Perspective

Product and Process Design for Structured Products

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Since its birth a century ago, the chemical engineering profession has well served the needs of the chemical industry. Commodity chemical businesses long dominated the chemical industry, and this greatly influenced the curriculum of undergraduate chemical engineering education. In turn, the chemical industry provided the major source of employment for chemical engineering graduates and rewarded many with satisfying careers.

Nevertheless, it is apparent that the chemical industry is now moving toward the manufacture and sale of higher value-added materials. This shift is more profound than simply a change from commodities to specialties; it is a move away from materials sold according to their purity, to materials sold for their performance behavior (Villadsen, 1997). These latter materials can been termed "chemical products" (Cussler and Moggridge, 2001).

Chemical products can be as varied as performance chemicals, formulated pharmaceuticals, semiconductors and other electronic products, household products, beauty or personal care products, and processed foods. Whether the customer for these products is an industrial user or an individual consumer, it is performance against the criteria of the customer, not a product's composition or purity, that determines its value. Not surprisingly, this trend in the chemical industry has been reflected in employment trends for new BS chemical engineers. 25 years ago, most chemical engineering graduates were hired by commodity chemical companies. Today, some chemical engineering departments report that over half of their BS graduates are entering product-oriented companies, e.g., those in the consumer products and semiconductor materials sectors (Dudukovic, 2003; Cussler and Moggridge, 2001; Westerberg and Subrahmanian, 2000).

The Institute Lecture at the AIChE Annual Meeting in November 2003 also echoed these trends. After commenting on the shift within the chemical industry from a process-centered orientation to a product-centered one, Stephanopoulos suggested that the chemical engineering profession is ill prepared for this change (Stephanopoulos, 2003). In response to these changes, an increasing number of chemical engineering departments have introduced courses in chemical product design, often using *Chemical Product Design* by Cussler and Moggridge (2001) as the main text. Some have suggested that Product Design should be the capstone course of an undergraduate chemical engineering education (Westerberg and Subrahmanian, 2000). This broadening of chemical engineering so as to incorporate product design should be applauded, as it brings fresh problems and new modes of thinking, thereby augmenting and enriching chemical engineering as a whole.

Nevertheless, chemical product design has historically been the domain of chemists, material scientists, and food technologists, whereas chemical engineers have focused on process design and development. So, it might rightly be asked why an employer should now hire chemical engineers for product design. Furthermore, if chemical engineers in the future will focus more and more on product design (in competition and/or collaboration with chemists, physicists, and material scientists), who will be trained to design the processes to make these products?

After 20 years of industrial R&D experience working on both new products and processes for a product-oriented company, I am observing new opportunities emerging in product design that build upon the traditional strengths of chemical engineers. In addition, contrary to the popular wisdom, process design can still add strategic value to the manufacture of chemical products.

While I believe these conclusions are valid across all product-oriented segments of the chemical industry, I will utilize examples involving "structured products". These include processed foods (e.g., ice cream, margarine, and peanut butter), household products (e.g., laundry detergents), and beauty or personal care products (e.g., soaps, shampoos, skin creams, and toothpaste). These are all complex multiphase materials, with microstructures on a scale of 0.1–100 μm. The properties of these materials are determined primarily, not by their overall composition, but rather by their microstructure. The microstructure, in turn, is determined by phase volumes, particle-size distributions and shapes, levels of structurants, including polymers, clays and surfactants, and process history (Edwards, 1998).

Design of Structured Products

Several articles have appeared in the literature proposing new methodologies for designing chemical products (Mog-

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gridge and Cussler, 2000; Westerberg and Subrahmanian, 2000; Wibowo and Ng, 2001; Wibowo and Ng, 2002; Cussler and Wei, 2003; Fung and Ng, 2003). In practice, large product-oriented companies utilize multidisciplinary teams with well-defined roles for product design. The overall procedure typically used is outlined below.

(1) Based on an analysis of consumer trends, a consumer need is identified, typically by market researchers and marketeers. As an example, a food company may conclude from growing consumer awareness of obesity problems that consumers have a need for food products that taste good and will help them lose weight. More specifically, this food company may conclude from market research studies that consumers would be interested in low carbohydrate desserts.

