Perspective

# Chemical Product Engineering: An Emerging Paradigm Within Chemical Engineering

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## Introduction

New product development is a crucial task for modern corporations. Facing an increasingly competitive and dynamic market, the ability to continuously identify customer needs and create products that meet such needs is essential to business success. As a result, researchers from fields such as management, marketing, industrial design and engineering have devoted their attention to new product development issues, and many references can be found in the literature covering this topic.[1-5]

New product development combines strategic and organizational actions with technical effort; the former dealing with the management of the development process, strategic placement and launch of the new product; the latter being chiefly concerned with the design of the product and its manufacturing process.

While in some industrial and engineering sectors, such as mechanical and electronic, the technical side of the development process has always been appreciated as a major issue, in the chemical process industries the systematic and efficient design of new products is a relatively recent concern. However, these industries, with chemical engineering as their technical support, seem to be making up for lost time, and chemical product engineering is a fast developing concept among both industrial and scientific communities.

The aim of this article is to provide a review of the scope of chemical product engineering by discussing its emergence within chemical engineering.

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## Chemical Engineering: Present and Future

The chemical process industries, which include the petroleum, fine chemicals, pharmaceuticals and health, cosmetics, household care, agro and food, environment and electronics sectors, have been facing dramatic social, economic and technical challenges, on a global and local scale. As a result, they have been undergoing deep and rapid changes in the scope of their activities, in the strategies adopted to remain profitable and achieve sustainable growth, and, hence, in the way they view the chemical engineering profession. Since many of the chemical products of today and tomorrow do not have much in common with those of twenty years ago, the portfolio of skills and technical knowledge required by chemical engineers has also been changing rapidly. Chemical engineering science and practice must address this new reality, updating its scope, and, hence, evolving from both educational and research perspectives.

In recent years, the chemical engineering community has become apprehensive about the way new generations of chemical engineers are being trained. Several references addressing these concerns can be found in the literature.[6-14]

The words of Danckwerts[15], which have often been echoed,[8,9,16-19] are now more applicable than ever:

"*It would be a great mistake to think of the content of chemical engineering science as permanently fixed. It is likely to alter greatly over the years, in response to the changing requirements of industry and to new scientific discoveries and ideas for their application.*"

According to Cussler and Wei[20], chemical engineers have to reinvent themselves in order to address the demands of the current industrial environment. Nonetheless, the core concepts of the discipline (unit operations, heat and mass transfer, equilibrium, thermodynamics, etc.) remain highly relevant, and an evolution rather than a revolution should be sought.[7,13,18,20,21] Chemical engineering has traditionally focused on the synthesis, design, optimization, operation and

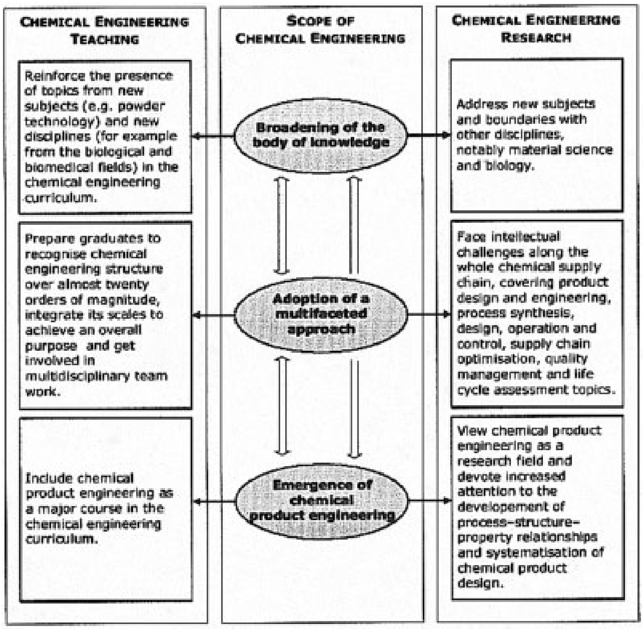


**Figure 1. Changes in chemical engineering and practice.**

control of processes that result in the transformation of raw materials into useful products. Such concerns remain highly significant from the industrial point of view. Furthermore, chemical engineering skills are varied and versatile, allowing one to tackle a wide range of problems found in diverse industrial sectors. Thus, the modern chemical process industries demand not only the development of new concepts and tools, but also a change in the usage in which chemical engineering skills are applied.

