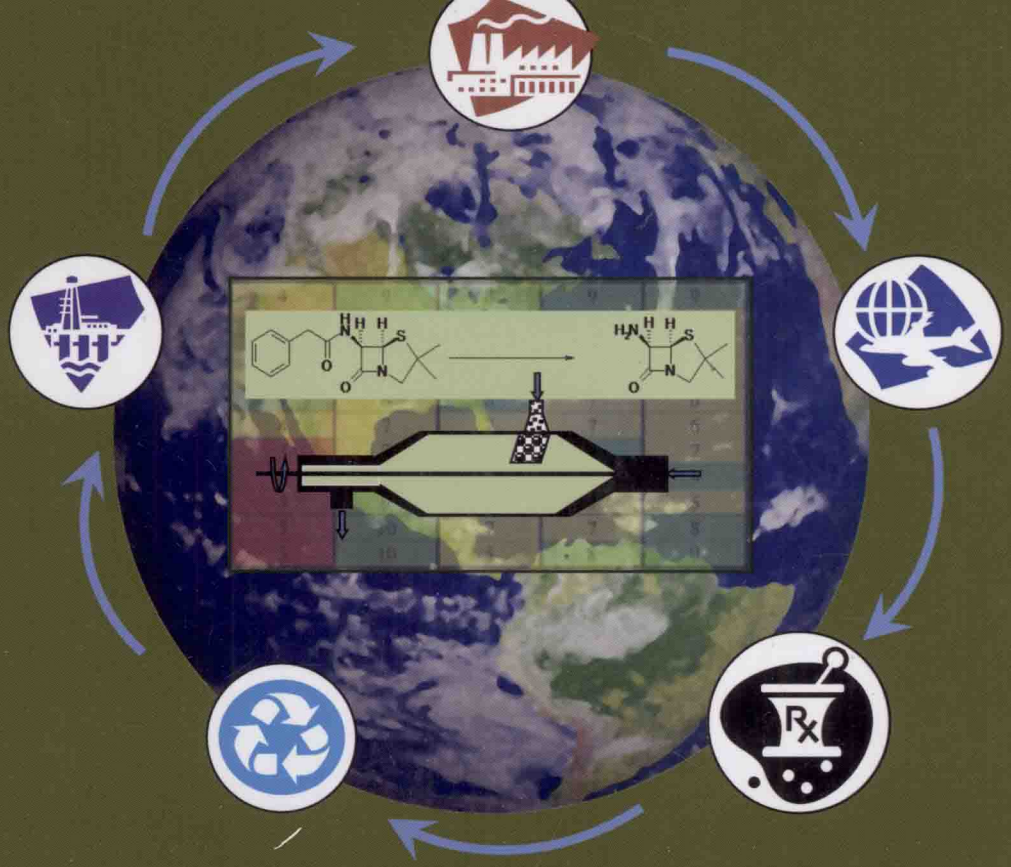

GREEN CHEMISTRY AND ENGINEERING

A Practical Design Approach

CONCEPCIÓN JIMÉNEZ-GONZÁLEZ *and* DAVID J.C. CONSTABLE

WILEY

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GREEN CHEMISTRY AND ENGINEERING

PREFACE

In the last decade, interest in and understanding of green chemistry and green engineering have increased steadily beyond academia and into the business world. Industries within different sectors of the economy have made concerted efforts to embed these concepts in their operations. Given our experience with green chemistry and green engineering in the pharmaceutical industry, we were initially approached by the publishers to edit a book on green chemistry in the pharmaceutical industry. This was a worthy proposal, but we felt that we had a greater opportunity and worthier endeavor to produce a book that would attempt to fully integrate green chemistry and green engineering into the academic curricula and that at the same time could serve as a practical reference to chemists and engineers in the workplace.

Green chemistry and green engineering are still relatively new areas that have not been completely ingrained in traditional chemistry and engineering curricula, but classes and even majors in these topics are becoming increasingly common. However, most classes in green chemistry are taught from an environmental chemistry perspective or a synthetic organic chemistry perspective, with neither approach addressing issues of manufacturing or manufacturability of products. Green engineering classes, on the other hand, tend to emphasize issues related to manufacturing, but do not treat reaction and process chemistry sufficiently, so these disciplines still seem to be disconnected. This lack of integration between chemistry, engineering, and other key disciplines has been one of the main challenges that we have had within the industrial workplace and in previous academic experiences.

