INTEGRATED DESIGN AND SIMULATION OF CHEMICAL PROCESSES

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COMPUTER-AIDED CHEMICAL ENGINEERING, 13

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PREFACE

In addition to high economic efficiency, Chemical Process Industries are confronted today with the challenge of sustainable development: the exploitation of the natural resources by the present society must not compromise the ability of future generations to meet their own needs. Sustainable development implies a profound change in developing and designing chemical processes, and implicitly in the education of designers. As an attempt to answer this challenge, the book deals with the design of innovative chemical processes by means of systematic methods and computer simulation techniques.

The current revolution in information technology, as well as the impressive progress in modelling and simulation has a significant impact on Process Design. Computer simulation is involved in all stages of a project, from feasibility studies, through conceptual design, to detailed engineering, and finally in plant operation.

In developing sustainable processes, the essential factor is the innovation capacity of chemical engineers to discover new processes and improve significantly the existing ones. The key to innovation is the integration of knowledge from different disciplines. It is also the distinctive feature of this work, in which the emphasis is set on the power of the conceptual methods incorporated in the new paradigm of *Process Integration*. Modern process design consists of developing not a unique flowsheet but alternatives, from which the best one is refined, integrated and optimised with respect to high efficiency of materials and energy, ecologic performance and operability properties.

This book aims is to treat the most important conceptual aspects of Process Design and Simulation in a unified frame of principles, techniques and tools. Accordingly, the material is organised in five sections, *Process Simulation*, *Thermodynamic Methods*, *Process Synthesis*, *Process Integration*, *Design Project*, and covered in 17 Chapters. Numerous examples illustrate both theoretical concepts and design issues. The work refers also to the newest scientific developments in the field of Computer Aided Process Engineering.

The book is primarily intended for undergraduate and postgraduate students in chemical engineering, as support material for various courses and projects dealing with Chemical Process Design and Simulation. The material can be customised to fulfil the needs of both general and technical universities. The work is intended also as a guide in advanced design techniques for practicing engineers involved in research, development and design of various chemical or related processes. The users of process simulators will find helpful guidelines and examples for an effective use of commercial systems.

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Writing this book has been a considerable challenge by the variety of topics and the amount of material. A large part of this book takes profit from the industrial experience acquired between 1982 and 1993 as consultant in process design and simulation for major French companies. In the last twenty years I had the privilege to work intensively with most of the simulation systems mentioned in this book, but also with other packages that unfortunately have not survived. Both the use of scientific principles in design and the systems approach in solving complex problems have deep roots in that industrial experience.

My first expression of gratitude is for my former teachers, as well as for my numerous colleagues from France, The Netherlands, Romania, Germany, England and USA, who helped me to progress along the years in this fascinating profession called Chemical Engineering.

I am grateful to the Department of Chemical Engineering at the University of Amsterdam, The Netherlands, for the excellent working conditions. I would like to express my gratitude to all my colleagues, particularly to Professors Alfred Bliek and Rajamani Krishna for their support and valuable advises.

The material of this book has been taught for about a decade at the University of Amsterdam. From a long list of former and actual PhD students who helped me with assistance during the course and design project I would mention only few names: Sander Groenendijk, Adrian Kodde, Sasha Kersten, Florin Omota. Susana Cruz was very obliging with the proofread of several chapters. In addition, Tony Kiss gave me a precious help to prepare simulation examples and to finish the document.

In particular I am pleased to acknowledge the important contribution of Dr. Sorin Bildea, now at the Technical University Delft, who is co-author of the chapters about Controllability Analysis and Integration of Design & Control.

Finally, I am indebted to my lovely family for the moral support and many-sided assistance during the hard work years needed to accomplish this book, most of all to my beloved wife and "editor-en-chief" Aglaia Dimian, as well as to my daughters Alexandra and Julia.

