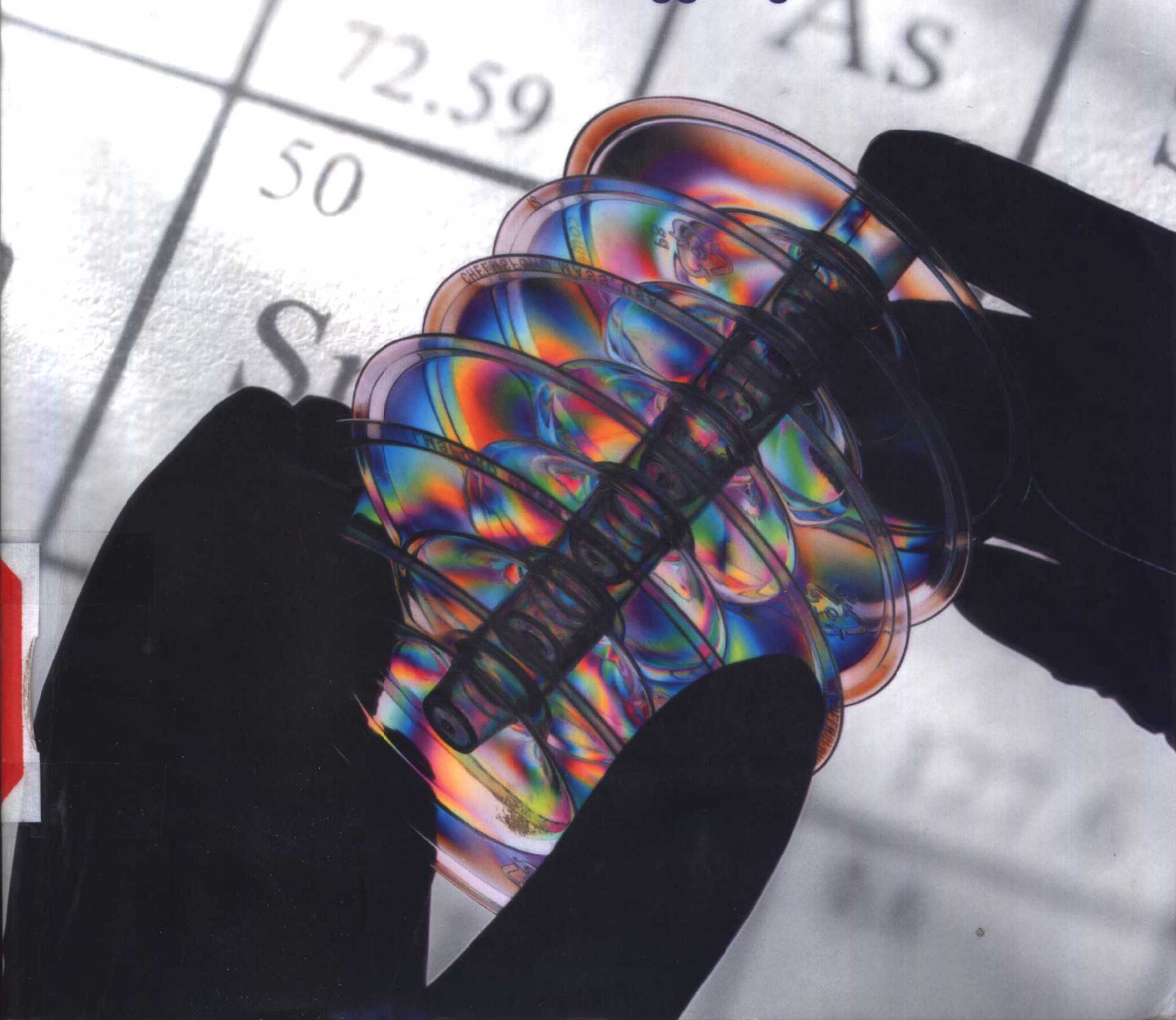
Chemical Product Design

E. L. Cussler G. D. Moggridge



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For Jia Yang Chen:
Thank you for giving
me the chance to work
with Chuanfang Yang.
Ed Cussler

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Preface

Since its inception in its modern form around the turn of the nineteenth century, the chemical industry has largely concerned itself with the manufacture of commodity chemicals. A commodity chemical is manufactured in very large quantities (at least 1,000 tons annually) and sold into a world market where the products of different companies are differentiated only by price; quality and composition are identical. Benzene, hydrogen, polyester, and titanium dioxide are examples. This industry has been immensely productive and successful, providing the major source of employment for trained chemists and chemical engineers as well as many from other disciplines.

