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Book Review

CHEMICAL PROCESS DESIGN

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The book "Chemical Process Design" is written by two authors Alexandre C. Diman and Costin Sorin Bildea. The first author, Alexandre C. Dimian, is Associate Professor for Process Design and Integration at the University of Amsterdam, The Netherlands, since 1993. He worked as a consultant for computer applications in process industries for 12 years in France, has accomplished numerous industrial projects, and has more than 100 refereed scientific papers as well as five books and three patents to his name. His research interests focus on the computer-aided design of chemical processes and, more recently, on biofuels and biorefinery applications.

The second author, Costin Sorin Bildea is currently Associate Professor at the University Politehnica Bucharest, Romania, where he teaches process control and various other chemical engineering courses. He has more than 50 published papers and conference presentations to his name and his research interests are in the fields of nonlinear dynamics and integration between process design and process control.

The present book deals with the conceptual design of chemical processes illustrated by case studies worked out by computer simulation. This book uses ample case studies to teach a generic design methodology and systematic design methods. Each project starts by analyzing the fundamental knowledge about chemistry, thermodynamics and reaction kinetics. Environmental issues are highlighted by analyzing the detailed chemistry. On this basis the process synthesis is performed. The result is the generation of several alternatives from which the most suitable is selected for refinement, energy integration, optimization and plant wide control.

Computer simulation is intensively used for data analysis, supporting design decisions, investigating the feasibility, sizing the equipment, and finally for studying process dynamics and control issues.

The book is structured in fifteen chapters and contains six appendixes. The first four chapters deal with the fundamentals of a modern process design, while their application is developed in the subsequent eleven case studies.

Chapter 1, *Introduction,* presents the concepts and metrics of sustainable development, as well as the framework of an integrated process design by means of two interlinked activities, process synthesis and process integration. Likewise, Chapter 1 brings into discussion the following issues, sustainable process design, sustainable development, concepts of environmental protection, production-integrated environmental protection, end-of-pipe antipollution protection, efficiency of raw materials, superstructure optimization, life cycle of a design project and others.

Chapter 2, *Process syntheses by hierarchical approach,* propose an efficient methodology aiming to minimize the interactions between the synthesis and integration steps. The hierarchical approach presented in this Chapter is a simple but powerful methodology for the development of process flow sheets. It consists of a top-down analysis organized as clearly defined sequence of tasks aggregated in levels. Each level handles a fundamental conceptual problem: input/output structure, reactor design, structure of separations and recycles, design of separation subsystems, energy and recourse integration, protection of environment, safety and hazard problems, as well as plant wide control issues.

At each level, systematic methods can be applied for the analysis and synthesis of subsystems.

Chapter 3 deals with *Synthesis and Separation System*. The goal in process synthesis of separations is the development of close-to-optimum flow sheets, in which both the feasibility and the performance of splits are guaranteed. Emphasis is placed on the synthesis of distillation systems by residue curve map methods.

Chapter 4 details the analysis of the *Reactor/Separation/Recycle Systems*. This topic is a significant one, since recycle of raw materials, energy integration and reduced size or the lack of buffer vessels are characteristics of modern plants. In such conditions, the interaction between units is so strong that a classical approach to control does not work. In this chapter two different approaches to plant wide control are discussed, namely controlling the material balance of the plant by using the self-regulation property or by applying feedback control.

Chapter 5 discusses the first case study *Phenol Hydrogenation by Cyclohexanone*. This introductory case study presents the key features of a conceptual process design by using the systematic methods presented in the previous chapters. The selected process is the manufacture of cyclohexanone, a key intermediate in the production of ε-caprolactam and adipic acid, which are basic materials for nylon-type polymers. In addition, the case study deals with waste reduction by design, with both economical and ecological benefits.

Chapter 6 is focused on case study *Alkylation of Benzene by Propene to Cumene*. This case study deals with the design and simulation of a medium size plant of 100 kton cumene per year. The goal is performing the design by two essentially different methods. The first one is a classical approach, which handles the process synthesis and energy saving with distinct reaction separations. In the second alternative a more innovative technology is applied based on reactive distillation.

Chapter 7 on *Vinyl Chloride Monomer Process* addresses the complexity of designing a large chemical plant with multireactors and an intricate structure of recycles. The goal of this case study is to illustrate some generic issues raised by the conceptual design of a large-scale process involving several reaction and separation sections interconnected in a complex plant with recycles.

Chapter 8 describes the case study associated with *Fatty-Ester Synthesis by Catalytic Distillation*. This case study investigates the possibility of applying reactive distillation to the synthesis of fatty-acid esters as a generic multiproduct process. A relevant characteristic of the technology should be the ability to remove the water selectively and continuously in order to shift the chemical equilibrium to full conversion. Since the catalyst manifests similar activities for several alcohols, the study investigates the possibility of designing a multiproduct reactive distillation column by slightly adjusting the operating conditions.