The consequent update in the scientific sphere of chemical engineering can be thought about in terms of three major trends:

1. broadening of the body of knowledge associated with the discipline;[8-11,16]
2. adoption of a multifaceted approach to products and processes;[6-9,12-14,16,22-31]
3. emergence of chemical product engineering as a well-established teaching and research field.

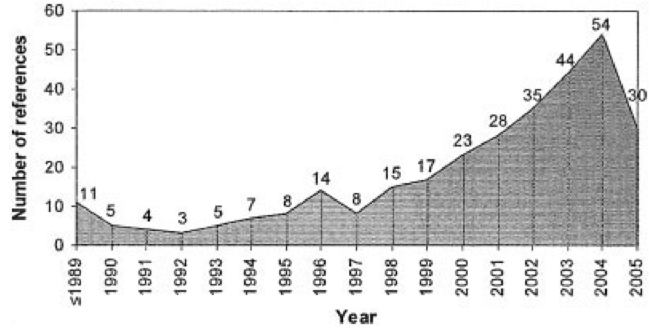


**Figure 3. References related to chemical product engineering published in the last 20 years.**

Each of these trends have direct implications for teaching and research (Figure 1).

## Chemical Product Engineering: An Emerging Paradigm

The emergence of chemical product engineering in the vocabulary of chemical engineering is closely related to the need for moving the design of chemical products from an empirical art toward a science. Chemical process industries have always launched successful products. However, in view of the dynamic and demanding markets companies have to deal with, more systematic approaches have to be adopted in order to guarantee competitiveness. As a consequence, chemical product engineering is becoming a well-established branch of chemical engineering. The concept has been emerging for the last decade (Figure 2). A recent review[36] counted over 300 references related to chemical product engineering available in the open literature (Figure 3). Exponential growth since 1997 is evident.

Some authors have discussed the history of chemical engineering in terms of two paradigms — unit operations (developed in the 1920s and 1930s) and transport phenomena (developed in the late 1950s) — and identified chemical product engineering as a possible third paradigm.[11,20,35] However, although some efforts have been made to elucidate the scope of chemical product engineering and position it in the context of chemical engineering,[8-12,14,24] the field is broad and developing

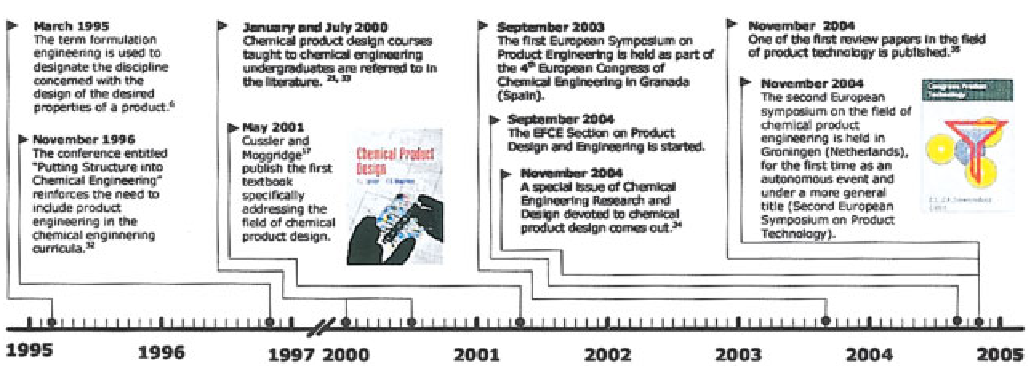


**Figure 2. Chronological diagram of important events marking the affirmation of chemical product engineering as a discipline within chemical engineering.**