(2) The consumer need must next be translated into a technical target. This is the process of "conceptual product design". Following the food earlier example, consumer scientists (e.g., psychologists and psychophysicists) may suggest that consumers would buy an ice cream that contained less than 5g of carbohydrates per serving. Note, however, that nothing has yet been said as to how (or even if) such a product can be made.

(3) The product concept must next be reduced to a physical prototype. This typically begins with the identification of some sort of novel "active ingredient" which may be a biological active (as in the case of an antiwrinkle skin cream), a chemical active (as in the case of a hair dye or a laundry detergent with bleach), or a physical active (such as a new structurant). Depending on the nature of the "active ingredient", it may be identified by biochemists, organic chemists, physical chemists, or food technologists. In the low carbohydrate ice cream example, a food technologist may suggest that ice cream could be sweetened with sucralose (a chlorinated sucrose) and sugar alcohols (e.g., sorbitol or mannitol) rather than sugar. However, as sugar not only serves to sweeten ice cream but also affects the product microstructure, the substitution of one ingredient for another is not trivial.

(4) Once identified, the "active ingredient" must be incorporated into a physical product prototype. This is usually done by physical chemists, materials scientists, food technologists, and chemical engineers. In the low carbohydrate ice cream example, a food technologist would actually make a batch of ice cream using the identified alternative sweetener.

(5) The prototype product must next be assessed for its performance against a variety of relevant criteria. Ideally this is a field test involving actual consumers, but in the early stages of prototype testing this may be done by laboratory tests to save time and money. For example, the efficacy of a self-tanning skin cream is best assessed by expensive and time-consuming clinical trials. Whereas clinical trials would surely be used in the final stages of product assessment, *in vitro* laboratory measurements may be adequate in the earliest stages, and *in vivo* tests on small panels may be adequate for later stages. Generally speaking, product assessment is done by what may be termed measurement scientists (e.g., analytical chemists, clinicians) and statisticians.

(6) On the basis of measured results, the physical prototype is experimentally refined, guided either by intuition, scientific understanding, or both. As with the initial prototype creation, this is usually done by physical chemists, materials scientists, food technologists, and chemical engineers. This, in turn, is followed by additional rounds of prototype assessment and refinement, as described above.

It must be appreciated that consumers usually want products that simultaneously meet several performance criteria. However, in the real world we usually cannot have everything we want, and so product design invariably involves multivariate trade-offs. For example, increasing the level of highly soluble ingredients in a soap bar may help provide for a rich creamy lather, but those same highly soluble ingredients may also lead to a rapid rate of wear and, thus, poor perceived economy. Hence, compromises must be made.

There will also be trade-offs in product design involving speed and cost. For example, additional rounds of prototype assessment and refinement may allow a product to simultaneously meet all the performance criteria to a greater degree, but this may slow down the product launch to the point where a competitor enters the market first, reducing potential market share and profits. Some products (e.g., ice cream) have seasonal demand, so that the launch must be ready for the season, or else it will not occur. Again, this limits the cycles of prototype assessment and refinement. Similarly, consumers usually have an upper limit as to what they will pay for a product, no matter how well it performs. So, a compromise must be made between performance and cost.

Due to the complexity of this multidisciplinary process, the various disciplines usually work apart, coming together periodically to compare notes and keep the entire team informed of progress. Typically, chemical engineers are not involved with the entire process of product design (Steps 1–6), but rather focus on prototype creation and refinement (Steps 4 and 6).

Of course, chemical engineers are not the only ones capable to create and refine prototypes, so why should chemical engineers add value to this process? The conventional answer to this question is that chemical engineers are good problem solvers, pragmatic, have the skills to do rigorous mathematical analysis, and are trained in systems thinking. However, these are all generic skills, and, hence, provide no guidance as to how (or if) the chemical engineering curriculum needs to change to become more relevant.

