Chemical Product Design

Second edition

The chemical industry is changing, going beyond commodity chemicals to a palette of higher value added products. This ground-breaking book, now revised and expanded, documents this change and shows how to meet the challenges implied. Presenting a four-step design process – needs, ideas, selection, manufacture – the authors supply readers with a simple design template that can be applied to a wide variety of products. Four new chapters on commodities, devices, molecules, and microstructures show how this template can be applied to products including oxygen for emphysema patients, pharmaceuticals like taxol, dietary supplements like lutein, and beverages that are more satisfying. For different groups of products the authors supply both strategies for design and summaries of relevant science. Economic analysis is expanded, emphasizing the importance of speed-to-market, selling ideas to investors, and an expectation of limited time in the market. Extra examples, homework problems, and a solutions manual are available.

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For Betsy and Liana, who tolerated numbered wine glasses.

Contents

List of Symbols

a	surface area per volume
A	area
b	constant
B	bottoms in distillation (Section 6.4)
c	total concentration
c_i	concentration of species "i", in either moles per volume or mass per volume
$\tilde{C}_p,\ \hat{C}_p$	molar and specific heat capacities respectively at constant pressure
$\tilde{C}_v,\ \hat{C}_v$	molar and specific heat capacities respectively at constant volume
d	diameter or other characteristic length
D	diffusion coefficient
D	distillate (Section 6.4)
D	decimal reduction time (Section 9.3)
E	activation energy
f	friction factor
F	feed
g	acceleration due to gravity
G	molar flux of gas
G	Gibbs free energy
G	crystal growth rate (Section 8.4)
Gr	Graetz number (d^2v/Dl)
h, h_i	heat transfer coefficients
H	partition coefficient
H	enthalpy
$\tilde{H},\ \hat{H}$	molar and specific enthalpies
HTU	height of transfer unit
IRR	internal rate of return
j_i	diffusion flux of solute "i", moles or mass per area per time
J_i	total flux of solute "i", moles or mass per time
k, k_{D}	mass transfer coefficient
k, k_{B}	Boltzmann's constant
k, k_{R}	reaction rate constant
k, k_{T}	thermal conductivity

K	equilibrium constant
K	overall mass transfer coefficient
K_{OW}, K_{OA}	partition coefficients between octanol and water or air (Section 2.4)
Kn	Knudsen number (λ/d)
l, L	length
l'	length of unused bed (Section 8.4)
L	molar flux of liquid
m	partition coefficient relating mole fractions in gas and liquid
m	molecular mass
M	total mass
$\tilde{M}_i$	molecular weight of species "i"
n_i	average number concentration per volume (Section 9.4)
N	number of ideal stages
$\tilde{N}$	Avogadro's number
N_i	number of particles in volume V
NPV	net present value
NTU	number of transfer units
p	pressure
$p(N_i)$	probability that volume V contains N_i particles (Section 9.4)
P	power
Pe	Péclet number (dv/D)
q	energy flux
q_i	concentration of solute "i" per mass of adsorbent (Section 8.4)
Q	heat
Q	volumetric flow
r	radius
r	correlation coefficient (Section 9.2)
r, r_i	rate of chemical reaction
R	gas constant
R_D	reflux ratio (Section 6.4)
Re	Reynolds number ($dv\rho/\mu$)
RIPP	acronym for separations of fermentation products (Section 8.2)
ROI	return on investment
S	entropy
Sc	Schmidt number (ν/D)
St	Stanton number (k_D/v)
t	time
T	temperature
U	overall heat transfer coefficient
$\hat{U}$	specific internal energy
v	velocity
V	volume
W	work
We	Weber number ($\rho v^2 l/\gamma$)
x, x_i	mole fraction in liquid
X	fraction conversion in chemical reaction
y, y_i	mole fraction in vapor
z	position

α	thermal diffusivity
α	relative volatility (Section 6.4)
γ	surface tension
γ_i	activity coefficient of species "i"
δ	thickness of thin layer, especially a boundary layer
δ_i	solubility parameter of species "i"
ε	void fraction
η	efficiency
θ	fraction of unused adsorption bed (Section 8.4)
κ	reciprocal of Debye length
λ	mean free path
μ	viscosity
μ_i	chemical potential of species "i"
ν	kinematic viscosity
ν	stoichiometric coefficient
ρ	density
σ	collision diameter
σ	concentration fluctuation (Section 9.4)
τ	characteristic time
τ	tortuosity
ϕ	volume fraction
φ	electrochemical potential
ω	angular velocity
ω	regular solution parameter
ω_i	weighting factor for attribute "i"

Preface

Since its inception around a century ago, the chemical industry has focused on the manufacture of commodities. A commodity chemical, produced at over 1000 tons per year, is sold into a world market where the products are differentiated only by price. Benzene, polypropylene, and titanium dioxide are examples.