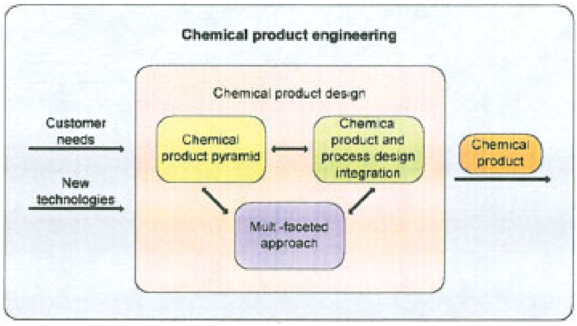


**Figure 4. Structure for chemical product engineering.**

in many directions, and a consensual structure for the discipline has not been achieved yet.[35] Such a structure is essential for its full acceptance as an autonomous and dedicated branch of chemical engineering science.

In the remaining sections, a possible structure for chemical product engineering is developed, and the main teaching and research challenges faced by chemical engineers in the context of this discipline are reviewed.

## Structure of Chemical Product Engineering

Chemical product engineering is a broad field, and to elucidate its scope diverse aspects must be simultaneously considered.

In this article, a new conceptual model for the discipline is proposed (Figure 4). The main aim of this model is to structure chemical product engineering in terms of fundamental and inter-related pillars, supporting the major objective of designing new chemical products. Three such pillars are suggested: (1) the chemical product pyramid; (2) the integration of chemical product and process design, and (3) a multifaceted approach.

In the proposed model chemical products are seen as a very diverse group, encompassing a great variety of structures and functions. Chemical product engineering deals with chemical-related products substantially different from commodity chemicals, which has traditionally been the main focus of chemical engineering. The term chemical product is used to differentiate them from commodity chemicals.

There is often confusion between chemical product design and chemical product engineering. In this article, it is argued that chemical product design is just one facet, albeit the central one, of chemical product engineering. Chemical product design can be seen as the operational and concrete task of converting consumer needs and new technologies into new chemical products. This is encompassed by a larger space of knowledge that corresponds to the chemical product engineering discipline.

From a practical point of view, the design of a new chemical product involves the embodiment of property, process and usage functions (which are systematized in a chemical product pyramid). It must be integrated with the design of a manufacturing process. The effective incorporation of the chemical product pyramid and process design to create a successful product marketed on a global scale demands the adoption of a multifaceted approach to products and processes.

In the following paragraphs, the proposed structure of chemical product engineering (as illustrated in Figure 4) is discussed in terms of the nature of chemical products, chemical product design and the three pillars supporting it.

### Chemical Products

In the chemical engineering context, product engineering has often been taken as synonymous with formulation engineering and, in this sense, associated with multifunctional products whose structure (in the range 0.1–100 $\mu$m) is specifically designed and manufactured to provide the functionality desired by customers. These products, which include shaped and bulk solids, semisolids, liquids and gases (Table 1), have been termed structured products,[7-12,14,32] engineered products,[24] dispersed systems,[37] chemical-based consumer products[38] or formulated products (as in this article). More recently, Voncken et al.[35] introduced the notion of product technology in an attempt to bring a broader designation to product engineering in the chemical engineering context.

