In celebration of George Stephanopoulos' 70th birthday and retirement from MIT

The Vista of Chemical Product Design in 2040

Ka Ming NG

Department of Chemical and Biomolecular Engineering

The Hong Kong University of Science and Technology
Clear Water Bay, Hong Kong

Acknowledgment: Kelvin Fung, Warren Seider, Danny Lewin, Bob Seader, Soemantri Widagdo, and Rafiqul Gani

2040 Vision of Process Systems Engineering, MIT, June 1-2, 2017

Part I
George – My Professor, My Mentor

Time	Relationship	Turning Point
1973-1976	Professor and Academic Advisor UG, University of Minnesota	• Introduced Prof Alkis Payatakes at the University of Houston to me as my graduate advisor to work on flow in porous media.
1989 Spring	Sabbatical advisor MIT	• Helped consolidate my interest in PSE to this date
2001 March	CTO Corp Sci & Tech Advisor, Mitsubishi Chemical	• Showed us how to organize product and process design around a business vision

Part II
Setting Product Design in Motion

- *G. Stephanopoulos*

  "Invention and Innovation in a Product-Centered Chemical Industry: General Trends and a Case Study,"

  AIChE 55th Institute Lecture (2003).

MITSUBISHI CHEMICAL

Cussler, Chem. Engr. Edu. 1999

DO CHANGES IN THE CHEMICAL INDUSTRY IMPLY CHANGES IN CURRICULUM?

E.L. Cussler
University of Minnesota • Minneapolis, MN 55455

Edward L. Cussler, Institute

Cussler & Wei, AIChE J. 2003

Perspective

Chemical Product Engineering

E. L. Cussler
Dept. of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455

James Wei
Chemical Engineering Dept., Princeton University, Princeton, NJ 08544

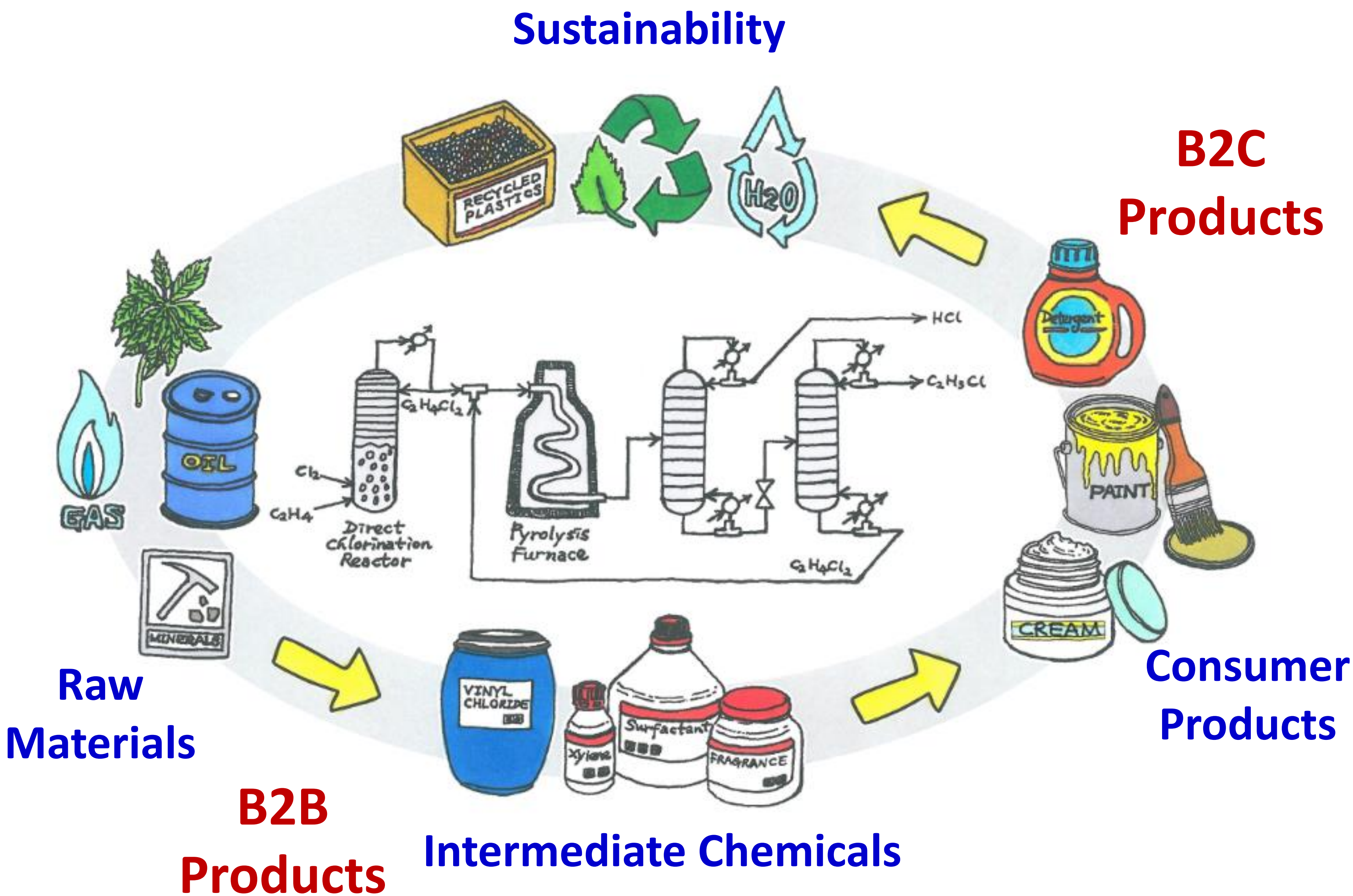
Hill, AIChE J. 2004

Perspective

Product and Process Design for Structured Products

Michael Hill
Unilever Research & Development - Edgewater, 45 River Road, Edgewater, NJ 07020

