Chemical Product Design:
What Is it? Why is it important? How is it done?

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What Is a Chemical Product?

Functional material which meets specific need
- Performance chemicals
- Semi-conductors
- Pharmaceuticals
- Paints
- Personal Care products
- Processed foods
- Household products
- Devices
## Commodities vs. Products

<table>
<thead>
<tr>
<th>Commodities</th>
<th>Products</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Compositional spec</td>
<td>• Performance spec</td>
</tr>
<tr>
<td>• Generic</td>
<td>• Differentiated</td>
</tr>
<tr>
<td>• Low margin</td>
<td>• High margin</td>
</tr>
<tr>
<td>• High volume</td>
<td>• Often low volume</td>
</tr>
<tr>
<td>• Process-centered</td>
<td>• Product-centered</td>
</tr>
</tbody>
</table>
Trend Affecting ChE Employment

Recent graduates continue to be hired by businesses producing:

- performance chemicals
- non-durable consumer goods
- formulated pharmaceuticals
- semi-conductor products
- etc. etc. etc.

Cussler & Wei, AIChE J, 49 1073
A Shift From Our Traditional Role

• Chemical engineering community traditionally responsible for process development and manufacturing

• Left product design/development to the chemists, who “threw product over the wall”

• Chemical engineers tracked product purity and costs; other product issues considered irrelevant
How are Chemical Products Developed?

- Industrial approach has been intuitive/experimental
  - Experienced product developer draws on vast knowledge of previous formulations/properties
  - Multivariate trade-offs determined through trial-and-error experimentation
  - Inefficient and resource intensive, typically involving hundreds of prototypes
- Process typically developed after formulation
  - Ignores large impact process conditions can have on product properties
  - Resulted in sub-optimal products
Accelerating Product Development

1. Design of Experiments (DOE)
   - Factorial experimentation
   - Statistical analysis of variance
   - Raises experimental efficiency, but impractical to include more than several variables at time
   - Best suited for narrowly defined problems
Accelerating Product Development

2. High-throughput experimentation (HTE)
   - Robotics
   - Combinatorial chemistry
   - Parallelization

Is this sufficient?

Courtesy of CCRI, University of Ottawa
What Determines Product Properties?

Physico-chemical properties of components

and

Microstructure, which is influenced by process history

Cryo-SEM micrographs of a lamellar structured hair conditioner manufactured under low deformation rates (left) and high deformation rates (right). Although having the identical formulation, viscosities differ by order of magnitude. (Edwards, IChemE NWBP 9, 1998)
And the Combinatorial Explosion

Consider a typical mass market hand cream:

<table>
<thead>
<tr>
<th>Formulation Decisions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Water (1)</td>
<td>1</td>
</tr>
<tr>
<td>Emollients (select 2 of 10)</td>
<td>10*9</td>
</tr>
<tr>
<td>Surfactants (select 2 of 10)</td>
<td>10*9</td>
</tr>
<tr>
<td>Humectants (select 1 of 6)</td>
<td>6</td>
</tr>
<tr>
<td>Polymers (select 2 of 10)</td>
<td>10*9</td>
</tr>
<tr>
<td>Active/emotive (select 1 of 3)</td>
<td>3</td>
</tr>
<tr>
<td>Fragrance (1)</td>
<td>1</td>
</tr>
<tr>
<td>Preservative (1)</td>
<td>1</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Processing Decisions:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Order of Addition</td>
<td>11!</td>
</tr>
<tr>
<td>Operational decisions (after each ingredient)</td>
<td></td>
</tr>
<tr>
<td>Change temp?</td>
<td>2^{11}</td>
</tr>
<tr>
<td>High sheer?</td>
<td>2^{10}</td>
</tr>
<tr>
<td>Emulsification configurations (2 stages)</td>
<td></td>
</tr>
<tr>
<td>Equipment selection (2 of 20)</td>
<td>20^2</td>
</tr>
<tr>
<td>Bypass?</td>
<td>2</td>
</tr>
<tr>
<td>Recycle?</td>
<td>2</td>
</tr>
</tbody>
</table>

10^{23} alternatives
High Throughput Experimentation is not the ultimate answer

- Parallelization raises experimental efficiency
- Yet infeasible to generate *massively* parallel alternatives
- Impractical to replicate process conditions at the scale of typical HTE operation

*How do we deal with the combinatorial explosion?*
Analogous to Process Design

Process designer needs to choose from $10^9$ potential designs

- Systematically identifies and eliminates inferior designs
- Eventually one or two designs proven by experimentation in pilot plant

Product designer needs systematic way to identify product designs while minimizing experimentation
Replace Traditional Product Dev’t?