Chemical process companies, and, hence, chemical engineers, have to deal with a wide range of products beyond commodity chemicals, which can be roughly classified into six categories: (1) specialty chemicals, (2) formulated products, (3) biobased concepts, (4) devices, and (5) virtual chemical products, and (6) technology based consumer goods. Specialty chemicals are pure compounds that, as opposed to commodity chemicals, are produced in small quantities (typically less than 1,000 tonnes/year), and are sold on the basis of a specific benefit or function. The evolution from commodities to specialty chemicals has been an enduring trend among chemical process industries. However, the shift in the activity of these industries over the last twenty years is more extensive than a change from commodity chemicals to specialty chemicals.[39] Formulated products (e.g., cosmetic and food consumer goods) now represent a large fraction of their business. These products can be defined as combined systems (typically with 4 to 50 components) designed to meet end-use requirements.[11] They are often multifunctional (because they accomplish more than one function valued by the customer) and microstructured or

**Table 1. Typical Forms of Formulated Products[38]**

| Physical Form | | Product Form | Examples |
|---|---|---|---|
| Solid | Shaped | Composites | Bar of soap |
| | | Capsules | Whale oil capsule |
| | | Tablets | Aspirin tablet |
| | | Solid foams | Styrofoam |
| | Bulk | Powders and Granules | Powdered detergent |
| Semi-solid | | Pastes | Toothpaste |
| | | Creams | Pharmaceutical cream |
| Liquid | | Liquid foams | Shaving foam |
| | | Macromolecular solutions | Dishwashing liquid |
| | | Microemulsions | Hair conditioner |
| | | Dilute emulsions and suspensions | Writing ink |
| | | Solutions | Perfume |
| Gas | | Aerosols | Hair spray |

**Table 2. Examples of Chemical Products**

| Category of Product | Illustration | | |
|---|---|---|---|
| | Class of Product | Example | Key Attribute |
| Specialty chemicals | Surfactant | Ammonium lauryl sulfate | Molecular structure |
| Formulated products | Cosmetic | Exfoliating gel | Microstructure |
| Biobased concepts | Drug | Alendronate sodium | Biological activity |
| Devices | Biomedical device | Blood oxygenator | Materials and assembly |
| Virtual chemical products | Software to simulate chemical processes | Aspen Plus® | Computational performance |
| Technology-based consumer goods | Health care consumer goods | Disposable diaper | Materials and assembly |

engineered (since their value derives significantly from their microstructure).[21,24] Biobased concepts, including innovative biomaterials, drugs (genomic and post genomic solutions), and tissue and metabolic engineering technologies, have increased in importance within the chemical process industries with the rise of healthcare and wellbeing concerns. The scope of the sector has also expanded to incorporate products that are not pure compounds, mixtures or particular materials. Devices that carry out a physical or chemical transformation, such as an electrolytic device used to convert salt into chlorinated pool disinfectant, and virtual chemical products[40] are the focus of a growing number of companies. Products such as post-it notes are consumer goods whose functionality is provided by a chemical/physical technology. This kind of product provides a promising and worthwhile extension of the activities of the chemical process industries.

The term chemical product is used in this article to encompass the wide range of goods chemical process companies deal with beyond commodity chemicals, generalizing and standardizing various notations that have been adopted in the literature.[11,19,21,40-42] Table 2 illustrates the different categories of chemical products.

Although the different categories of chemical products have little in common, based on their appearance or performance, similarities between them do exist in terms of development and manufacturing. The term chemical product engineering should then designate the framework of knowledge, approaches, methodologies and tools employed to analyze, develop and produce the whole range of chemical products and not focus solely on formulated products.

## Chemical product design

While the systematisation of product design is a relatively recent concern in chemical engineering, it is better established in some of its sister disciplines, such as mechanical, electrical, computer and biomedical engineering, where customisation is heavily emphasized.[3,5]

By adapting procedures used in these disciplines, Cussler and Moggridge[17] developed the concept of chemical product design, an holistic approach to the design and development of new chemical products, comprising four essential steps: (1) identification of needs that should be met by the product; (2) generation of product ideas which potentially satisfy the needs identified; (3) selection of the most promising product idea, and (4) development of a process to manufacture the desired product. Other frameworks specifically addressing the design of chemical products have also been proposed.[20,33,38,39,42] The chemical product design frameworks proposed in the literature are mainly associated with a market-pull view of the development process. However, technology-push strategies also create significant development opportunities. Besides, in accordance with the multifaceted approach that constitutes one pillar supporting chemical product engineering (Figure 4), the discipline is concerned with the entire process of discovery, design, development, manufacturing and marketing of chemical products. Thus, the concepts of chemical product design and chemical product engineering should not be seen as synonymous, just as the traditional concepts of process design and chemical engineering have not been seen as equivalents.