The Chemical Supply Chain



Challenges and Trends in Industry

- For private chemical companies, it is hard to secure sufficiently high profit margin by manufacturing commodity chemicals (B2B) alone, partly because of the gyration in raw material cost and the competition from state-owned companies.
- To survive and to prosper, they have to focus on B2C products that have entry barriers and sufficiently large market size for the effort to be worthwhile.
- Specifically, they have to sell new B2C products (if marketing channels are available) or link up with companies that sell B2C products - EV batteries, solar panels, touch panels, smart windows, printed electronics, and so on.

Consumer-Centered Products

New products that provide “a sustainable condition that is comfortable for people, society, and the Earth, transcending time and generations.” Kaiteki Institute, MCHC.

All other chemical companies have been heading in the same direction!

2013 Innovation Metrics (dollars in millions)

Metric	Full Year 2013
Total U.S. patent applications	1,755**
U.S. patents granted	1,041
New products commercialized	1,753
Sales from new products*	$10,061
% Sales from new products*	28%
Total R&D expense	$2,153
R&D as % of sales	6%

** Sales from new products launched within past four years*

*** Includes legacy Danisco and excludes any Performance Coatings*

DuPont Data Book

B2B vs. B2C Products

	B2B (Commodity)	B2C (Consumer Centered)
Nature of products	Simple or complex molecules	Novel molecules; **formulated** products; **functional** products; **devices**
Product design	Primarily purity	**Ingredients** and **structures**
Product lifecycle	Decades	**Month / Year**
Team	Primarily chemists and chemical engineers	A **multidisciplinary team** of marketing personnel, financial specialists, lawyers, electronic engineers, mechanical engineers, chemists and chemical engineers.
Financial goal	Cost reduction	**New sources of revenue**
Unit operations	Traditional – distillation, crystallization, extraction, absorption, adsorption, etc.	**Unconventional** – granulation, milling, nanomization, etching, lamination, physical vapor deposition, inkjet printing, etc.
Technical focus	Process design and optimization	Improved product **performance** and **quality**
Knowledge	Well-structured	**Fragmented** so far

A Historical Note: Mass Transfer Operations by Robert E. Treybal 1968

Preface

1. *The Mass-transfer Operations* 1

PART ONE DIFFUSION AND MASS TRANSFER

2. *Molecular Diffusion in Fluids* 15
3. *Mass-transfer Coefficients* 38
4. *Diffusion in Solids* 77
5. *Interphase Mass Transfer* 92

PART TWO GAS-LIQUID OPERATIONS 125

6. *Equipment for Gas-Liquid Operations* 126
7. *Humidification Operations* 176
8. *Gas Absorption* 220
9. *Distillation* 281

PART THREE LIQUID-LIQUID OPERATIONS

10. *Liquid Extraction* 407

PART FOUR SOLID-FLUID OPERATIONS 489

11. *Adsorption and Ion Exchange* 491
12. *Drying* 569
13. *Leaching* 628

PART FIVE THE LESS CONVENTIONAL OPERATIONS 677

14. *The Less Conventional Operations* 678

Index 699

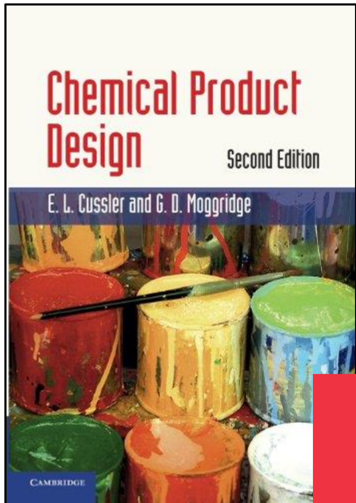
CHAPTER FOURTEEN THE LESS CONVENTIONAL OPERATIONS

The operations considered in this chapter involve, with a few exceptions, solid-fluid contact of various kinds. While some have been applied industrially, they are not commonly used and in most cases their technology is relatively undeveloped. Only a brief, qualitative discussion will be given, to indicate their field of usefulness and some of the problems they entail.