We suggest in Chapter 1 that this industry had its Golden Age in a period of a couple of decades just after World War II, with growth equivalent to that of the modern software industry. Since the 1970s, market growth has slowed and companies began to concentrate on consolidation and economies of scale. In the past decade a significant shift has occurred in the chemical industry, in which most new resources are now devoted to the design and manufacture of chemical products, rather than the traditionally dominant commodity chemicals. This change is reflected in the employment of new graduates from our universities. Thirty years ago most went into commodity-based companies. Now the majority start work on chemical products.

The change of direction of the British company ICI in the late 1990s is an exemplar of this shift from commodities to chemical products. Since the 1920s the mainstay of Britain's bulk chemical industry, ICI no longer manufactures polyester, fertilizer, or ethylene; instead it now makes perfumes, flavorings, and coatings for the electronics industry.

Commodities of course continue to be made – the world needs toluene, ammonia, and methanol just as it always has. However, commodities are made by a dwindling number of ultra-efficient companies, which employ relatively few people; profits remain good, if cyclical, but no longer lead to a large-scale need for chemists and engineers. Often these companies are private, allowing them more easily to ride the trade cycles typical of commodity businesses.

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So we have argued that there has been a rapid shift in focus in the chemical industry in the past decade, away from commodities and into chemical products; but what is the distinction between these two? We distinguish chemical products from commodities in three ways: quantity manufactured, value, and differentiation in the marketplace. Chemical products are produced in small quantities (usually much less than 1,000 tons per year). The archetype is the active ingredients of drugs, only a few kilograms of which may be required annually to command a market worth millions of dollars. Chemical products are high value added and sell at a high margin, whereas commodities typically sell for a few hundred dollars per ton at a marginal profit of a few percent. This high value added reflects our third difference: chemical products are differentiated in the marketplace primarily by performance and quality, rather than price. A company's advantage is often sustained by patent protection, or it may rely on trade secrets and a technological lead. This form of differentiation makes chemical products vulnerable to improved competition: patents may expire; the competition's technology may get better. As a consequence, chemical products are expected to have a short lifetime, typically a decade or less.

Clearly this is interesting, but does it affect chemists and engineers? Yes. Because of their different nature, chemical products are designed and manufactured in very different ways from commodities. They are usually made in batch, in generic equipment used for many different products. Much of the training of chemical engineers is directed at the optimization of large-scale, purpose-built plants: this is irrelevant for the type of process normally required for chemical product manufacture. Furthermore, because of the short lifetime in the market of chemical products and the premium on being first to market, chemical product industries require rapid, new designs. We argue that this has led to a cultural shift in the industry away from specialization and toward integrated design teams. Where the traditional chemical engineer has been restricted to the design, commissioning, and optimization of a plant with a predetermined purpose, the modern counterpart can expect to be involved in the design procedure right from its inception through to the marketing of the product. The process design we teach chemical engineering students seems limited in this context.

Thus the changes in the chemical industry have had a very substantial impact on the type of work an engineer or chemist can expect to do. We have just stated that much of what has been seen as the core of chemical engineering education is of only marginal relevance to the new industry. Are we therefore arguing that our discipline is now irrelevant, or that it has already made the necessary changes in response to the changing needs of industry? Our answer to both these questions is an emphatic no. We believe the chemical engineering curriculum has changed remarkably little in the past 50 years, ignoring the major changes in industry. Indeed that is why we wrote this book. However, we also believe that the core skills of chemistry and chemical engineering are ideally suited to the design of chemical products.

In his presidential address to the Institution of Chemical Engineering in 1966, P. V. Danckwerts said, "It would be a great mistake to think of the content of chemical engineering science as permanently fixed. It is likely to alter greatly over the years, in response to the changing requirements of industry and to new scientific discoveries and ideas for their application." We believe academic chemical engineering has done well at responding to the latter; computerized optimization, for example, is now a standard part of design courses, and modern equations of state are normal in the teaching of thermodynamics. However, in terms of responding to the changing requirements of industry, we believe chemical engineering education has done almost nothing. A glance at an old course syllabus or textbook or a consultation with retiring academics reveals that the basic structure of chemical engineering curricula is essentially unchanged in the past thirty years, that many parts of a 1950 course are completely familiar, and that the essential elements are recognizable even in the first systematic textbooks of the 1920s.

Does this matter? After all, the teaching of basic geometry has not changed much in the past couple of millennia, but it is as useful today as ever. We wish to emphasize that this is to a large extent true of the underlying science in chemical engineering too. The principles that have served so well in process design are applicable to the new challenges of chemical products. We hope that this has been brought out by the numerous examples in the book. Indeed, we believe that chemical engineers are uniquely well placed to exploit the new emphasis on chemical products; our discipline has always drawn together the technology of other areas into a coherent engineering subject, united by thermodynamics, heat and mass transfer, and unit operations; and this discipline is an ideal background for those involved in developing chemical products. Chemical product design offers chemical engineering education the opportunity to share in a renaissance, integrating our well-established skill set into the new challenges of the chemical industry.

