sustainable design. It advocates the exploration of maximum energy recovery within the process through process-process heat exchange prior to resorting to external utility requirements. Its strength lies in the ability to set energy targets before commitment to design. Moreover, its graphical nature allows the designer to guide the optimisation process, which is not necessarily the case with mathematical approaches. This finally results in an energy efficient heat exchanger network (HEN). It still remains one of the major advances in chemical engineering even today. However, this contribution was aimed at continuous processes at steady state and ignored the impact of time dependent interventions as traditionally encountered in batch processes. This omission was not seen as a major drawback in process integration within the chemical engineering community, since continuous processes have largely been perceived to be much more energy intensive than their batch counterparts. The concept of process integration was later extended to mass exchanger networks with the ultimate goal of waste minimisation in 1989 where it also proved to be a major contribution. Again, the focus at the early stages of this advancement was on continuous rather than batch processes for similar reasons.

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Whilst methods for scheduling batch processes advanced steadily throughout the 2 quarters of the last century, process integration aspects pertaining to energy and waste minimisation still remained largely isolated from the mainstream research. There were indeed a few contributions in this regard, but their impact remained minimal for one main reason. They were largely a direct adaptation of the techniques developed for continuous processes, which meant that the time dimension had to be directly or indirectly suppressed in the analysis, thereby resulting in somehow inaccurate results. Stringent environmental legislation and the growth of batch processes in the industrial sector have necessitated research on the development of process integration techniques that are particular to batch processes. Since the beginning of this century, significant advances have been made in this regard. It is becoming clear, however, that batch processes, unlike continuous processes, are more amenable to mathematical than graphical analysis. This situation arises mainly from the added time dimension that makes it difficult to confine batch process analysis to 2 dimensions as traditionally encountered in graphical methods.

This textbook presents a comprehensive overview of some of the milestones that have been achieved in batch process integration. It is largely based on mathematical techniques with limited content on graphical methods. This choice was deliberately influenced by the observation made in the foregoing paragraph, i.e. in order to handle time accurately mathematical techniques seem to be more equipped than their graphical counterparts. The book is organised as follows.

- Chapter 1 gives an overview of batch processes.
- Chapter 2 introduces the reader to the basis of all the mathematical techniques presented in this textbook. The mathematical techniques are founded on a recipe representation known as the state sequence network (SSN), which allows the use of states to dominate the analysis thereby reducing the binary dimension.
- Chapter 3 presents a synthesis technique for multipurpose batch plants and further introduces an unexplored operational philosophy so called Process Intermediate Storage (PIS) operational philosophy.
- Chapter 4 presents a technique for wastewater minimisation in batch plants with single contaminants.
- Chapter 5 addresses the optimum design of intermediate water storage in multiproduct and multipurpose batch plants.
- Chapter 6 presents a technique for wastewater minimisation in multipurpose batch plants characterised by multiple contaminants.
- In Chapter 7 a mathematical technique that takes into account presence of multiple reusable water storage vessels is presented.
- A near-zero effluent approach is presented in Chapter 8. In particular, this chapter focuses on a special class of batch plants wherein water is a major constituent of the final product.
- Chapter 9 presents a mathematical technique for wastewater minimisation through exploitation of idle processing units, which is a unique and largely inherent feature of batch plants.

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• Heat integration is addressed in Chapter 10 and 11. Chapter 10 focuses on direct heat integration whilst Chapter 11 on indirect heat integration.

 Lastly, Chapter 12 presents graphical techniques in wastewater minimisation of batch processes as well as a brief comparison between graphical and mathematical techniques. The comparison aims to highlight the necessity of time in batch plants.

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Acknowledgments

This work could not be brought to life without the help of several people who gave guidance, assisted with research material and kept me focused throughout the writing of this textbook. Most of these people are my current and former students who have worked tirelessly in understanding batch processes. First and foremost, I would like to thank my recent PhD graduate student Dr Jacques Gouws with whom we shared a very common vision from the onset of his research. All the seeds of ideas I shared with him landed on a fertile ground and grew rapidly to applicable methodologies that have been adopted and implemented for industrial benefit. Perhaps in the same league is Mr Thomas Pattinson who put significant effort in the development of the formerly unexplored operational philosophy in batch plants, viz. Process Intermediate Storage (PIS) operational philosophy.

I am sincerely grateful to many of my recent students who had to edit some of the sections of this book whilst keeping with my demands on their research. In no particular order, at the fore of my mind in this regard are, Miss Bola Adekola, Miss Jane Stamp, Mr. Tim Price, Mr. Donald Nonyane, Mr. Vhutshilo Madzivhandila, Mr Vincent Gololo and Mr Esmael Reshid. Indeed, I am deeply indebted to my former supervisor, Dr Frank Zhu, who instilled in me love for batch operations and highlighted the urgency of generating appropriate techniques for these operations. He is also the one who introduced me to the world of mathematics and always mentioned that in every step of the way I must never compromise beauty for there is no permanent place in this world for ugly mathematics – confirming the famous mathematician Godfrey Harold Hardy's observation.