This industry had its Golden Age from 1940 to 1980, with growth equivalent to that of the modern software 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. Sometimes, these companies are private, allowing them more easily to ride out the trade cycles typical of commodity businesses. Increasingly, the companies are associated with national oil companies and so have captive petroleum-based feedstocks, the most common raw materials for these commodity products.

More recently, as market growth has slowed, chemical companies without these captive feedstocks have moved towards higher value added products. These products are distinct from commodities in three ways: quantity, value, and structure. They are produced in small quantities, often less than 10 tons per year. The archetype is the active ingredients of a drug, where a few kilograms can command millions of dollars. These higher value added products are made of ingredients which cost a tenth or less of their selling price. These products gain their value from a molecular or micro structure which gives them better performance.

A company's advantage in making these products does not come from having a cheap, reliable feedstock. The advantage comes from a better product. The company does not sustain its position by always becoming a more efficient producer. The company keeps its advantage by continuous innovation, by patent protection, and by trade secrets. It needs better chemistry and engineering, all the time.

The movement of chemical companies towards higher value added products is reflected in the employment of new graduates, most of whom start work not on commodities, but on specialty chemical products. However, most new graduates

are trained largely, if not exclusively, to serve the commodity chemical industry. To train these graduates more effectively, traditional education of chemical professionals must expand. The expanded education must not focus on the traditional question, "How should we make this commodity product?" The expanded education should focus on what is increasingly the more relevant question, "What high value added products are we going to make?"

This book describes chemical product design, and so attempts to fill part of the educational gap between the commodity chemical industry and the new, more fragmented, high value added chemical product industry. The book is divided into two parts. First, we present a template for chemical product design, which starts to answer the question about what we should make. Second, we apply the template to different types of chemical products.

Thus, the first part of the book requires chemists and engineers to go beyond their traditional role of how they will make a chemical commodity chosen by others. This part assumes that these chemists and engineers will be working as part of a project team. Such teams will include those representing marketing, research, manufacturing, and sales. This first part of the book expands material in the first edition. While the book aims to help engineers think about these other aspects of the chemical enterprise, it may also introduce non-engineers to ideas and constraints of engineering. Understanding this introduction requires knowledge of calculus and chemistry.

The second part of the book, which is new to this second edition, is specific to particular parts of the chemical industry. For example, Chapter 6 reviews commodities, Chapter 8 centers on active ingredients, like pharmaceuticals, and Chapter 9 includes personal-care products. Those already working in one product area may find some chapters are more useful than others. Those who seek an overview should be able to gain from all parts.

One market for the book is those trained in commodity chemicals but now involved with other types of chemicals with higher added value. The book also is suitable as a text for university courses. We and others have used the material in this book in a required course, originally taught along the same lines as chemical process design. Such courses involved lectures, use of process simulators, and one large report written by teams of students. All found teaching and learning the material challenging. However, although our courses have always been highly rated, we believe that the courses were not wholly satisfactory. While we could point to a few students whose work was so strong that it attracted venture capital, we always knew that the students' average experience was uneven.

As a result, we now use the book's content in two different ways, which we find more effective than imitating courses in chemical process design. First, we teach a separate course of about forty classes restricted to product design. The classes are split between lectures and smaller recitations, where the specific problems are discussed. The students do not write one large report, but six to ten shorter reports. They are encouraged to develop ideas as teams, but they are expected to write each report individually. In the second type of new course, we teach about twelve classes as a supplement to chemical process design. Again, about half of

these are lectures; again, each student writes not one but three or four individual essays. Both of these strategies work better for us.