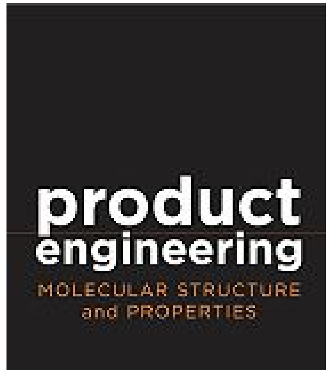
FRACTIONAL CRYSTALLIZATION

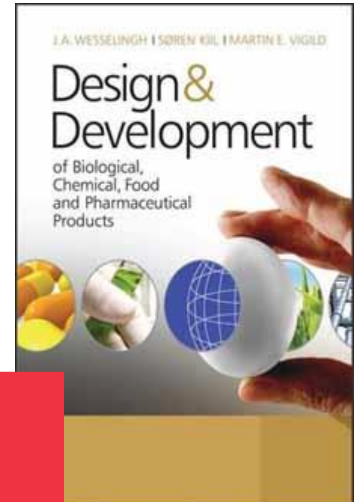
The common crystallization process is a solute-recovery operation rather than a fractionation, such as the crystallization of a nonvolatile solid from a solution with a volatile solvent. If it is done by progressively cooling the saturated solution, mass transfer from the bulk solution to the crystal surface and transfer of sensible heat and heat of solution in one fashion or another are involved. In most cases, solute and solvent are insoluble in the solid state, and this gives rise to an equilibrium diagram of the sort shown in Fig. 14.1.

Product Design Texts

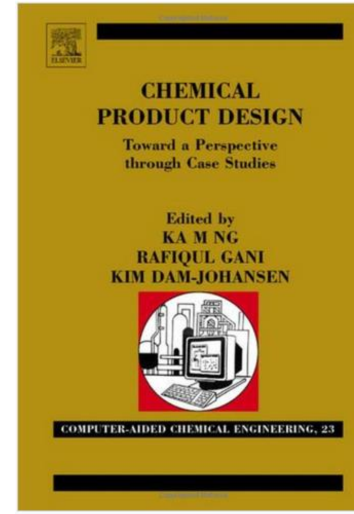


2001, 2011

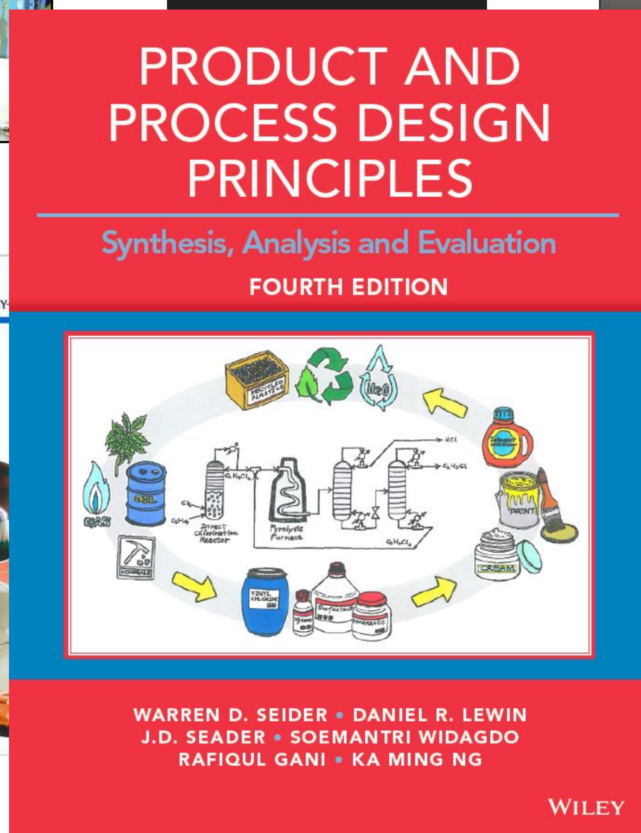


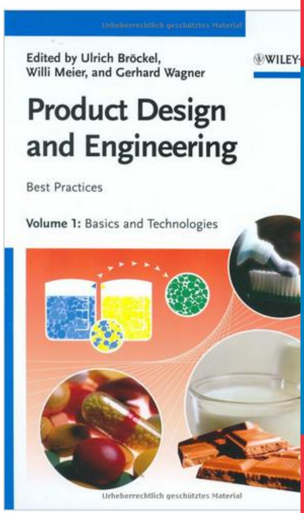


2007

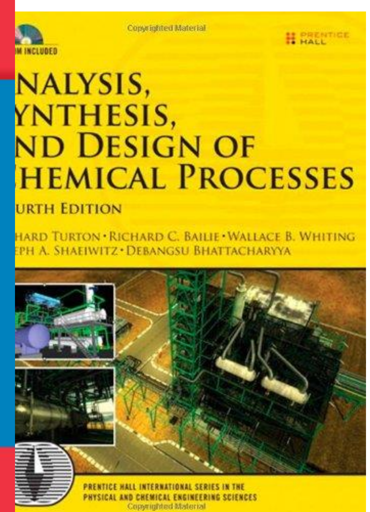


2007

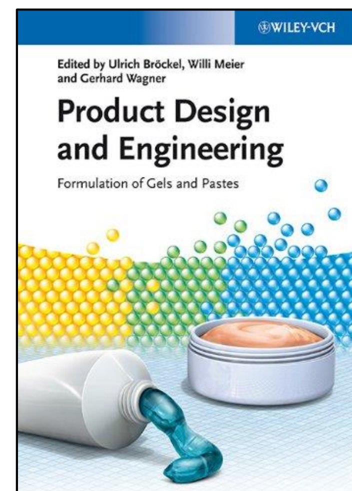




2007



2012



2013

Part III
A Personal View of Product Design Research

Multidisciplinary Hierarchical Product Design Framework

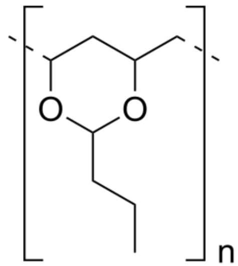
Phases and Job Functions

Job function	Phase I Product Conceptualization	Phase II Detail Design & Prototyping	Phase III Product Manufacturing & Launch
Management	Project management		
Business and Marketing	Market study		Product launch
Research and Design	Product design	Prototyping	
	Process design		
Manufacturing	Feasibility study	Engineering design	Plant startup
Finance and Economics	Economic analysis		