Some may argue that the current chemical engineering curriculum adequately develops the generic skills, and, hence, the curriculum should not change, even if graduates never use the specific knowledge content. Ironically, this is the same argument that has been made for university students to study classical Greek and Latin (Cussler, 2003).

However, it is the unique skills of chemical engineers, not just the generic skills that are responsible for the demands for our services. These specific skills include a working knowledge of thermodynamics, fluid flow, heat transfer, mass transfer, and applied economics (Churchill, 2004). This is especially true in the design of structured products, where I have observed that traditional chemical engineering technical skills have a definite place.

As noted above, product design usually consists of an iterative process: make the prototype, assess it in use, and refine the prototype. However, the use of the product by a consumer is itself a "process" in the chemical engineering sense, insofar as it involves applied stresses, temperature gradients, physicochemical hydrodynamics, mass transfer, etc. Since an improved understanding of what happens during product use will facilitate prototype refinement, a fundamental chemical engineering process analysis of product use should serve as a critical part of product design.

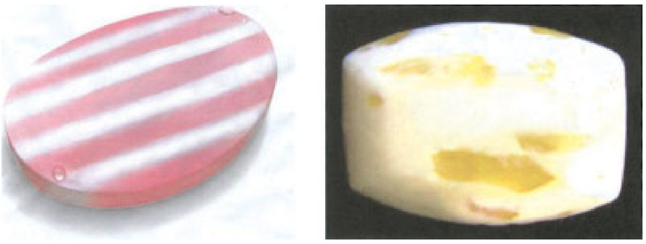

Figure 1. Recent examples of product innovation through processing (Courtesy of Unilever).

Design of Processes for Structured Products

It has been observed the the primary economic driver for a successful chemical product is speed to market, not low cost or efficient manufacture (Cussler and Wei, 2003). Some have interpreted this to mean that process design is not strategically important to these products, and, hence, does not deserve much effort. However, several studies have shown that process design remains a potential source of competitive advantage that successful companies exploit strategically (Pisano, 1997; Pisano and Wheelwright, 1995; Chadha, 1998).

This is certainly true in the manufacture of structured products. For example, an inadequate understanding of how process scale-up affects a particular product's properties can lead to major launch delays at the eleventh hour, much to a company's dismay. This may not just involve the loss of the competitive advantage of being first to market, but in the case of a product with seasonal demand, this may even involve the total loss of a market opportunity. For example, it is too late to launch a new ice cream product if the summer has already passed.

Process design can also bring competitive advantage in cost. The traditional wisdom says that a new product should be launched as quickly as possible, even if the product's profit margin is low due to an inefficient manufacturing process. It is generally believed that since processing knowledge increases over time, both manufacturing efficiencies and profit margins will naturally improve. Sadly, however, these improvements are only incremental and are often inadequate to ensure long-term profitability. This is because early process design decisions constrain later process improvements. Indeed, a company may be loath to discard an entire manufacturing process after having made a capital investment for the initial process. However, designing a process correctly at the start creates the most leverage for maintaining profit margins.

Process design can also be an enabler of product innovation. Some new products demand new processes if they are to be manufactured at commercial scale. Figure 1 depicts two such products, soap bars that were recently launched by a large multinational consumer products company. These soap bars could never have been manufactured at commercial scale without the simultaneous design of new processes, which are now protected by patents (Aronson et al., 2004; Coyle et al., 2002). This highlights the need for concurrent product and process design.

Concurrent product and process design is especially critical for structured products as process conditions during manufacture will greatly influence their microstructure and, hence, their properties. Figure 2 shows micrographs of two hair conditioning products having identical formulation, but manufactured under different process conditions (Edwards, 1998). While differences in product microstructure are obvious from the micrographs, a difference will also be apparent to the consumer as the viscosities of these products differ by an order of magnitude.

Changes in microstructure due to processing are often unavoidable. This is because manufacturing processes typically require both product flow and temperature gradients, thereby inducing stresses on the product. This, in turn, causes such phenomena as droplet deformation, breakup, or coalescence, changes in crystal size or distribution, and structure realignment, all of which will alter product properties. Since processing of structured products usually alters their properties, process design cannot be decoupled from product design for these products.

