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

The Vista of Chemical Product Design in 2040

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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

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


DO CHANGES IN THE CHEMICAL INDUSTRY IMPLY CHANGES IN CURRICULUM?

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

Cussler & Wei, AIChe J. 2003

Hill, AIChe J. 2004

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

Perspective
Product and Process Design for Structured Products
Michael Hill
Unilever Research & Development • Edgewater, 45 River Road, Edgewater, NJ 07020
The Chemical Supply Chain

Sustainability

B2C Products

Consumer Products

Intermediate Chemicals

B2B Products

Raw Materials

B2C Products

Vinyl Chloride
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!

<table>
<thead>
<tr>
<th>2013 Innovation Metrics (dollars in millions)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Metric</td>
<td>Full Year 2013</td>
</tr>
<tr>
<td>Total U.S. patent applications</td>
<td>1,755**</td>
</tr>
<tr>
<td>U.S. patents granted</td>
<td>1,041</td>
</tr>
<tr>
<td>New products commercialized</td>
<td>1,753</td>
</tr>
<tr>
<td>Sales from new products*</td>
<td>$10,061</td>
</tr>
<tr>
<td>% Sales from new products*</td>
<td>28%</td>
</tr>
<tr>
<td>Total R&amp;D expense</td>
<td>$2,153</td>
</tr>
<tr>
<td>R&amp;D as % of sales</td>
<td>6%</td>
</tr>
</tbody>
</table>

* Sales from new products launched within past four years
** Includes legacy Danisco and excludes any Performance Coatings
# B2B vs. B2C Products

<table>
<thead>
<tr>
<th>Nature of products</th>
<th>B2B (Commodity)</th>
<th>B2C (Consumer Centered)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple or complex molecules</td>
<td>Novel molecules; <strong>formulated</strong> products; <strong>functional</strong> products; <strong>devices</strong></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Product design</th>
<th>Primarily purity</th>
<th><strong>Ingredients</strong> and <strong>structures</strong></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Product lifecycle</th>
<th>Decades</th>
<th><strong>Month / Year</strong></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Team</th>
<th>Primarily chemists and chemical engineers</th>
<th>A <strong>multidisciplinary team</strong> of marketing personnel, financial specialists, lawyers, electronic engineers, mechanical engineers, chemists and chemical engineers.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Financial goal</th>
<th>Cost reduction</th>
<th><strong>New sources of revenue</strong></th>
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</thead>
</table>

<table>
<thead>
<tr>
<th>Unit operations</th>
<th>Traditional – distillation, <strong>crystallization</strong>, extraction, absorption, adsorption, etc.</th>
<th><strong>Unconventional</strong> – granulation, milling, nanomization, etching, lamination, physical vapor deposition, inkjet printing, etc.</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Technical focus</th>
<th>Process design and optimization</th>
<th>Improved product <strong>performance</strong> and <strong>quality</strong></th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Knowledge</th>
<th>Well-structured</th>
<th><strong>Fragmented</strong> so far</th>
</tr>
</thead>
</table>
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

- Chemical Product Design
- Design & Development of Biological, Chemical, Food and Pharmaceutical Products
- PRODUCT AND PROCESS DESIGN PRINCIPLES: Synthesis, Analysis and Evaluation
- Product Design and Engineering: Best Practices
- Product Design and Engineering: Formulation of Gels and Pastes

Editions:
- 2001, 2011
- 2007
- 2009
- 2012
- 2013
Part III
A Personal View of Product Design Research
## Multidisciplinary Hierarchical Product Design Framework