Job function	**Phase I** Product Conceptualization	**Phase II** Detail Design & Prototyping	**Phase III** Product Manufacturing & Launch
Management	**Project management** ▪ *Set product development objective-time chart* ▪ *Secure the necessary human, financial and physical resources*	▪ Identify service issues ▪ Recruit salespersons ▪ Recruit production personnel ▪ *Monitor project progress and spending*	▪ Consider business alliances ▪ *Manage design changes*
Sales and Marketing	**Market study** ▪ *Collect consumer preferences* ▪ *Identify product attributes* ▪ *Study competing products*	▪ Develop marketing plan ▪ *Identify a family of products* ▪ Test marketing	**Product launch** ▪ Develop promotional and launch materials ▪ Firm up key buyers or sales channels
Research and Design	**Product design** ▪ *Choose ingredients and base-case formula* ▪ *Identify product structure* ▪ *Measure physical and chemical properties of product* ▪ *Specify product technical requirements* ▪ *Identify technical challenges and opportunities*	**Prototyping** ▪ *Fabricate prototype* ▪ *Characterization of prototype* ▪ *Stability tests* ▪ *Performance tests* ▪ *Study product safety*	▪ *Continue product improvement* ▪ *Investigate related products* ▪ *Consider development of technology platform*
	▪ *Process conceptual design*	**Process design** ▪ *Synthesize manufacturing process*	▪ *Continue process optimization*
Manufacturing	**Feasibility study** ▪ *Estimate product cost* ▪ *Identify sources of raw materials* ▪ *Investigate patent issues* ▪ *Study environmental impact*	**Engineering design** ▪ *Perform scale-up studies* ▪ *Procure necessary equipment* ▪ *Perform engineering design* **Economic analysis** ▪ *Perform make-buy analysis*	**Plant startup** ▪ *Obtain regulatory approvals* ▪ *Plant startup* ▪ Develop inventory control scheme
Finance and Economics	▪ *Calculate internal rate of return and other financial metrics* ▪ Evaluate opportunity cost	▪ *Facilitate make-buy analysis* ▪ Evaluate all tax issues	▪ Update economic return ▪ Manage cash flow

Classification of Products – Molecular (1)

- Molecules

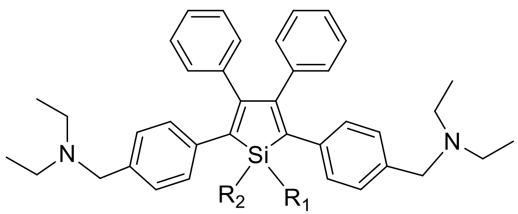


Polyvinyl butyral

Nanoparticles

IR blocking and sound-absorbing auto safety windshield

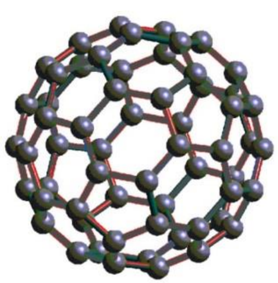
- Functional Molecules

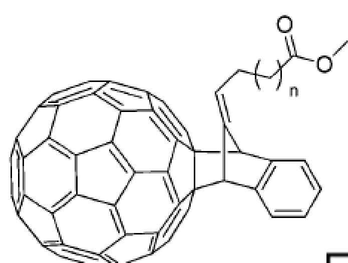


Aggregation induced emission molecule

Biosensors

- Nanomaterials





$IC_{60}MA$-2C n=1
$IC_{60}MA$-3C n=2
$IC_{60}MA$-4C n=3

Fullerene and its derivatives

Organic photovoltaic

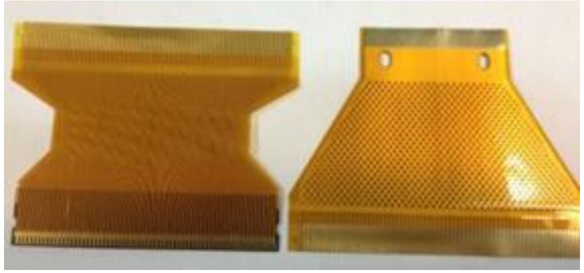
Formulated Products (2)

Formulated products are obtained by mixing selected components together to get the desired product attributes.