Process Synthesis for Structured Products

Recognizing the potential impact of processing, how are new processes to make structured products designed? Before a new process is ever designed, the product is conceptually designed, so that the actual product is prespecified in terms of performance attributes and/or physical attributes. Even when the intention is for product and process design to be concurrent, the product formu-

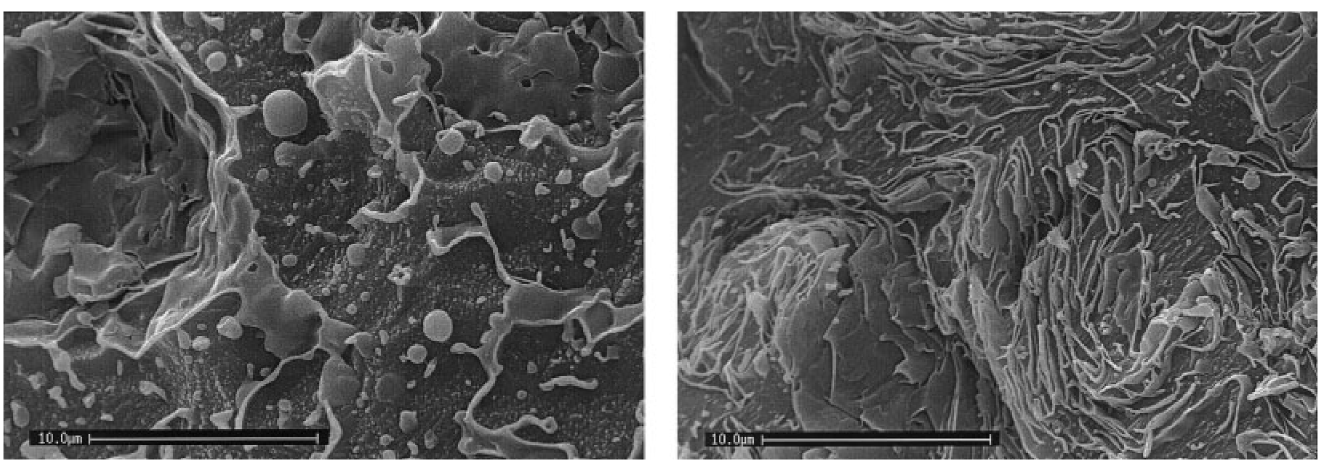

Figure 2. Cryo-SEM micrographs of a lamellar-structured hair conditioner manufactured under low deformation rates (left) and high deformation rates (right) (Edwards, 1998).

lation is often largely set before a process is considered. Furthermore, capital investment for these products is often constrained, either by the costs themselves or by timing considerations. As a result, radical process design is rare, and process design for these products often becomes a retrofit problem.

Once an initial prototype is assembled, the actual process design is invariably done by analogy, either to the bench recipe or to processes for similar products. For example, the process engineer may try to replicate in the pilot plant the process that the formulator used at the bench, i.e., follow the same basic operations in the same order. Or the process engineer may choose a pilot plant process that is known to work well for products that are similar to the prototype. Both approaches, of course, are similar to the way chemical plants used to be designed prior to the invention of process synthesis techniques. Nevertheless, there is a need for a better way to design processes to make structured products. I will illustrate this need with three examples.

Soap Bars

Soap, commonly defined as the salt of a fatty acid, is the reaction product of aqueous caustic soda with fats and oils, which are esters of fatty acids and glycerin. As commercial soap manufacturers derive these fats and oils from natural sources (e.g., beef tallow, coconut oil), the resulting soap contains the salts of several fatty acids, typically ranging in alkyl chain length from C8 to C18. Soap bars also contain multiple phases, including various types of crystal hydrates and lyotropic liquid crystal. Hence, the multiple components are divided among the various phases. This is further complicated through the fact that observed phases may be metastable. The desired microstructure typically calls for the various components to be distributed across the various phases in a specified, nonequilibrium manner (Hill and Moaddel, 2004).