We do not wish to suggest wholesale changes to the curriculum, although undoubtedly some alterations are appropriate. What we do argue is that an evolution is needed in the way in which design is taught, in order to prepare our students for the types of career many will have. Design of large-scale continuous plants is simply no longer what most engineers do. An expanded design experience should prepare students for the more diverse and flexible roles they are now expected to perform in industry.

In order to achieve this we have described a four-step design procedure: needs, ideas, selection, and manufacture. This procedure gives the book its structure. Similar procedures have long existed in mechanical engineering and business studies. We have adapted these to the needs of chemical product design; we hope that in doing so we have reflected the unique technology involved in the chemical industry. We passionately believe that in this industry design must be led by chemical technology.

Our four-step procedure can of course be no more than a template, a starting point from which to proceed. It suggests a helpful structure with which to organize design: it is a heuristic from which to start, not a description of a complete or perfect strategy. It must be adapted to individual cases – every product is unique. It will naturally be appropriate to emphasize different stages for different products. Although we have presented the design procedure as four steps in series, this too is an oversimplification. Frequently, elements of the different steps will proceed in parallel. More often than not, we will return to earlier stages in the light of later conclusions. Chemical engineers understand the value of recycle loops in enhancing efficiency; this applies to the design procedure just as it does to chemical reactors. Despite its evident simplicity, we do believe that providing an intellectual framework for design is an important and valuable contribution to both teaching and practice.

Suggestions and Acknowledgments

We believe that the material in this book can be used in three different ways. First, it can supplement a conventional, two-semester course on chemical process design. This course will normally include a project for student teams, a project that can include process design, product design, or both. We recommend that the product design material be taught after the material on process design, because we feel that students benefit from learning more quantitative process synthesis before trying to make qualitative decisions concerning products.

Second, the material in this book can also be used in a one-semester course on product design. We suggest that such a course should be about one-third lectures and two-thirds tutorials on design projects. Although the lectures should be spread throughout the semester, they should be more frequent at the beginning of the course. Finally, the material in the book can be used for a short course containing lectures alone, though we believe that this may be less effective for inexperienced students of uneven ability.

We are indebted to many who helped us write this book. We benefited from the encouragement of Professor John Bridgwater, who arranged our collaboration at the University of Cambridge, and to Keith Carpenter of Astra-Zeneca, who partially supported it. We were strongly influenced by the excellent book *Product Design* by Ulrich and Eppinger, which showed us how this subject could be effectively taught in mechanical engineering. We benefited from discussions with Professor James Wei of Princeton University and Professor Hans Wesselingh of the University of Groningen. We are grateful to Liz Thompson and Shirley Tabis, who did much of the typing. Finally we would like to thank our students, who were generously tolerant as we shaped a few slogans into an educational experience.

E. L. Cussler & G. D. Moggridge
Cambridge, U.K. 3 May, 2000

Notation

a	area per volume
A	area
c	total concentration
c_i	concentration of species "i"
$\hat{C}_p$, $\tilde{C}_p$	specific and molar heat capacities at constant pressure
$\hat{C}_v$, $\tilde{C}_v$	specific and molar heat capacities at constant volume
d	characteristic length, e.g., pipe diameter
D	diffusion coefficient
f	fraction extracted
f	friction factor
F	force
$\mathcal{F}$	Faraday's constant
g	gravitational acceleration
G	Gibbs free energy
G	gas flux, in mass per area per time
G	crystal growth rate
h	individual heat transfer coefficient
H	enthalpy
H	partition coefficient; often a Henry's law constant
H	feed flux in extraction
j_i	diffusion flux of species "i"
k, k_D	mass transfer coefficients
k, k', k''	rate constants for chemical reactions
k_B	Boltzmann's constant
k_{surface}	rate constant for a surface reaction
k_T	thermal conductivity
K	overall mass transfer coefficient
K, K'	equilibrium constants
K_a	association constant, especially for a weak acid
Kn	Knudsen number (λ/d)
l	size, for example of a turbulent eddy or an adsorbent bed
l'	length of unused bed
L	liquid flux, in mass per area per time