Chemical product design can be defined as a systematic procedure or framework of methodologies and tools whose aim is to provide a more efficient and faster design of chemical products able to meet market demands. Chemical product engineering is the whole science and art of creating chemical products, a much larger concept encompassing chemical product design. In other words, chemical product engineering can be seen as the general background of knowledge and practice supporting the concrete task of designing chemical products and their manufacturing processes.

## Chemical product pyramid

A crucial feature of chemical products is that customers generally do not judge their value based on technical specifications, but rather according to functionality and performance attributes, such as smell and handling properties. These attributes, used to express and characterize the quality of the product from the customer perspective, are usually referred to as quality factors. Because quality factors are often inherently qualitative and subjective, quantitative parameters have to be developed to model them. These are called performance indices.

Performance indices (and therefore quality factors) are determined by three main factors: (1) the composition and physicochemical properties of the materials forming the product; (2) product structure, which is dependent on the manufacturing process, and (3) product usage conditions.

The dependence between performance indices and product composition, product ingredients' properties and product structure (when applicable) has been mathematically systematized through the concept of property function, initially proposed by Rumpf.[43]

An interesting example to illustrate the concepts of quality factor, performance index and property function comes from perfumery. The performance of a fragrance, which relates to its olfactory perception, has been empirically described in terms of four quality factors: impact (measures the efficacy of the fragrance during the first instants after application); diffusion (refers to the distance over which the fragrance is perceived

Table 3. Illustration of the Concepts of Property Function, Process Function and Usage Function

| Quality Factor | Performance Index | Key Material Physico-Chemical Properties and Compositions | Key Product Structural Attributes | Property Function | Key Process Variables | Process Function | Key Usage Variables | Usage Function |
|---|---|---|---|---|---|---|---|---|
| (i) Pharmaceutical ointment[47,48] | | | | | | | | |
| Controlled release of the active ingredient | Concentration of the active ingredient in the plasma (mean error of temporal profile over target nominal value) | Partition coefficient of the active ingredient between the continuous phase and the dispersed phase<br>Diffusion coefficient of the active ingredient through the continuous phase | Droplet size | Mass transfer model describing transference of the active ingredient from the ointment to the blood, comprising a series of interphase equilibria and diffusion processes | Mixing speed<br>Mixing time | Droplet break-up model balancing interfacial tension and disruptive forces | Time between applications<br>Quantity applied<br>Skin surface of application<br>Patient blood volume | Dynamic model able to predict the concentration of active ingredient in the plasma depending on the values assumed for specific usage conditions |
| (i) Paint formulation (P. Saraiva, unpublished data, January 2006.) | | | | | | | | |
| Paint aesthetics on the wall | Paint whiteness (expressed in terms of panel evaluation against standards) | Pigments concentration<br>Resin concentration | Homogeneity (expressed in terms of a dispersion statistics) | Statistical models, derived from laboratory data, relating the paint whiteness to the mass fractions of pigment and resin | Mixing speed<br>Mixing time | Statistical model relating the paint homogeneity to mixing time and mixing speed | Number of coats<br>Application temperature and humidity<br>Substrate conditions<br>Wall washing practices | Statistical models, derived from experimental data, relating the paint whiteness to the paint application conditions and practices and wall uses |

soon after application); tenacity (expresses the long-term efficacy of the fragrance) and volume (relates to the distance over which the fragrance is noticed some time after application). The odor value can be used to quantitatively express the performance of the fragrance (performance index). Recently, Mata et al.[44] applied thermodynamics and transfer phenomena fundamentals to develop a model (property function) relating the odor value of a fragrance to its composition, volatility and threshold concentration of its components, and activity coefficients expressing the interaction between the fragrant components and the solvent.