The process of making soap bars can be thought of as in two stages: soap making and soap finishing (Villela and Surányi, 1996; Spitz et al., 1996; Spitz, 1996; Burke, 1996). Consider process synthesis for each of these.

Soap making takes crude fats and oils, aqueous caustic soda, and water as inputs, and produces neat soap, crude glycerin, and waste as outputs (Villela and Surányi, 1996). Neat soap is a lamellar liquid-crystalline phase, typically comprised of 65% soap and 35% water (Hill and Moaddel, 2004; Burke, 1996). It is the most concentrated form of soap that is easily pumpable, and, hence, serves as a good dividing point between soap making and soap finishing. It should be apparent that soap making is all about chemical reactions and separations. Thus, process synthesis for soap making is amenable to modern process design techniques.

However, soap finishing is very different in essence. Process input streams are neat soap, active ingredients, emotives, fragrance, color and preservatives. The output streams should be soap bars (of the desired microstructure and properties) and the excess water. This is all about physical transformations and the creation/evolution of microstructure, well beyond modern process synthesis techniques.

Given the complexities of the desired product, the soap finishing process will involve heating/cooling, removing excess water, macromixing, micromixing, recrystallizing, and shaping of the bars (usually by extrusion). Key questions are: What is the best order of these operations? What equipment should be used, and in what order?

Margarine

Margarine is a water-in-oil emulsion with a network of solid fat crystals. The water droplets need to be small enough to avoid phase separation and microbial growth. In addition, although fat crystals can exist as either of three polymorphs (α, β' and β, in order of increasing stability), only one crystal morphology (β') will produce margarine that is not sandy or grainy (Alexandersen, 1996; Chrysam, 1996).

The margarine process takes as input streams fats and oils, water, milk protein, food polymers (like guar and carageenan), and flavorings, and has as an output stream margarine with the desired properties. As with soap finishing, this is all about physical transformations and the creation/evolution of microstructure.

More specifically, the margarine process will involve heating/cooling, premixing, mixing, melting/crystallizing, emulsification, creating a droplet distribution, and shaping of the final product (either by extrusion or molding). Key questions are: What is the best order of these operations? What equipment should be used, and in what order?

Skin Creams

Skin creams are emulsions, usually water-in-oil, sometimes with a network of solid crystals. The ingredient list may be long, with as many as 50 ingredients, some of which may be sensitive to degradation by heat, oxidation, or shear (Barnett, 1972; Strianse 1972, Griffin, 1974; Barton, 2002; Shai et al., 2001).

Input streams for the skin cream process typically include water, stearic acid, surfactant, waxes, polymers, and various emotives and/or biological actives. The one output stream is the skin cream with the desired properties. The process must achieve the correct physical transformations and, thereby, create the desired microstructure.

The skin cream process typically involves heating/cooling, premixing, mixing, melting/crystallizing, emulsification, and creating a desired droplet distribution. Key questions are: What is the best order of these operations? What equipment should be used, and in what order? For that matter, should this be any different from margarine processing? If so, why?

As these examples illustrate, the numerous process steps involved with the processing of structured products create the potential for an enormous number of process alternatives. There is currently no coherent methodology to select the best

Table 1. Some Heuristics for Skin Cream Manufacture

1. Dissolve all hydrophylic ingredients in water prior to emulsification.
2. Heat/melt all hydrophobic ingredients prior to emulsification.
3. Powders that are difficult to wet should be prewet if possible, using an available liquid.
4. Heat the water mixture prior to emulsification.
5. Do not add head-sensitive or volatile ingredients to any mixture that will be heated until after that mixture has cooled.
6. Do not add shear-sensitive ingredients until after emulsification.
7. Additives that increase mixture viscosity should be added as late as possible.
8. Avoid pH extremes (<4 or >9) if polymeric thickeners are present.
9. Avoid high electrolyte activity if polymeric thickeners are present.

Implications for Chemical Engineering Education

The need for product and process design for structured products has several implications for the undergraduate chemical engineering curriculum. For example, chemical engineering undergraduates may not realize that they already have the technical skills needed to analyze product use simply because they have never been given examples of such problems to solve. So it would be helpful to illustrate process analysis with examples of product use alongside more traditional process examples.