Å Becomes first phase of Product Development

Å Product design should specify a small set of formulations likely to meet requirements, confirmed or refined through experimentation

Å Allows experimental program of chemical product development to be more focused
Chem Engineers Should Be Good at This

Â Designing a product is not just about knowing physical properties of compounds and mixtures

- When product is used, often subjected to stresses, temperature and concentration gradients, etc.
- Behavior often controlled by transport phenomena, reaction kinetics, thermodynamics: “a process”
- A good product designer understands same principles as good process designers

Â Same fundamental knowledge base needed to understand product manufacture can help in designing products
<table>
<thead>
<tr>
<th>Similarities &amp; Differences</th>
<th>Process Design</th>
<th>Product Design</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Process Design</strong></td>
<td>Product is specified but process is not</td>
<td>Neither product nor process is specified</td>
</tr>
<tr>
<td></td>
<td>Search technique to select among process alternatives</td>
<td>Search technique to select among product alternatives</td>
</tr>
<tr>
<td></td>
<td>Focus on models of manufacturing process</td>
<td>Focus on models of product properties</td>
</tr>
<tr>
<td></td>
<td>Goal is lowest cost manufacturing process</td>
<td>Goal is added value through enhanced product properties</td>
</tr>
</tbody>
</table>
Product Design Algorithm

Cussler & Moggridge*:  
1. Identify customer needs  
2. Generate ideas to meet those needs  
3. Select among the ideas  
4. Manufacture the product

* Chemical Product Design, 2nd Ed (2011)
The Devil is in the Detail

Å Creativity techniques can help, but need more than just brainstorming and selection

Å Need a generic methodology to systematically transform each novel approach into set of product alternatives, and quantitative analysis of those alternatives
Designing Homogeneous Products

Properties result solely from components and not a product microstructure generated during processing

Product and process can be designed sequentially rather than simultaneously
Aircraft Deicing Fluid
What must this product do?

- Melt ice under ambient conditions
- Liquid of appropriate viscosity
- Adequate wetting/spreading
- Non-corrosive
- Biodegrade at acceptable rate
- Etc.
What Basic Mechanism?

Â- Heat generation?

*Open system; likely refreeze*

Â- Freezing point depression?

*If depression is sufficient*

Â- Prevent ice from sticking?

*Sufficient by itself?*
Design Strategy

• Select a freezing point depressant with acceptable biodegradation rate as main component

• Viscosity, wetting/spreading and non-corrosion assured through additives
Use of Physical Property Models

Â Model for fp depression (eutectic behavior)

\[ \ln \frac{1}{\gamma_i x_i} = \frac{\Delta h_i^f}{RT_{m_i}} \left( \frac{T_{m_i}}{T} - 1 \right) \]

Â Models for biodegradation rate and oxygen demand

Â Search for acceptable candidates
Structured Chemical Products

Complex, multiphase materials with properties determined by physico-chemical properties of components and product microstructure

- Emulsions
- Granulated powders
- Compressed powders
- Extruded solids
- Suspensions
- Other complex fluids
Designing Structured Products

- Microstructure determined by interaction of components and manufacturing process

- Since microstructure influences properties, product and process must be designed simultaneously

- A generic design methodology should systematically generate alternatives, and quantitatively analyze those alternatives
Available Techniques

Heuristics
- Systematically generate/eliminate alternatives
- Good designs that are quickly found usually preferred over slow-to-find optimal solutions
- Required when data are limited, e.g. early stages of design

Mathematical Programming
- Optimize set of all potential alternatives
- Useful when sufficient data available
Conclusions

Å Chemical Product Design is the identification of a small set of formulations likely to meet performance specifications, and which can be confirmed or refined through experimentation.

Å Product Design can accelerate new product development well beyond capabilities of experimentation alone.