Alexandre C. Dimian

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Nomenclature

The symbols given bellow are general. Supplementary notations are explained in context.

a	activity (kmol/m^3)
A	heat exchange area (m^2)
A_c	cross-sectional area
B	bottom product flow rate
c_i	molar concentration (kmol/m^3) of component I
C_i	dimensionless concentration
C_P	molar heat capacity at constant pressure (kJ/kmol/K)
C_V	molar heat capacity at constant pressure (kJ/kmol/K)
d	diameter (m^{-1})
d_p	particle diameter
D	distillate flow rate (kmol/s)
Da	Damköhler number $Da = kc_A^{n-1}\tau$
E	activation energy (kJ/kmol)
f_i	fugacity of component i (bar)
F	total molar feed flow rate (kmol/s)
F_i	partial molar flow rate of component i
F_T	temperature correction factor for shell & tubes heat exchangers
g	acceleration due to gravity (9.81 m/s)
G	mass feed flow rate (kg/s)
G	molar Gibbs free energy (kJ/kmol)
h	specific enthalpy (kJ/kg, kJ/kmol), heat transfer coefficient (W/m^2K)
H	molar or mass enthalpy (kJ/mol, kJ/kg)
H_i	Henry coefficient of component i
$\Delta H_{R,i}$	enthalpy of reaction with reference to component i
k	reaction constant [(kmol/m^3)$^{1-n}$$s^{-1}$]
k_0	pre-exponential Arrhenius factor [(kmol/m^3)$^{1-n}$$s^{-1}$]
K_a, K_c, K_f, K_x	reaction equilibrium constant (activity, concentration, fugacity, molar fractions)
K_i	K-factors or K-values
L	liquid flow rate (kmol/s or kg/s)
m	mass amount (kg)
M_i	molar weight of component i
n	molar amount (kmol)
N_c, N_{eq}, N_v	number of components, equations and variables
N_{min}	number minim of theoretical stages
P	pressure (bar)
$P_{v,i}$	vapour pressure of component i
P_c	critical pressure (bar)
t	time (s)
T	temperature (K or °C)
T_c	critical temperature (K or °C)
ΔT_{ad}	adiabatic temperature change (K or °C)
ΔT_{min}	minimum temperature approach (K or °C)
ΔT_{LM}	logarithmic mean temperature difference (K or °C)

Q	heat duty (kW)
Q_t	heat transferred (kW)
Q_v	volumetric flow rate (m^3/s)
r	radius
r_j	rate of reaction ($kmol/m^3/s$) of component j
R	universal gas constant, (R=8.31451 J/mol/K)
R_{min}	minimum reflux ratio
S	entropy (kJ/mol/K)
u	superficial fluid velocity (m^3/m^2s)
U	internal energy (kJ/kmol), overall heat transfer coefficient
v	velocity (m/s)
V	volume (m^3), vapour flow rate (kmol/s or kg/s)
V_c	critical volume (K)
V_R	reaction volume (m^3)
W	work (kJ), power (kW)
W_s	shaft work in compression, expansion
x	molar fractions of liquid phase
X_A	fractional conversion of the component A
y	molar fractions of vapour phase
z	molar fractions of feed stream, length co-ordinate (m)
Z	compressibility factor

Greek symbols

α	relative volatility
α, β	reaction orders
δ	width
∂	differential operator
Δ	finite difference operator
ε	error
γ	liquid activity coefficient
λ	thermal conductivity (W/mK)
μ_i	chemical potential of component i
ξ_j	molar extent of reaction j
η	fluid viscosity, efficiency in general
ω	accentric factor
ρ	density (kg/m^3)
σ	surface tension (N/m)
ν	stoichiometric coefficient
ϕ_i	fugacity coefficient of component i
τ	reaction time (s^{-1}), constant time (s^{-1})
θ	dimensionless time

CONTENTS

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Chapter 1

INTEGRATED PROCESS DESIGN

1.1 INTRODUCTION

1.1.1 Motivation

The products manufactured by the Chemical Process Industries (CPIs) are of greatest importance for the modern society. Chemical processes are born from the imagination of researchers and engineers. The person in charge with transforming a valuable idea in laboratory or on paper into an industrial competitive process is the designer. Its first motivation is the creation of new processes, or improving significantly the existing ones. The creative effort must be rewarded by substantial economic advantages. Thus, innovation and efficiency are key motivations for designers.