Chapter 9 considers the design of an *Isobutane / Butene Alkylation* plant, following the hierarchical approach methodology. A special attention is addressed to the reaction/separation/recycle structure of the flowsheet, showing how plantwide control considerations are introduced during the early stages of conceptual design. An important part of this chapter has been devoted to robustness. The tools used in this chapter include numerical methods for solving systems of nonlinear equations and tracing the dependence upon one parameter by continuation methods.

Chapter 10 deals with *Vinyl Acetate Monomer Process*. The vinyl acetate monomer (VAM) is large-scale chemical mostly used in manufacturing polyvinyl acetate, the basic ingredient in water-soluble acrylic paints. Higher production efficiency of VAM can be achieved by upstream integration with the production of low-cost acetic acid, as well as by downstream integration with the manufacturing of polyvinyl acetate and polyvinyl alcohol. Likewise, this chapter demonstrates the benefit of solving a process design and plantwide control problem based on the analysis of the reactor / separation / recycle structure.

Chapter 11 *Acrylonitrile by Ammoxidation of Propene* presents the synthesis of flowsheet in which a difficult separation problem dominates. Acrylonitrile (AN) is one of the leading chemicals with a worldwide production and the important applications are acrylic fibers, thermoplastics, technical rubbers, adiponitrile, etc. About 90% of the worldwide AN is manufactured today by the ammoxidation of propene. In this reaction, significant amounts of highly toxic species form, such as HCN, acetonitrile (ACN) and heavy nitriles. Their removal from aqueous mixtures is difficult, as reflected in elevated water-treatment and energy costs. Different separation methods are employed from simple flash and gas adsorption to extractive distillation for splitting azeotropic mixtures. The problem is tackled by an accurate thermodynamic analysis.

Chapter 12 deals with *Biochemical Process for NO_x Removal*. Most of the existing processes of nitrogen oxide removal are chemically based requiring high temperature or expensive catalysts. Biotechnology can provide an alternative for chemical-based cleaning processes this time the function of the catalyst being played by micro-organisms. In this case study the authors have simulated and designed an industrial-scale BioDeNO_x process. Rigorous rate-based models of the adsorption and reaction units have been presented, taking into account the kinetics of chemical and biochemical reactions, as well as the rate of gas-liquid mass transfer. This chapter demonstrates that bringing together chemistry, microbiology and engineering results in the development of an efficient process for removal of NO_x from flue gases.

Chapter 13 tackles *PVC Manufacturing by Suspension Polymerization*. The selected case study illustrates a typical problem of product design.

This application illustrates the key features of a product design in the field of polymer technology, such as building the polymerization recipe and the reactor operating procedures necessary to achieve different polymer grades. The link between these aspects is realized by means of detailed kinetic modeling of the polymerization reaction, including the molecular-weight distribution. Reactor-design issues are examined from the viewpoint of heat-transfer intensification. These elements are imbedded in a dynamic reactor model with control-system implementation, simulated in Matlab. The results are expressed as profiles in time of temperature, concentrations of monomer and initiator.

Chapter 14 *Biodiesel Manufacturing*, presents the biofuels. Biofuels have at least five merits: reduce the energetic dependence of nation with respect to fossil resources acting as stabilizing factors in a global market environment; reduce the global pollution by less CO_2 ; enable recycling various potentially energetic industrial and domestic wastes; creating new jobs in rural areas and sustainable economic growth. This chapter presents a classification of alternative transportation fuels in terms of origin and ecological efficiency and the economic aspects. Also it is completed which manufacturing processes, batch, catalytic, hydrolysis, esterification and the enzymatic processes. From the chemistry viewpoint the raw materials for biodisel are quite homogeneous, being based on triglycerides. The fuel obtained has superior combustion features and good CO_2 balance being sometimes called "second-generation" biodisel. The quality of biodiesel is regulated by standards, the content of free and bound glycerol is most important.

Chapter 15 deals with *Bioethanol Manufacturing*. Bioethanol is a valuable ecological fuel than can be used in blending with gasoline and diesel. This chapter presented economic and ecological aspect of biofuels. Bioethanol can be produced from a large variety of natural renewable materials, such as agricultural crops, land and forest products, as well as from industrial and domestic waste, such as paper, textile and beverages. The selected case study illustrates biorefinery concept and fermentation processes. The case study handles the design of bioethanol plant based on lignocellulosic biomass following the NREL technology (The National Renewable Energy Laboratory) and making use of simulation in Aspen Plus.

Each chapter of the book contains an up-to-date well documented list of references. The book is written in contemporary way and includes many illustrations which make the text more useful for specialists in chemical process design. Also it is completed with Annexes on the analysis of reactive mixtures by residue curve map, design of heat exchangers, selection of construction materials, steam tables, vapor pressure of typical chemical components and conversion table for the common physical units. The book is aimed for a wide audience interested in the design of innovative chemical processes, especially chemical engineering students completing a process or plant design project. Likewise, postgraduate students and PhD students will find advanced and thought-provoking process-design methods. The information presented in the book may be useful for the continuous education of specialists, i.e. professional designers and R&D engineers.

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