### Phases and Job Functions

<table>
<thead>
<tr>
<th>Job function</th>
<th>Phase I Product Conceptualization</th>
<th>Phase II Detail Design &amp; Prototyping</th>
<th>Phase III Product Manufacturing &amp; Launch</th>
</tr>
</thead>
<tbody>
<tr>
<td>Management</td>
<td></td>
<td></td>
<td>Project management</td>
</tr>
<tr>
<td>Business and Marketing</td>
<td></td>
<td></td>
<td>Market study</td>
</tr>
<tr>
<td>Research and Design</td>
<td>Product design</td>
<td>Prototyping</td>
<td>Product launch</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Process design</td>
</tr>
<tr>
<td>Manufacturing</td>
<td>Feasibility study</td>
<td>Engineering design</td>
<td>Plant startup</td>
</tr>
<tr>
<td>Finance and Economics</td>
<td></td>
<td>Economic analysis</td>
<td></td>
</tr>
<tr>
<td>Job function</td>
<td>Phase I</td>
<td>Phase II</td>
<td>Phase III</td>
</tr>
<tr>
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<td>-----------</td>
</tr>
<tr>
<td>Management</td>
<td>Product Conceptualization</td>
<td>Detail Design &amp; Prototyping</td>
<td>Product Manufacturing &amp; Launch</td>
</tr>
</tbody>
</table>
| 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 | Product launch | |
| Market study | - Collect consumer preferences  
- Identify product attributes  
- Study competing products | - Develop marketing plan  
- Identify a family of products  
- Test marketing | - Develop promotional and launch materials  
- Firm up key buyers or sales channels |
| Research and Design | Product design | Prototyping | |
| 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 | - Fabricate prototype  
- Characterization of prototype  
- Stability tests  
- Performance tests  
- Study product safety | - Continue product improvement  
- Investigate related products  
- Consider development of technology platform |
| Manufacturing | Feasibility study | Engineering design | Plant startup |
| Feasibility study | - Estimate product cost  
- Identify sources of raw materials  
- Investigate patent issues  
- Study environmental impact | - Perform scale-up studies  
- Procure necessary equipment  
- Perform engineering design | - Obtain regulatory approvals  
- Plant startup  
- Develop inventory control scheme |
| Finance and Economics | Economic analysis | | |
| Economic analysis | - 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

• Functional Molecules
  - Aggregation induced emission molecule

• Nanomaterials
  - Fullerene and its derivatives
  - IR blocking and sound-absorbing auto safety windshield
  - Biosensors
  - Organic photovoltaic
Formulated Products (2)

*Formulated products* are obtained by mixing selected components together to get the desired product attributes.
**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 performing reactions, fluid flow, heating/cooling, and/or separations.

A water filter consisting of activated carbon and ion exchange resins

A humidity sensor with nanopores

An air purifier decomposes VOCs using UV-TiO$_2$ catalysts
Systematic approaches, procedures, methods and tools for designing the entire spectrum of chemical products are being developed.
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

**Company**
- Revenue
- Product
- Employment, energy-saving, & taxes
- Incentives

**Consumer**
- Incentive
- Regulation

**Government**
- Regulations

**Objectives**
- Consumer satisfaction

**Objectives**
- Quality of life
- Public safety
- Competitiveness of society
The Grand Product Design Model
The optimal product that satisfies multiple objectives

Max \([e, \text{CSR}, \text{and so on}]\)

subject to

- \(q \leftarrow T_q(p, s, u)\) (Quality model)
- \(p \leftarrow T_p(x)\) (Property model)
- \(s \leftarrow T_s(x, pd)\) (Process model)
- \(c_m \leftarrow T_{cm}(x, pd)\) (Cost model)
- \(P_{prms} \leftarrow T_{prms}(q; Y)\) (Pricing model)
- \(e \leftarrow T_e(c_m, c_{nm}, P_{prms})\) (Economic model)
- \(\text{CSR} \leftarrow T_{CSR}(x, pd, c_m, c_{nm})\) (Corp. Soc. Resp. model)
- \(c^L \leq f(p, s, u, x, pd, q, c_m, c_{nm}, P_{prms}) \leq c^U\) (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
<table>
<thead>
<tr>
<th>Subject</th>
<th>Present</th>
<th>2040</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit Operations</td>
<td>Distillation, extraction, and so on</td>
<td>Coating, aggregation, etching, breakage, solids formation,</td>
<td>Progress in solids processing has been slow</td>
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<tr>
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<tr>
<td>Process Design</td>
<td>Process synthesis and simulation</td>
<td>Product synthesis and simulation (Bio, materials, and sustainability)</td>
<td>Prediction of product microstructure is in its infancy</td>
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<tr>
<td>Transport Phenomena</td>
<td>Flow in pipes and packed beds</td>
<td>Transport in functional products and devices</td>
<td>Need a new BSL focusing on products</td>
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<tr>
<td>Mathematics</td>
<td>Methods of solution</td>
<td>Use of product design tools</td>
<td>In progress: CFD, gPROMS, Comsol, Mathlab</td>
</tr>
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<td></td>
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<tr>
<td>Thermodynamics</td>
<td>Prediction of VLE, SLE, and so on</td>
<td>Prediction of properties such as wettability, UV absorptivity, etc.</td>
<td>Many research opportunities in formulation science</td>
</tr>
</tbody>
</table>
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