Skin Cream

Die Attach Adhesive

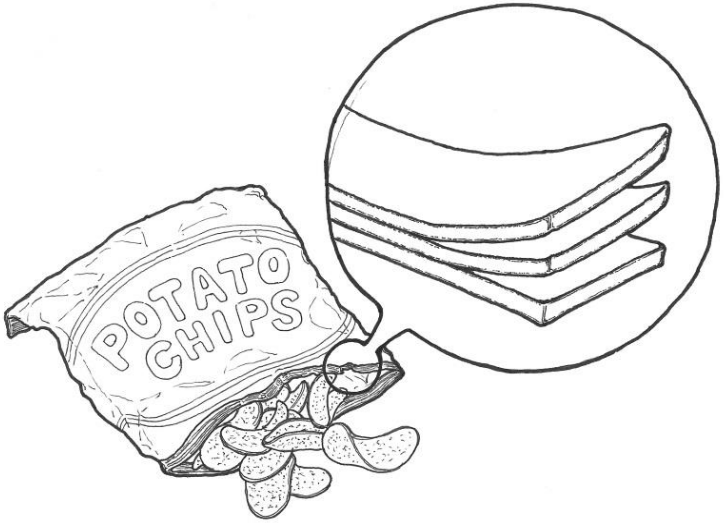
NP Conductive Inkjet Ink ⇨



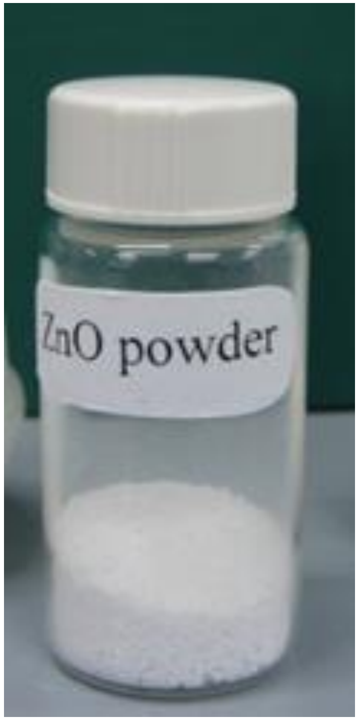
PCB

Functional Products (3)

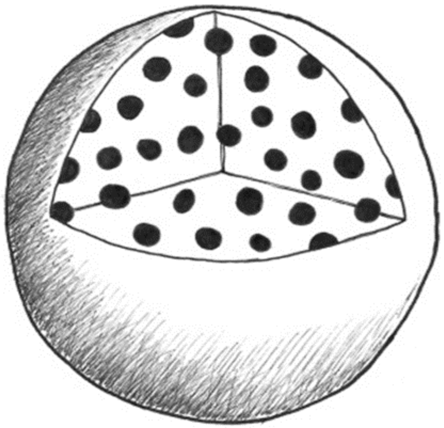
Functional products are those chemical products made up of materials that perform a desired function



Food packaging is made up of three main layers – outside print layer, adhesive layer and inside barrier layer.



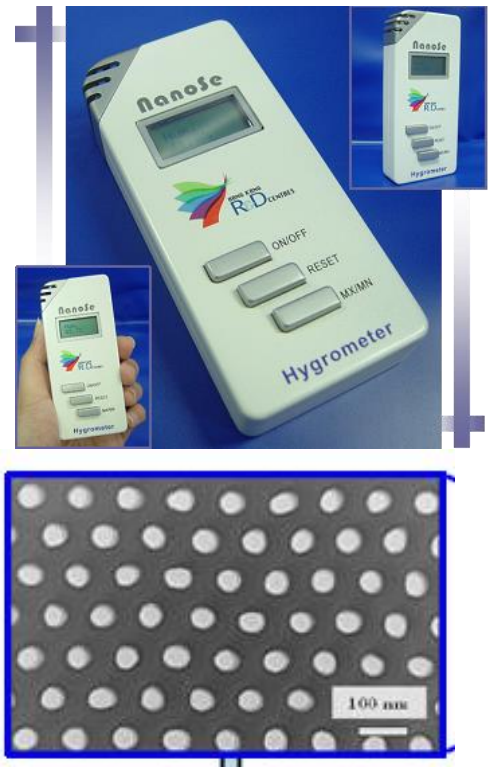
Nano ZnO used in transparent sunscreen



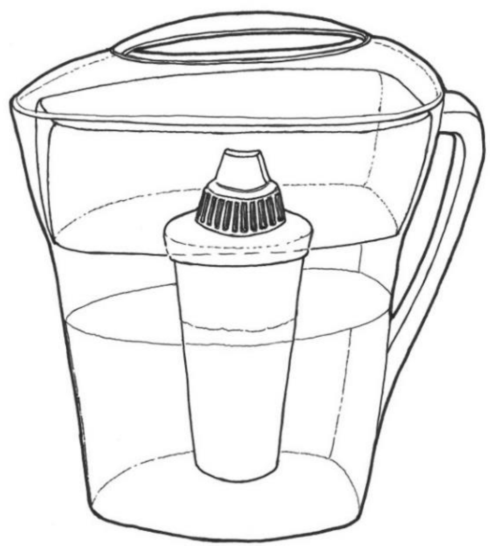
Controlled release herbicide granule

Chemical Devices (4)