However, in the today's business and social environment we may add another dimension to creativity. Much more than in the past, the designer should be concerned about the rational use of resources and the preservation of the natural environment. The process has to be novel, efficient, and competitive in a global business environment, but also sustainable. The immediate conclusion is that the job of a designer is becoming increasingly complex and challenging. The designer has to integrate in his project a large number of constraints, and to deal often with contradictory aspects. For example, the selection of the suitable chemistry should avoid hazards and unsafe reactions. The process should be compact and economical in energetic consumption, but offer flexibility and ready to accept other raw materials or other specifications of products. The optimal combination of so many aspects gives highly *integrated processes*. The design of complex processes implies the availability of adequate conceptual methods and of powerful computer-based tools, which form nowadays the core of Process Systems Engineering.

Hence, in the today's world the key issue for CPIs is the innovation. We believe that the creativity cannot be left as a skill of some gifted persons or some powerful organisations. Creativity should be accessible to anyone having the basic professional knowledge and motivation for discovery. Creativity can be enhanced by systematic learning and training, thus is a teachable matter. It not excludes but reinforces the skills and motivation of individuals. The intellectual support for enhancing creativity is the use of systematic design methods. A systematic approach has at least two merits: 1) Provide guidance in identifying what is and what is not feasible; 2) Not a single solution but several alternatives are generated, corresponding to the decisions that the designer has to take. After ranking, following some performance criteria, as for example the Total Annual Cost, the most convenient alternative is refined and optimised. A remarkable feature of the systematic methods available nowadays is that these can set quasi-optimal targets well ahead the detailed sizing of the equipment.

The assembly of the systematic methods applied to chemical processes forms the new design paradigm designated today by *Process Integration*. Its application relies on the intensive use of *Process Simulation*. Combining design and simulation allows the designer to understand the behaviour of complex systems, to explore several alternatives, and on this basis to propose effective innovative solutions.

1.1.2 The road map of the book

The book contains five sections, each of several chapters, in total seventeen. The road map depicted in Fig. 1.1 allows the reader an easy orientation in different topics. Because the emphasis is on the design process, a large avenue links the introductory chapter on *Integrated Process Design* with the section devoted to *Design Project*, the final goal. The activities on the right side deal with the logistic issues regarding computing tools and methods, grouped in two blocks devoted to *Process Simulation* and *Thermodynamic Methods,* respectively. The other two blocks on the left side handle conceptual activities, namely *Process Synthesis* dealing with the architectural design, as well as *Process Integration* handling the development of subsystems and the allocation of resources, and their optimisation in the frame of the whole process. A rapid tour along this roadmap will allow the user to be informed about the key issues in each chapter before she or he will take more time for a longer stay.

The tour begins with the chapter on *Integrated Process Design.* The key topic is the *Sustainable Development* and its implications on the design of chemical processes, as *Production-Integrated Environmental Protection.* Integrated Process Design is described as the marriage of two types of activities: Process Synthesis - architectural design, and Process Integration - development and optimisation of subsystems in a flowsheet. This distinction, although somewhat artificial, serves in fact to better structuring of the chapters devoted to learn the logical development of a design. This chapter describes also concepts from systems engineering useful in the managing engineering projects.