In addition to our teaching in universities, we have presented this material as short courses to several companies. We have found that different people have trouble with different parts of product design. Inexperienced students are wonderful at generating new product ideas, but they have trouble making estimates which let them quickly select among possible alternative products. Experienced chemists and engineers have no trouble making quick estimates and sensible selections, but they are less effective at suggesting new ideas. Despite these differences, both groups have benefited from and enjoyed their efforts to get better at chemical product design using the methods described in this book. We challenge you, either as a professor or as a student: while this material is hard to teach and hard to learn, it will often be among the most satisfying parts of your education. Have fun with your designs.

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. 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. Finally, we would like to thank our students, who have been generously tolerant as we shaped a few slogans into an educational experience.

E. L. Cussler and G. D. Moggridge
Cambridge, UK

"I have been anticipating the launch of this book since Dr. Moggridge told me back in 2009 that he had been working on the second edition. This is the long-awaited update of the book which was the first of its kind in the chemical engineering literature. The book had served as the foundation of my chemical product design course. Cussler and Moggridge's clear writing style and abundance of real-world examples in the book make it a must-have for any faculty interested in this fast emerging field of product design in chemical engineering."

Sin-Moh Cheah, Singapore Polytechnic

"Nowadays, Chemical Process Industries mostly produce products with target end use properties, and not simply molecules. This textbook offers the opportunity, for students, chemists, engineers or professors, to discover the framework, methodology and building concepts of the emerging 'chemical product design' discipline. The 2nd edition proposes an increased number of relevant and novel examples, treated thanks to a unique common approach. This reference textbook should be strongly recommended to anyone who wants to take into account the evolution of the chemical industry, and its incidence on teaching applied chemistry or chemical engineering."

Eric Favre, ENSIC, Nancy, France

"After their pioneering first edition on 'Chemical Product Design', Cussler and Moggridge have produced a second edition in which they have adopted a more systematic approach to this topic, which should make it easier to teach at the undergraduate level in chemical engineering courses, and more readable by industrial practitioners. The authors describe a four-step design strategy, involving a template composed of needs, ideas, selection, and manufacture that can be applied in principle to any product, from commodities to novel devices to molecular products to microstructures. The authors have also expanded the economic analysis to emphasize the importance of speed-to-market. Any instructor teaching a course on product design will find this book to be a very useful textbook. Industrial practitioners should find this book to be an excellent reference for promoting innovation in their organizations."

Ignacio E. Grossmann, Carnegie Mellon University

"There is a difficult transition from asking 'How do we make this commodity more cheaply?' to asking 'What should we be making in the first place?', but Cussler & Moggridge clearly guide the way. This is the seminal textbook on Chemical Product Design, demonstrating how chemical engineering fundamentals can be effectively applied to product design. The new and expanded material in the second edition greatly improves the text, illustrating how to apply their design template with industrially relevant problems. I highly recommend this book to everyone in the field of chemical product design and development."

Michael Hill, Columbia University

"Back in 2001 Cussler and Moggridge pioneered Chemical Product Design and introduced its first ever textbook. Now, one decade later, they do it again, through a substantially revised new edition that covers a broader range of topics

(chapters for different product categories, coverage of business idea evaluation/presentation tools, defining future trends and establishing sets of final commandments for chemical product development), and will for sure become the book of reference in this field for the forthcoming years, a mandatory presence in many many shelves, including mine!"

Pedro Saraiva, University of Coimbra

"This second edition of a pioneering and well-received book has been carefully updated and enlarged by the addition of four new exemplifying chapters. Appearing 10 years ago as the first text on chemical product design, the book has been an important source of inspiration for chemists and chemical engineers. The systematic treatment of this diverse discipline and the many practical examples make the book very useful as an introductory text for both a university course and for practicing engineers."

Søren Kiil, DTU-Chemical Engineering

"The book builds on the well established four-step design process presented in the ground-breaking first edition. New additions emphasize the differences in design and manufacturing characteristics of molecules, micro-structured products and devices as opposed to chemical commodities. Students and practitioners may find this an invaluable introduction into the methodology of chemical product design and the use of engineering principles to support the screening and selection of product options."

Ton Broekhuis, University of Groningen

"Revisions to the second half of this excellent text by Cussler and Moggridge have made the book even more relevant and valuable to the challenge of contemporary chemical product design"

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