I am also deeply indebted to the following people who have offered guidance in various roles; as mentors, as friends and as family. Professor Ferenc Friedler, the Dean of Information Technology at the University of Pannonia in Hungary who has been my longstanding mentor, since I met him in 2000 in Los Angeles. He has always been the source of intellectual support and a reliable sounding board to most of my ideas. My former supervisors, Professor Chris Buckley and Mr Chris Brouckaert for their faith in me during my very early stages of research. Professor Toshko Zhelev from the University of Limerick in Ireland who has always had time to listen, criticise and encourage constructively since our first encounter in 1997 in South Africa. His patience with me still remains unprecedented. Professor Mahmoud El-Halwagi, the author of the foreword to this book, who I did not

xiv Acknowledgments

have to meet in person to derive inspiration from him. My true interest in Process Integration started whilst reading his book on 'Pollution Prevention through Process Integration' in 1997. I read each of its 314 pages with great passion. Mr Thanda Sibisi, my former science and mathematics teacher, who instilled in me the love and understanding for these two wonderful subjects and further advised me to pursue chemical engineering at my most desperate moment. My wife Bongiwe 'Mabongi' Dube and my children, Ntsika and Olwanda (the bunnies), who have been very understanding of my absence even when I am physically in their midst. Lastly, but certainly not the least, my dear parents who were beginning to understand the challenges of batch process integration towards the end of writing this book.

Let me not forget the mention of those who have provided fuel for my research vehicle to propel to the fore – the financial sponsors. Predominant among these are Dr Sibisi, the President and CEO of the Council for Scientific and Industrial Research (CSIR), Mr. Cyril Gamede, the Operations Director of African Explosives Limited (AEL) and Mr. Leon Kruger, the Operations Director of Johnson and Johnson (Pty) Ltd. My heartfelt thanks also go to the Water Research Commission (WRC) of South Africa.

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Chapter 1 Introduction to Batch Chemical Processes

Overview Batch processes are mostly suited to low volume high value added products that are usually characterised by common recipes, which render them amenable to sharing of equipment units. Due to their intrinsic adaptation to sudden changes in recipe, they are processes of choice in volatile or unstable conditions that have become regular in global markets. This chapter provides the background information on batch chemical processes, which constitutes the basis for the forthcoming chapters. Only the essential elements of batch plants are captured with references, where necessary, to further sources of information for the benefit of the reader.

1.1 Definition of a Batch Process

Any process which is a consequence of discrete tasks that have to follow a predefined sequence from raw materials to final products is a batch process. This predefined sequence is commonly known as a recipe. The primary features of any comprehensive recipe are the quantities of materials that have to be processed by individual tasks as well as the duration of each task within the recipe. The secondary features are the operating conditions of the various tasks, and in less common circumstances, the locality or geographic position of the task at hand. In processes wherein safety is of great concern, it might be necessary to perform a particular task in a designated area equipped with relevant safety features.

In reality, it is the *discreteness* of tasks that differentiates batch processes from their continuous counterparts. To illustrate, Fig. 1.1a shows a typical batch reactor with all the tasks comprising the entire batch reaction. On the other hand, Fig. 1.1b depicts a typical continuous reactor at steady-state. The discreteness of tasks in Fig. 1.1a is evident, which is not the case in Fig. 1.1b. Consequently, it is fair to deem batch processes 'distributed in time', whilst continuous processes, at steady-state, are 'frozen in time'.

Another illustration for the distinction between batch and continuous process is depicted in Fig. 1.2. The discreteness of tasks that characterise a batch process is evident in Fig. 1.2a. The use of storage becomes necessary when the completion of

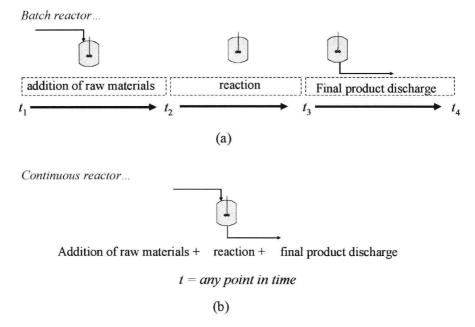


Fig. 1.1 (a) Batch vs (b) continuous reaction

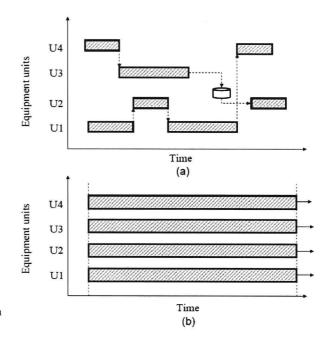


Fig. 1.2 (a) Batch vs (b) continuous process operation