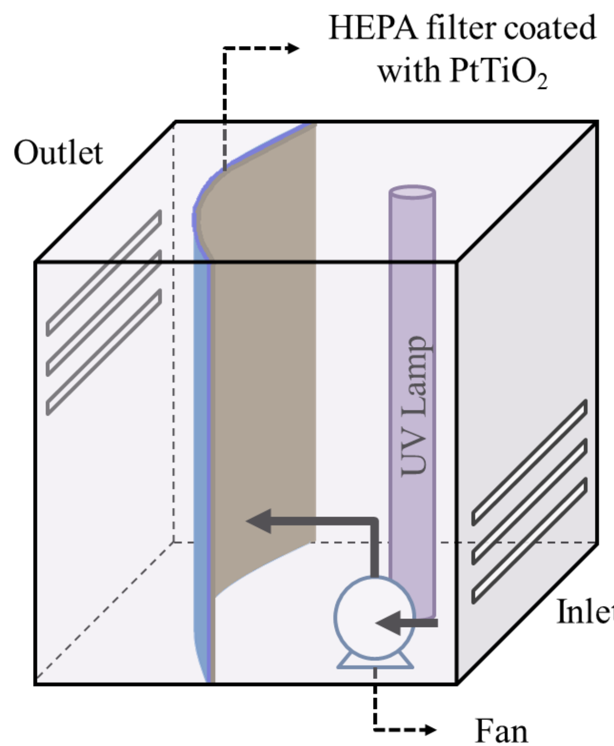
Chemical devices are those chemical products that achieve certain objectives by <u>performing</u> reactions, fluid flow, heating/cooling, and/or separations.



A humidity sensor with nanopores

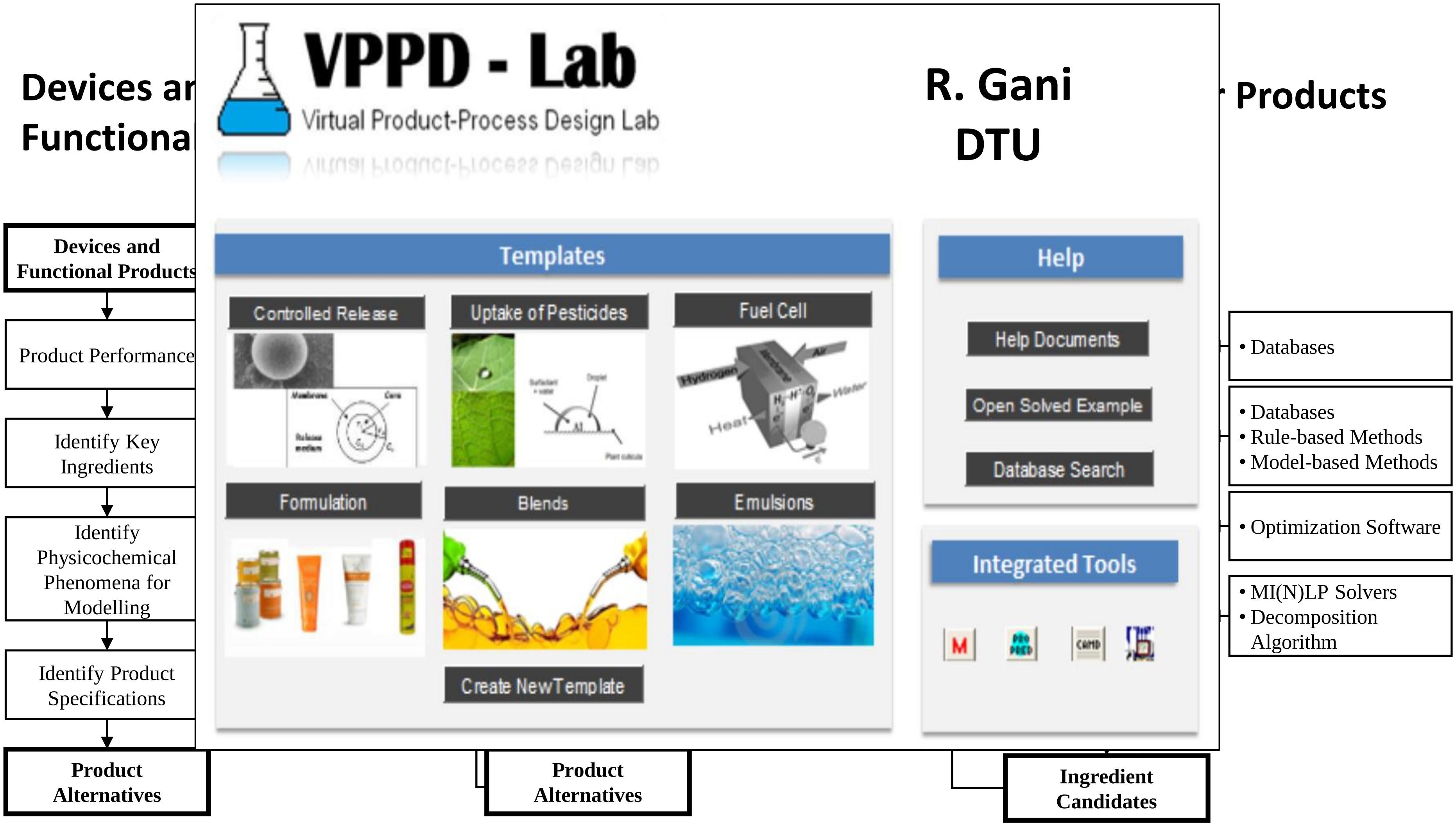


A water filter consisting of activated carbon and ion exchange resins



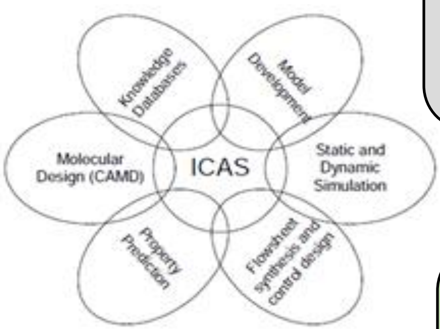
An air purifier decomposes VOCs using UV-TiO_2catalysts

Systematic approaches, procedures, methods and tools for designing the entire spectrum of chemical products are being developed.



