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

Commodities
- Compositional spec
- Generic
- Low margin
- High volume
- Process-centered

Products
- Performance spec
- Differentiated
- High margin
- Often low volume
- Product-centered

Trend Affecting ChE Employment

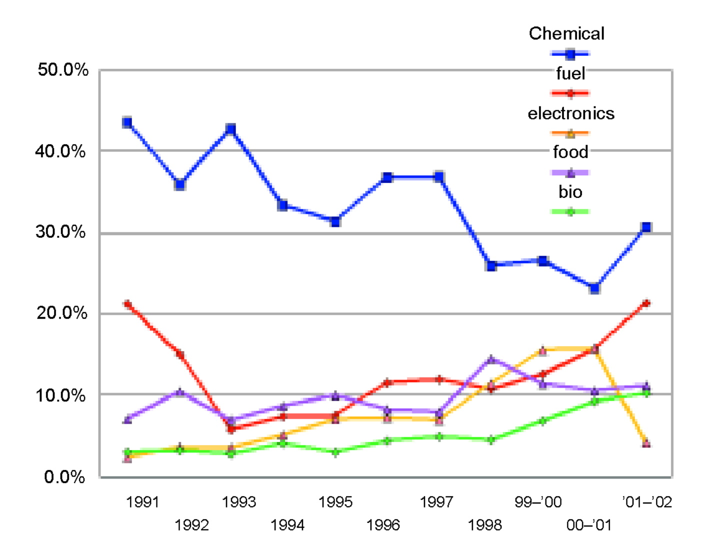


Figure 1. Recent employment of Bachelor's level chemical engineers.

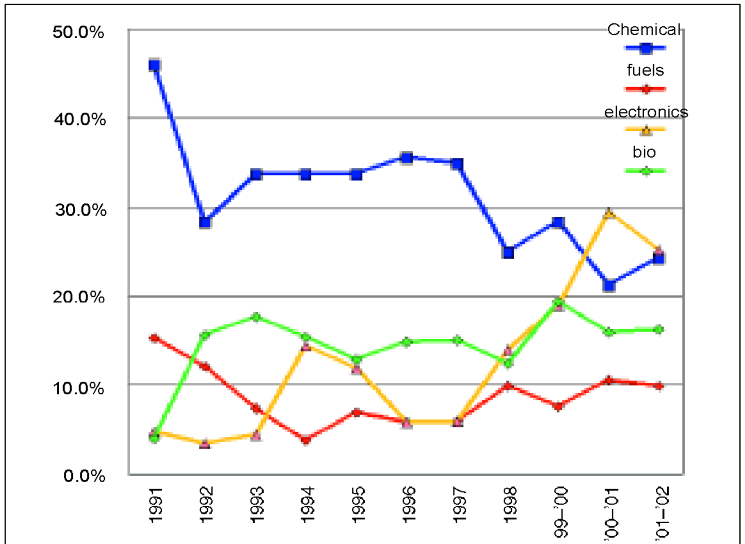


Figure 2. Recent employment of doctoral level chemical engineers.

Cussler & Wei, *AIChE J,* **49** 1073

Recent graduates continue to be hired by businesses producing:

Åperformance chemicals

Ånon-durable consumer goods

Åformulated pharmaceuticals

Åsemi-conductor products

Åetc. etc. etc.

A Shift From Our Traditional Role

Å Chemical engineering community traditionally responsible for process development and manufacturing

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

Å Chemical engineers tracked product purity and costs; other product issues considered irrelevant

How are Chemical Products Developed?

- Å 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
- Å 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)

   Å Factorial experimentation

   Å Statistical analysis of variance

   Å Raises experimental efficiency, but impractical to include more than several variables at time

   Å Best suited for narrowly defined problems

Accelerating Product Development

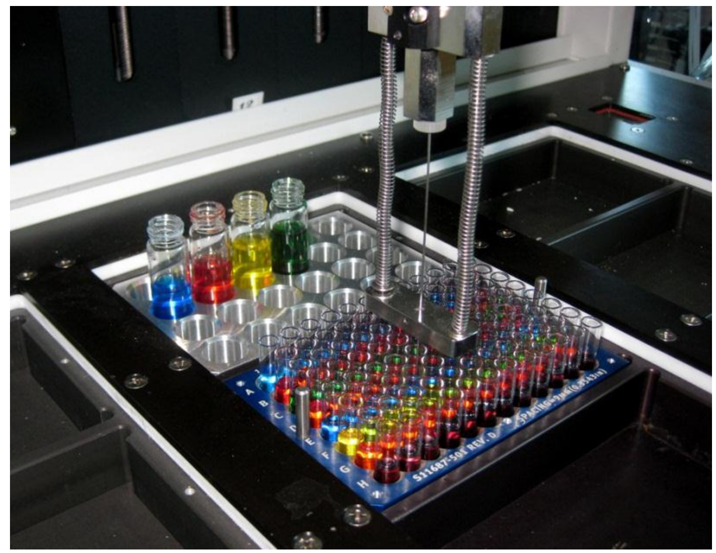
2. High-throughput experimentation (HTE)

Å Robotics

Å Combinatorial chemistry

Å Parallelization

Is this sufficient?