The first part of the book presents generic principles and techniques in *Process Simulation* that enable an innovative and efficient use of any commercial software. Chapter 2 serves as *Introduction in Process Simulation.* Particular attention is paid to the systems analysis of a design problem by means of simulation, commonly called *flowsheeting.* This chapter presents elements of the software architecture, as well as the main integrated commercial systems. Chapter 3 develops in larger extent the *Steady state Flowsheeting.* Major topics include the description of generic flowsheeting capabilities, as degrees of freedom analysis, treatment of recycles, and use of control structures. Mastering the flowsheeting techniques allows the user to get valuable insights into more subtle aspects, as plantwide control problems. Chapter 4 is devoted to *Dynamic Flowsheeting,* nowadays a major investigation tool in process operation and process control.

It is largely recognised that inappropriate thermodynamic modelling is the most important cause of failure in computer-aided design. That is why a section of the book - *Thermodynamic Methods* - reviews theoretical principles and practical aspects regarding the computer-based methods for physical properties and phase equilibria. Chapter 5 describes the *Generalised Computational Methods* for *PVTx* systems, largely based nowadays on the use of equations of state. Chapter 6 develops the computation of *Phase Equilibria* by various thermodynamic models, classified in equation of state and liquid activity models. Particular attention is paid to the regression of model parameters from experimental data.

After having solved the logistic elements, the third part of the book - *Process Synthesis* - enters in the core of the design. This part teaches how to invent process flowsheets by a generic approach based on systems analysis and systematic methods. Chapter 7 develops in detail the systematic development of flowsheets by applying the *Hierarchical Approach*. The emphasis is set on the material balance envelope formed by the sub-systems of reactions and separations connected by recycles. Reactor-Separator -Recycle structure is the basis for further integration of units with respect to low energetic consumption and good controllability properties. Additional chapters are devoted to deeper analysis of the sub-systems for reaction and separations. Chapter 8 dealing with the *Synthesis of Reaction Systems* is particularly important. The key issue is the reactor selection and its integration with the other units. Stoichiometry and thermodynamic calculations can supply valuable insights to designer, even when kinetic data are not available. Chapter 9 presents the *Synthesis of Distillation Systems*, particularly the treatment of the azeotropic mixtures. Particular attention is given to the new systematic technology based on Residue Curve Maps.

Process Integration part addresses the combination of units in an optimal system from the point of view of energetic consumption, controllability properties and environmental performance. The principles of achieving optimal energy consumption are addressed in the Chapter 10 devoted to *Pinch Point Analysis*. Chapter 11 deals with *Practical Energy Integration* by presenting specific techniques for saving energy. The next two chapters develop new challenging issues concerning the integration between design and control. This topic corresponds to the requirements set to modern plants with respect to high flexibility in manufacturing, but safe and robust controllability characteristics. Chapter 12 review basic concepts in process dynamics and control with emphasis on *Controllability Analysis*. Chapter 13 is devoted to *Plantwide Control*, a recent concept dealing with the strategy of controlling the whole plant and its relation with the design of units.

The last part, *Design Project*, addresses specific subjects for carrying out conceptual design projects. Chapter 14 discusses teaching aspects in *Process Integration*, as the organisation of courses and design projects, at both undergraduate and postgraduate levels. The *Economic Evaluation* of design projects is treated in Chapter 15 from the perspective of profitability analysis. Chapter 16 develops some guidelines for the *Selection and Sizing of Process Equipment*, namely reaction vessels, separation columns, heat exchangers, and devices for the transport of fluids. The last Chapter 17 presents two comprehensive *Case Studies* illustrating the design and simulation of complex plants, including full dynamic simulation with control implementation. Helpful information for design projects is given in Appendices.

This book can be used as support in teaching Process Design and Simulation. The chapters 1-3, 7, 10-11 and 14-17 are suitable for setting up an undergraduate course in Process Integration. Complementary courses or self-study could be necessary for upgrading the knowledge in thermodynamics (Chapter 5-6) and chemical reaction engineering (Chapter 8). Advanced material is more suited in postgraduate or continuous education courses, particularly the chapters 4, 9, 12-13, and 17. The best manner to consolidate the knowledge and skills in process engineering is working out a *Design Project* for a complete plant.

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