Methods and Tools Supporting Product Design Procedures

ICAS from DTU



Ingredients, x

Active ingredients
Supporting ingredients
(solvents, additives)

Process design, pd

Operating conditions, pd_{op}

Temperature
Pressure
Agitation speed

Process flowsheet, pd_{fs}

Unit operations
Equipment geometry
Materials of construction

Property model

Process model

Material properties, p

Physical properties
Chemical properties
Biological properties

Product structure, s

Particle size distribution
Phase volume fraction
Particle shape
Macro form

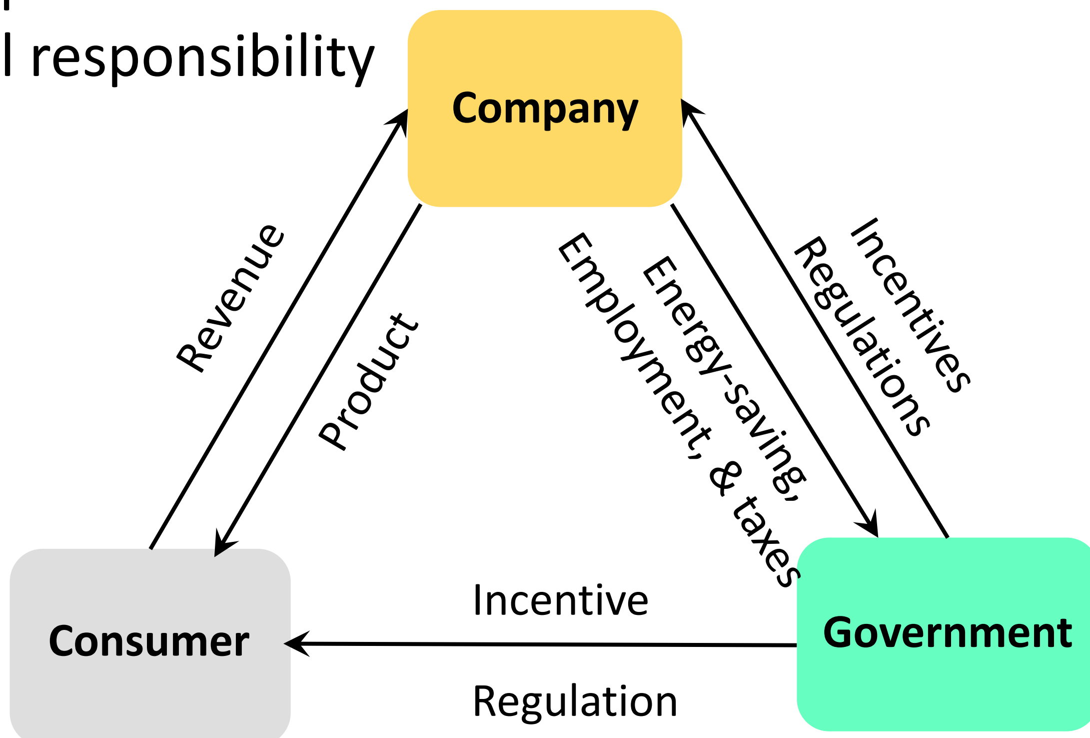
Quality model

Product quality, q

How do we know that the identified product can make a profit? What is the product cost and price? Does it satisfy consumer preference and company strategy? Does it follow government policies and regulations?

Company-Consumer-Government Relationships

Objectives
Net present value
Social responsibility



Objectives
Consumer satisfaction

Objectives
Quality of life
Public safety
Competitiveness of society

The Grand Product Design Model
The optimal product that satisfies multiple objectives