In the case of chemical products, in contrast to commodities, product structure often has a preponderant influence over functionality and end-use properties. The desired product structure requires selection of the proper product ingredients, but is often determined largely by the manufacturing process. Consider chocolate — the crystal form of the cocoa butter, which is determined by the tempering process during manufacture, is key to product quality since it determines chocolate melting point and, therefore, the mouth feel. The relationship between process conditions and structural attributes of a chemical product can be quantified by a process function, the definition being analogous to that of a property function.

In addition to product composition, product ingredients' properties and product structure, the circumstances under which a chemical product is used also affect its perceived quality. Parameters describing the way the customer uses the product (such as the magnitude of shear forces as body lotion is applied and quantity of perfume employed) and environmental conditions under which product usage takes place (for example, temperature, humidity level and substrate over which a paint is applied) cannot be directly controlled. Under the Taguchi notation,[45] they correspond to noise factors affecting product performance and, therefore, demanding robustness from the product.[46] Adopting the same reasoning as for the definition of property and process functions, usage functions relating performance indices to customer interaction parameters and usage environmental conditions can also be established.

The concepts of quality factor, performance index, property function, process function and usage function as well as the connection between them are illustrated in Table 3 through simplified examples, based on two chemical products.

Three approaches can be followed to derive property functions, process functions and usage functions. When the underlying phenomena behind the relationships are well understood, theoretical expressions can be obtained from a detailed analysis and rigorous modeling. This approach has been successfully applied to derive functions expressing transport phenomena. Order-of-magnitude analysis, based on a description of the phenomena supported by simplifying assumptions, is an alternative approach to obtain functions when a full scientific elucidation of the system is not available. Comparison of causal and opposing effects in solids handling is an example of this approach. For cases, such as that of systems involving solids, in which the underlying physical phenomena are poorly understood, empirical models can be determined through applied statistical approaches.[38,49]

The idea of a chemical product pyramid is introduced in this article to systematize the relationships between the product recipe, materials' physico-chemical properties, process variables, product structural attributes, usage variables and product

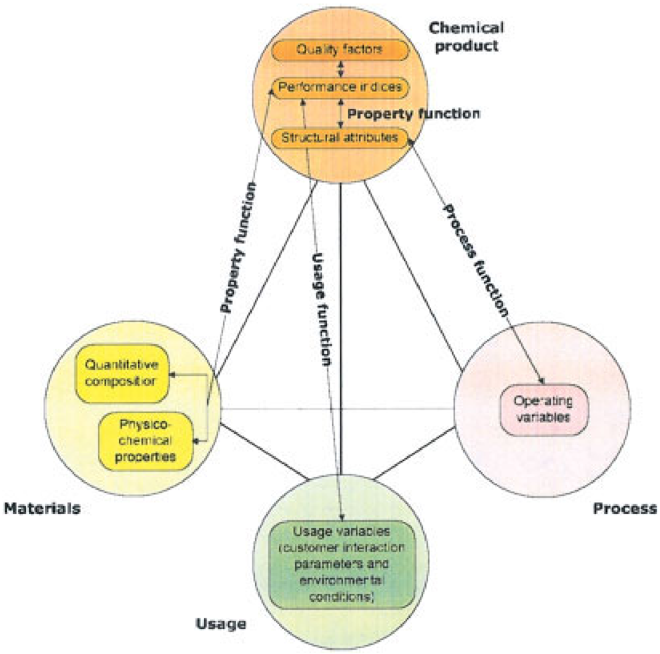


**Figure 5. Chemical product pyramid.**

quality factors (Figure 5). The base of the three-sided pyramid is defined by the materials space, process space and usage space, which determine the chemical product space occupying the top of the pyramid. Connections between and within these spaces are established by property functions, process functions and usage functions. This pyramid corresponds to the technical core of chemical product engineering — in practical terms, the discipline is concerned with the development of property functions, process functions and usage functions and their application, through simulation and optimization, to the design and manufacture of chemical products with end-use properties valued by the customer.