m	total mass transferred
m	molecular mass
m	equilibrium constant between phases
$\tilde{M}$	molecular weight
n	total number of moles
n_i	total flux of species "i"
$\bar{n}_i$	average assessment of product "i"
n_{ij}	assessment of product "i" by consumer "j"
N	particle concentration, number per volume
N_i	interfacial flux of species "i"
$\tilde{N}$	Avogadro's number
NTU	number of transfer units
p	pressure
p_i	vapor pressure of pure component "i"
pH	$-\log_{10}[H^+]$, where $[H^+]$ is the proton concentration
pK_a	$-\log_{10}[K_a]$, where K_a is the association constant
P	power
q	heat flux, energy per area per time
Q	heat
r	reaction rate, moles per volume per time
r	crystal radius
R	gas constant
Re	Reynolds number (dv/ν)
s_{ij}	score of factor "i" for idea "j"
S	entropy
Sh	Sherwood number (kd/D)
t	time
t_B, t_E	breakthrough time in and exhaustion time in adsorption
T	temperature
U	internal energy
U	overall heat transfer coefficient
v	velocity
V	volume
$\underline{V}_i$	partial molar volume of species "i"
W	work
W	volume of adsorbent
We	Weber number $(\rho v^2 \delta/\sigma)$
x_i	mole fraction of species "i", especially in a liquid
y_i	mole fraction of species "i", especially in a gas
z_i	electrical charge on species "i"
α	thermal diffusivity
$\dot{\gamma}$	strain rate (dv/dz)
δ	thickness, often of a thin film
δ_i	solubility parameter
ε	void fraction
η	electrochemical overpotential
λ	mean free path

μ	viscosity
μ_i	chemical potential of species "i"
ν	kinematic viscosity
Π	osmotic pressure
ρ	density
σ	collision diameter
σ	surface tension
τ	characteristic time
τ	shear stress
ϕ, ϕ_i	volume fraction of species "i"
φ	electrochemical potential
ω	angular speed
ω	activity parameter
ω_i	weighting fraction for factor "i"
Ω	correction factor in estimating thermal conductivity

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Chemical Product Design

Until recently, the chemical industry has been dominated by the manufacture of bulk commodity chemicals such as benzene, fertilizers, and polyester. Over the past decade a significant shift has occurred. Now most chemical companies devote their resources to the design and manufacture of specialty, high value-added chemical products such as pharmaceuticals, cosmetics, and coatings for the electronics industry. The jobs held by chemical engineers have also changed to reflect this altered business. However, the training of chemical engineers has remained static, emphasizing traditional commodities.

This ground-breaking text starts to redress the balance between commodities and higher value-added products. It expands the scope of chemical engineering design to encompass both process design and product design. The authors set forth a four-step procedure for chemical product design – needs, ideas, selection, and manufacture – using numerous examples from industry to illustrate the discussion. The book concludes with a brief review of economic issues.

Chemical engineering students and practicing chemical engineers will find this text an inviting introduction to chemical product design.

E. L. Cussler is Distinguished Institute Professor, Department of Chemical Engineering and Materials Science, University of Minnesota. He is a past president of the American Institute of Chemical Engineers and the author of *Diffusion*, published by Cambridge University Press.

G. D. Moggridge is lecturer, Department of Chemical Engineering, University of Cambridge. His research ranges broadly from new adsorbents to the control of zebra mussels.

Contents

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1

An Introduction to Chemical Product Design

This chapter explains what this book is about and why its subject is important. This is a book about the design of chemical products. In our definition of chemical products, we include three categories. First, there are new specialty chemicals that provide a specific benefit. Pharmaceuticals are the obvious example. Second, there are products whose microstructure, rather than molecular structure, creates value. Paint and ice cream are examples. The third category of chemical products is devices that effect chemical change. An example is the blood oxygenator used in open-heart surgery.

The nature of chemical product design is described in Section 1.1. Product design emphasizes decisions made before those of chemical process design, a more familiar topic. Chemical product design is a response to major changes in the chemical industry that have occurred in recent decades. These changes, described in Sections 1.2 and 1.3, involve a split in the industry between manufacturers of commodity chemicals and developers of specialty chemicals and other chemical products. The former are best served by process design, and the latter by product design.

The fourth section of this chapter outlines the product design procedure that we will use in the remainder of the book. This procedure is a simplification of those already used in business development. Such a simplification clarifies the basic sequence of ideas involved. Moreover, the simple procedure allows us to consider in considerable detail the technical questions implied in specific products. This technical approach is suitable for those with formal training in engineering and chemistry, and may also be challenging for those whose training is largely in business.

1.1 What Is Chemical Product Design?

Imagine four chemically based products: an amine for scrubbing acid gases, a pollution-preventing ink, an electrode separator for high-performance batteries, and a ventilator for a well-insulated house.

These four products may seem to have nothing in common. The amine is chemically well defined: a single chemical species capable of selectively reacting with

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