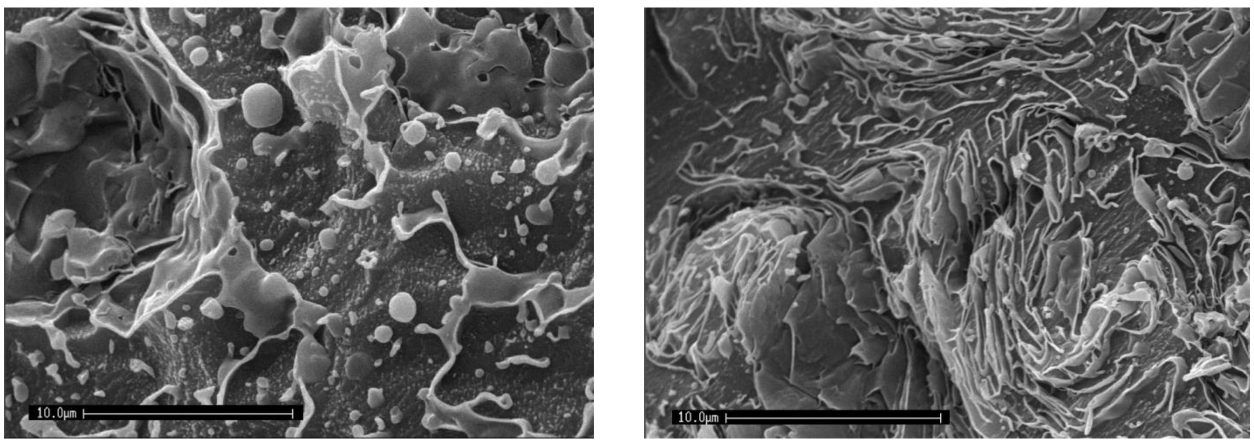
Courtesy of CCRI, University of Ottawa

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:

Formulation Decisions	
Water (1)	1
Emollients (select 2 of 10)	10*9
Surfactants (select 2 of 10)	10*9
Humectants (select 1 of 6)	6
Polymers (select 2 of 10)	10*9
Active/emotive (select 1 of 3)	3
Fragrance (1)	1
Preservative (1)	1
Processing Decisions:	
Order of Addition	11!
Operational decisions (after each ingredient)	
Change temp?	2^{11}
High sheer?	2^{10}
Emulsification configurations (2 stages)	
Equipment selection (2 of 20)	20^{2}
Bypass?	2
Recycle?	2

10^{23} alternatives

Accelerating Product Development

- Å 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

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

  ï Systematically identifies and eliminates inferior designs

  ï Eventually one or two designs proven by experimentation in pilot plant

Å 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

Å 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

Å Same fundamental knowledge base needed to understand product manufacture can help in designing products

Similarities & Differences

Process Design

- Product is specified but process is not
- Search technique to select among process alternatives
- Focus on models of manufacturing process
- Goal is lowest cost manufacturing process

Product Design

- Neither product nor process is specified
- Search technique to select among product alternatives
- Focus on models of product properties
- Goal is added value through enhanced product properties

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*, 2^{nd} 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?

ÅMelt ice under ambient conditions

ÅLiquid of appropriate viscosity

ÅAdequate wetting/spreading

ÅNon-corrosive

ÅBiodegrade at acceptable rate

Åetc.

What Basic Mechanism?

ÅHeat generation?

Open system; likely refreeze

ÅFreezing point depression?

If depression is sufficient

ÅPrevent ice from sticking?

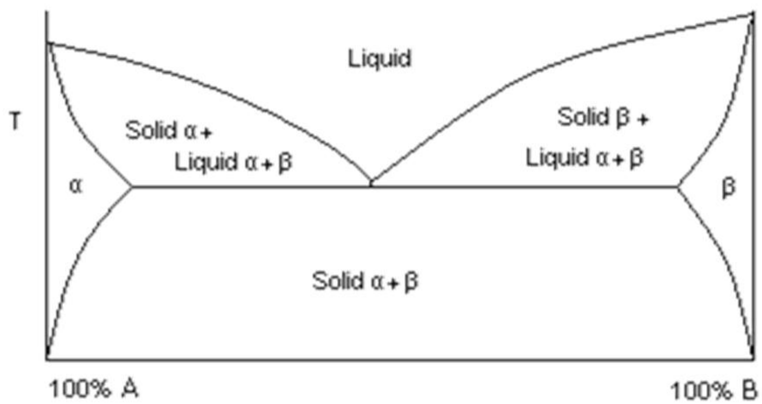
Sufficient by itself?

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

ÅModel for fp depression (eutectic behavior)



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

ÅModels for biodegradation rate and oxygen demand

ÅSearch for acceptable candidates

Structured Chemical Products

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

ÅEmulsions
ÅGranulated powders
ÅCompressed powders
ÅExtruded solids
ÅSuspensions
ÅOther complex fluids

Designing Structured Products

Å Microstructure determined by interaction of components and manufacturing process

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

Å 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