Ice cream can be used to illustrate the idea of a chemical product pyramid. Ice cream is valued by consumers for its flavor, its creaminess and smoothness, and its coolness; these are its quality factors. Flavor is determined primarily by the ingredients used — a property function would relate the ingredient recipe to empirical descriptions of flavor perception. Smoothness and creaminess are controlled as much by processing conditions as by the nature of the ingredients — the keys are the stabilization of air bubbles by fat particles, and keeping ice crystals below about 100 $\mu$m in size. A process function would describe this. The consumers' perceptions of both flavor and texture are strongly modulated by environmental and use factors. In particular the storage history affects ice crystal size by Ostwald ripening. Serving temperature, ambient conditions and general ambiance also influence perceived flavor and texture. This could be described by a usage function. The property and process functions should be controlled to ensure that the product quality factors are robust to variations in the usage function.

## Chemical product and process design integration

Superficially, chemical product engineering and process engineering might appear to be two fully independent disciplines. However, they are closely related to each other and should be viewed from an integrated perspective, rather than sequentially. Chemical product engineering covers the whole conversion process of customer needs and new technology discoveries into marketable products. Since product characteristics are strongly dependent on processing, it makes sense to adopt a view of product development centered on the integration of product and process engineering.

The strategies adopted to develop processes for the manufacture of chemical products have some differences to process engineering associated with the production of commodity chemicals, which is considered mature and has traditionally been the focus of chemical engineering curricula. In contrast to classical process technology, the economics of chemical products are strongly dependent on short lifetimes in the market. At the same time, the value of a chemical product is usually much greater than that of its raw materials, and, therefore, the emphasis on efficient processing is reduced. The phased approach (involving conceptual design, basic design, detailed design, procurement and construction), which has proved so successful for the design of plants for commodity chemicals, is not suitable for the design of processes for chemical products. These products are often not very well defined in physical terms, and the speed with which they are developed, produced and introduced into the market is a key factor in success. An approach to process design emphasising speed over optimization is, therefore, appropriate for chemical products.

An example illustrating the advantages of integrating chemical product and process design is provided by Bernardo and Saraiva,[50] who optimized the development of a cosmetic lotion (oil-in-water emulsion). In this application, the optimization problem incorporated the product quality as assessed by customers, a model relating the viscosity of the lotion to its composition, and a model linking process design and operation with product composition and microstructure. The solution identified the optimal lotion composition and process specifications, with product and process design decisions interacting strongly. An objective function accounting for both product quality and process costs was appropriate. The integrated chemical product and process design solution was shown to be superior to that obtained when chemical product design and process design were handled separately.

## Multifaceted approach

A final concept important in structuring chemical product engineering is that of a multiscale approach to products and processes.[6-9,12-14,16,22-31] In the context of the model proposed in this article (Figure 4), this concept complements those of the chemical product pyramid and the integration of chemical product and process design.

The quality and competitiveness of a chemical product marketed at a megascale is defined at the nano and microscale of its compounds and microstructure, as well as at the meso and macroscale of the manufacturing and distribution processes. Therefore, chemical product engineering is strongly dependent on a multiscale perspective. The ultimate aim of the discipline is the translation of phenomenological laws and models, expressed by property, process and usage functions, into commercial product technology. This requires the understanding of the relationship between macroscopic performance and micro-

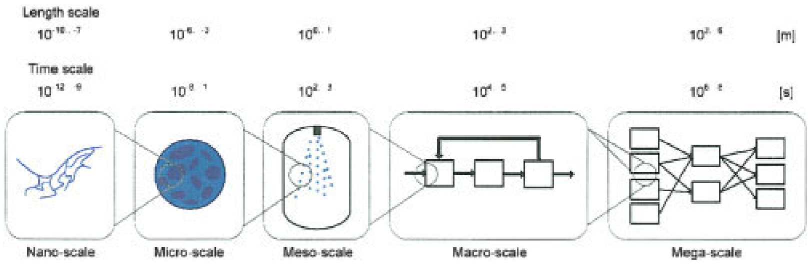


**Figure 6. Length and time scales in the development of a powdered detergent (adapted from Edwards[51]).**

scopic properties, and the ability to synthesize problems over length and time scales spanning many orders of magnitude. In the words of Charpentier,[12] chemical product engineering can be seen as the triplet molecular processes — product — process engineering.