For example, principles of fluid mechanics and rheology can be used to analyze the flow of toothpaste from a tube under an applied force. Principles of transport phenomena can be illustrated by an analysis of the degradation of sensitive ingredients caused by the diffusion of reacting species and/or thermal effects. The same principles can also be used to analyze transdermal delivery (involving simultaneous diffusion and enzymatic reaction), or powder dissolution under conditions of limited solubility.

Learning chemical engineering principles through analysis of various examples of product use will greatly broaden the thinking of new graduates and better equip them for careers in product design.

In addition, as structured products are typically powders, emulsions or colloids, it would be helpful if the undergraduate chemical engineering education included more exposure to these types of materials, including an introduction to surface science, non-Newtonian fluids, and powder properties.

While chemical engineers will have an increasing role in product design, process design will continue to be important. However, the context of process design courses should expand to include processes for chemical products, including structured products. This would require that the process design curriculum include material on the nature of chemical products, such as elements of product microstructure. The effects of processing on product microstructure should also be included, e.g., principles of droplet breakup and coalescence.

Financial analysis is also essential and should be assured adequate attention. In addition, a unit operations laboratory course would do well to require some performance specification, or an element of good manufacturing practice (GMP).

process alternative. This suggests the need for a comprehensive framework to systematically design a process to manufacture any given structured product. As this generic problem is analogous to process synthesis for chemical processes, the same techniques may be useful.

While numerous process synthesis methodologies have been described in the literature (Han et al. 1996), there are two primary approaches: (1) systematic reduction of the number of alternatives through heuristics, and (2) optimization of the set of all potential alternatives through mathematical programming.

Heuristic-based approaches are particularly appealing as heuristics are already used in the design of processes to make structured products. Some typical heuristics for Skin Cream processing are shown in Table 1. Although these heuristics may be helpful, they are not comprehensive and may at times conflict. Hence, heuristics require a framework if they are to be more useful for process synthesis.

One popular comprehensive heuristic framework for chemical process synthesis is the hierarchical decomposition methodology developed by Douglas (Douglas, 1988; Douglas and Stephanopoulos, 1995). Hierarchical decomposition has already been expanded to cover process design for mayonnaise and salad dressings (Meeuse et al., 2000), demonstrating that this technique can provide an acceptable framework for structured products. However, other heuristic frameworks may also be relevant, including Means-Ends Analysis (Siirola, 1996).

Less progress has been made using mathematical programming to optimize process design for structured products. Yet, mathematical programming has been successfully applied, not only to chemical process design (Grossmann, 1996), but also to simultaneous molecular design/process design (Hostrup et al., 1999; Linke and Kokossis, 2002). This strongly suggests that mathematical programming could be expanded to cover processes for the manufacture of structured products, and perhaps even simultaneous product and process design.

However, two significant hurdles impede the application of mathematical programming to these problems. First, complete scientific elucidation of the underlying chemical and physical phenomena behind many structured products and their processes is still lacking, and the relevant data which could be used to further that scientific understanding are maintained as carefully guarded secrets within industry. This limited understanding makes rigorous modeling difficult (Wintermantel, 1999; Wibowo and Ng, 2002). Second, property models for structured products do not exist in a form that lends itself to computer-aided design (Grossmann and Westerberg, 2000; Wesdorp, 2002). Progress against both fronts will be crucial if mathematical programming techniques are to be useful in designing processes to manufacture structured products.

Conclusions

As the chemical industry moves toward the manufacture and sale of chemical products, new opportunities arise for chemical product design. Chemical product design has historically been the domain of chemists, material scientists, and food technologists while most chemical engineers focused on process design. However, there are new opportunities for chemical engineers in product design, both in process analysis of product use, and in concurrent product/process design. The latter is especially important as process design capabilities can offer strategic competitive advantage in speed-to-market, cost, and product innovation. Chemical engineers can therefore contribute substantially to product design alongside the physical chemists, materials scientists, and food technologists, in addition to their unique role in process design.

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