As a consequence of these experiences, we decided to write this book to bridge the great divide between bench chemistry, process design, engineering, environment, health, safety, and life cycle considerations. We felt that a systems-oriented and integrated approach was needed to evolve green chemistry and green engineering as disciplines in the broader context of sustainability. To achieve this, we have organized the book in five main sections.

- Part I. Green Chemistry and Green Engineering in the Movement Toward Sustainability. Chapters 1 to 4 set the broader context of sustainability, highlighting the key role that green chemistry and green engineering have in moving society toward the adoption of more sustainable practices in providing key items of commerce.
- Part II. The Beginning: Designing Greener, Safer Chemical Synthesis. Chapters 5 to 8 address the key components of chemistry that will contribute to the achievement of more sustainable chemical reactions and reaction pathways. They also provide an approach to materials selection that promotes the overall greenness of a chemical synthesis without diminishing the efficiency of the chemistry or associated chemical process.
- Part III. From the Flask to the Plant: Designing Greener, Safer, More Sustainable Manufacturing Processes. Chapters 9 to 15 provide those key engineering concepts that support the design of greener, more sustainable chemical processes.
- Part IV. Expanding the Boundaries: Looking Beyond Our Processes. Chapters 16 to 20 introduce a life cycle thinking perspective by providing background and context for placing a particular chemical process in the broader chemical enterprise, including its impacts from raw materials extraction to recycle/reuse or end-of-life considerations.
- Part V. What Lies Ahead: Beyond the Chemical Processing Technology of Today or Delivering Tomorrow's Products More Sustainably. Finally, Chapters 21 to 25 provide some indication of trends in chemical processing that may lead us toward more sustainable practices.

To help provide a practical approach, we have included examples and exercises that will help the student or practitioner to understand these concepts as applied to the industrial setting and to use the material in direct and indirect applications. The exercises are intended to make the book suitable for both self-study or as a textbook, and most exercises are derived from our professional experiences.

The book is an outgrowth of our experience in applied and fundamental research, consulting, teaching, and corporate work on the areas of green chemistry, green engineering, and sustainability. It is intended primarily for graduate and senior-level courses in chemistry and chemical engineering, although we believe that chemists and engineers working in manufacturing, research, and development, especially in the fine-chemical and pharmaceutical areas, will find the book to be a useful reference for process design and reengineering. Our aim is to provide a balance between academic needs and practical industrial applications of an integrated approach to green chemistry and green engineering in the context of sustainability.

Acknowledgments

We thank all our colleagues who have contributed directly or indirectly to our journey toward sustainability, and whose ideas and collaborations throughout the years have contributed to our own experience in the areas of green chemistry and green engineering. We also express our gratitude to GlaxoSmithKline, in general, and to James R. Hagan, in particular, for their support and encouragement.

We also give special thanks to Rafiqul Gani and Ana Carvalho from the Computer Aided Process-Product Engineering Center, Department of Chemical and Biochemical Engineering at the Technical University of Denmark, for their comments, reviews, and contributions to Chapter 12; to Mariana Pierobon and BASF for their helpful comments and for allowing us to use one of BASF's eco-efficiency assessments as an example in the life cycle chapters; to Sara Conradt for allowing us to use a sample of her masters thesis as an example of LCA outputs; and to Tom Roper and John Hayler at GSK for their feedback on green chemistry throughout the years. Finally, we want to thank *Chemical Engineering* magazine, the American Chemical Society, Springer Science and Business Media, Elsevier, John Wiley & Sons, the Royal Society of Chemistry, and Wiley-VCH for permission to reproduce some printed material.