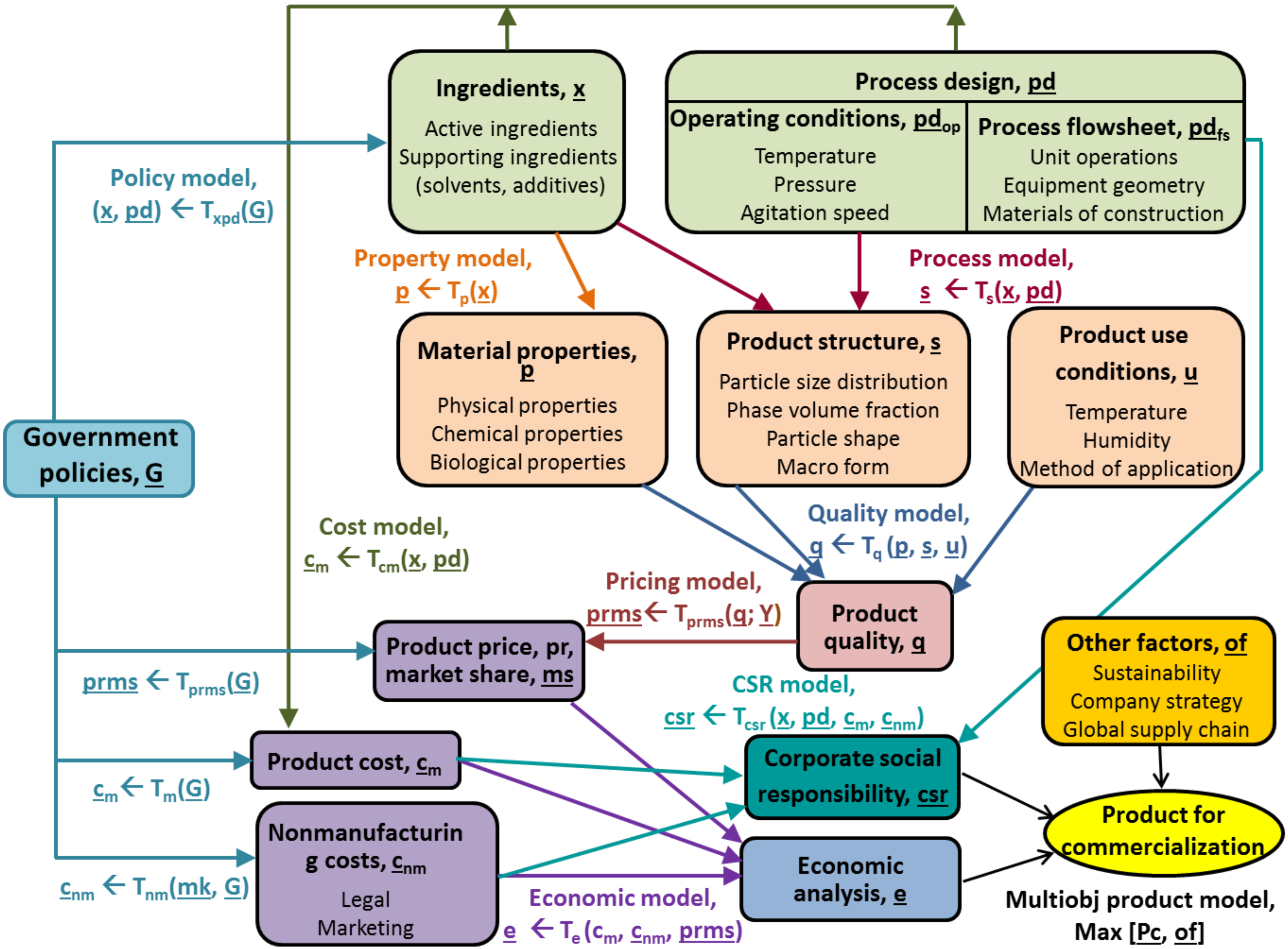
$$\text{Max } [\underline{e}, \underline{\text{CSR}}, \text{ and so on}]$$

subject to

$\underline{q} \leftarrow T_q(\underline{p},\underline{s},\underline{u})$	(Quality model)
$\underline{p} \leftarrow T_p(\underline{x})$	(Property model)
$\underline{s} \leftarrow T_s(\underline{x},\underline{pd})$	(Process model)
$\underline{c}_m \leftarrow T_{cm}(\underline{x},\underline{pd})$	(Cost model)
$\underline{P}_{prms} \leftarrow T_{prms}(\underline{q};\underline{Y})$	(Pricing model)
$\underline{e} \leftarrow T_e(\underline{c}_m,\underline{c}_{nm},\underline{P}_{prms})$	(Economic model)
$\underline{\text{CSR}} \leftarrow T_{CSR}(x, pd, \underline{c}_m,\underline{c}_{nm})$	(Corp. Soc. Resp. model)
$\underline{c}^L \leq \underline{f}\,(\underline{p}, \underline{s}, \underline{u}, \underline{x}, \underline{pd}, \underline{q}, \underline{c}_m, \underline{c}_{nm}, \underline{P}_{prms}) \leq \underline{c}^U$	(Model parameter constraints)

These transformation relations, T, are obtained from model-based methods, rule-based methods, databases, tools and experiments.

The Grand Product Design Model (Ctd)



Part IV
The Vista of Product Design in 2040

Evolution of the Chemical Engineering Curriculum

Subject	Present	2040	Remarks
Unit Operations	Distillation, extraction, and so on	Coating, aggregation, etching, breakage, solids formation,	Progress in solids processing has been slow
Process Design	Process synthesis and simulation	Product synthesis and simulation (Bio, materials, and sustainability)	Prediction of product microstructure is in its infancy
Transport Phenomena	Flow in pipes and packed beds	Transport in functional products and devices	Need a new BSL focusing on products
Mathematics	Methods of solution	Use of product design tools	In progress: CFD, gPROMS, Comsol, Mathlab
Thermodynamics	Prediction of VLE, SLE, and so on	Prediction of properties such as wettability, UV absorptivity, etc.	Many research opportunities in formulation science

Expansion of the Chemical Engineering Profession

- The chemical engineers (bachelor's degree graduates) with a broaden outlook and entrepreneurship will more likely participate in market sectors other than petrochemical – auto, agricultural, packaging, electronics, renewal energy, and so on.
- They will actively participate in product formulation and will operate plants with unconventional processing techniques.
- Many will be involved in designing products that can be sustained; e.g. use of aqueous binder in EV Li-ion batteries can greatly simplify the recycle process.
- They will contribute more directly to meeting societal needs – comfort and convenience for consumers, CSR, and so on

Product design will help integrate faculty focusing on basic sciences and propel chemical engineering to a new height (with new textbooks) by 2040!

To: Prof G. Stephanopoulos

From: UM student 1976

Re: Final design report