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December 2009

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PART I

GREEN CHEMISTRY AND GREEN ENGINEERING IN THE MOVEMENT TOWARD SUSTAINABILITY

1

GREEN CHEMISTRY AND ENGINEERING IN THE CONTEXT OF SUSTAINABILITY

What This Chapter Is About Green chemistry and green engineering need to be seen as an integral part of the wider context of sustainability. In this chapter we explore green chemistry and green engineering as tools to drive sustainability from a triple-bottom-line perspective with influences on the social and economic aspects of sustainability.

Learning Objectives At the end of this chapter, the student will be able to:

- Understand the need for the development of greener chemistries and chemical processes.
- Identify sustainability principles and associate standard chemical processes with the three areas of sustainability: social, economic, and environmental.
- Identify green chemistry and green engineering as part of the tools used to drive sustainability through innovation.
- Understand the need for an integrated approach to green chemistry and engineering.

1.1 WHY GREEN CHEMISTRY?

$$A + B \rightarrow C \tag{1.1}$$

Reactant A plus reactant B gives product C. No by-products, no waste, at ambient temperature, no need for separation. Is it really that easy?

Green Chemistry and Engineering: A Practical Design Approach, By Concepción Jiménez-González and David J. C. Constable

If industrial chemical reactions were that straightforward, chemists and engineers would have significantly more time on their hands and significantly less excitement and fewer long hours at work. Chemists know that this hypothetical reaction is not the case in real life, as they have less-than-perfect chemical conversions, competing reactions to avoid, hazardous materials to manage, impurities in raw materials, and the final product to reduce. Engineers know that in addition to conquering chemistry, there are by-products to separate, waste to treat, energy transfer to optimize, solvent to purify and recover, and hazardous reaction conditions to control. At the end of this first reality check, we see that our initial reaction is a much more complicated network of inputs and outputs, something that looks more like Figure 1.1.

Green chemistry and green engineering are, in a very simplified way, the tools and principles that we use to ensure that our processes and chemical reactions are more efficient, safer, cleaner, and produce less waste by design. In other words, green chemistry and green engineering assist us in first thinking about and then designing synthetic routes and processes that are more similar to the hypothetical reaction depicted in equation (1.1) than to the more accurate reflection of current reality shown in, Figure 1.1.

What are the drivers in the search for greener chemistries and processes? Engineers and scientists have in their capable hands the possibility of transforming the world by modifying the materials and the processes that we use every day to manufacture the products we buy and the way we conduct business. However, innovation and progress need to be set in the context of their implications beyond the laboratory or the manufacturing plant. With the ability to effect change comes the responsibility to ensure that the new materials, processes, and designs have a minimum (or positive) overall environmental impact. In addition, common sense suggests that there is a strong business case for green chemistry and engineering: linked primarily to higher efficiencies, better utilization of resources, use of less hazardous chemicals, lower waste treatment costs, and fewer accidents.

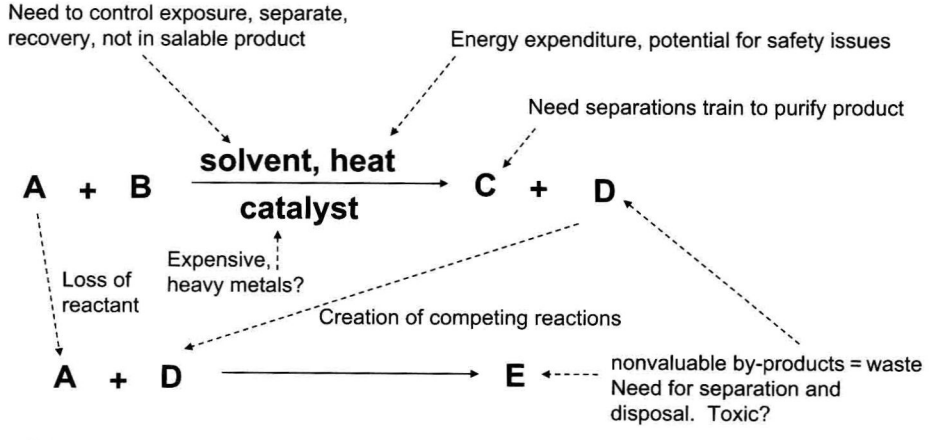

FIGURE 1.1 Simplified vision of some of the challenges and realities of designing a chemical synthesis and process.