The development of a powdered detergent[38] illustrates the need to adopt a multifaceted approach in chemical product design (Figure 6). Considerations defined at the megascale of markets and business determine the quality required for the product. Recent market trends indicate a shift from low-density to high-bulk density powdered laundry detergents, which are advantageous for transport and storage. As a cleaning agent, the product is expected to effectively remove water-insoluble grease and dirt from the clothes. Bleaching activity is also attractive to customers. Due to environmental considerations, it is desirable that the product is readily soluble in cold water, and has lower foaming and stronger suspension capabilities than existing detergents, being suitable for use in washing machines operating at 40 °C and with low-water consumption. The selection of the product recipe at the molecular scale is crucial to achieve the desired product functionality. A surfactant with a low critical micelle concentration and a Kraft point lower than the washing temperature has to be incorporated in the washing powder so that it removes hydrophobic materials and performs well at low concentrations and low washing temperatures. A bleaching agent should also be included in the product. Conventional bleaches, such as peroxygen compounds cannot be used because they are incompatible with the surfactant due to their oxidative power, and are not particularly effective in cold water. Under these circumstances, inactivated bleach such as sodium perborate, which transforms into the active per acid bleach as it dissolves in water, is a convenient alternative. Other ingredients, namely bleach activators, whitening agents and fragrances, have also to be incorporated in the product. In addition to the recipe, product structural characteristics defined at the microscale contribute to its end-use properties. In order to achieve quick dissolution in water and good flow properties, the size of the powder particles should be kept small, within a narrow distribution and above a minimum value, below which problems due to particle cohesion may occur. Particle-size distributions in the range 300–900 $\mu$m are desirable. A high-bulk density of the powder should be achieved by controlling individual particle porosity — particle porosities of about 5 % guarantee a bulk density of approximately 800 kg/m$^3$. The detergent manufacture process, which is defined at the macroscale, involves four main operations. First, the product ingredients are mixed to form a slurry, which is then spray-dried to form a powder. Because this powder has a low-bulk density, it has to be processed in a high-shear mixer, where shear is applied to fracture the porous spray-dried particles forming smaller and less porous ones. The desired particle-size distribution is achieved by agglomerating the small particles with the aid of a liquid binder. A final drying step is conducted to remove excess liquid. Each of the operations involved in the manufacturing process needs to be controlled so that the desired product structure is achieved. For example, the air/liquid flow ratio, relative air velocity at the nozzle and liquid viscosity are key operating variables in the spay-drying operation, determining the particle-size characteristics of the spray-dried powder. The detergent manufacturing process integrates a site with multiple plants connected to suppliers, warehouses and distribution centers, which is ultimately part of a commercial enterprise driven by global business considerations (megascale).

Concurrent with the adoption of a multiscale approach, the implementation of chemical product engineering requires an extension of chemical engineering into topics that have traditionally been studied separately (e.g., rheology, powder technology and materials science), as well as strong multidisciplinary collaborations among chemical engineers, scientists and other professionals. According to Westerberg and Subrahmanian,[33] success requires a mixture of many talents: business, fine arts, social sciences, basic sciences (e.g., chemistry, physics and biology) and chemical engineering technology, to which quality management and quality engineering tools can be added.[52]

## Teaching Chemical Product Engineering

The chemical engineering community has begun to recognize the need to teach chemical product engineering as part of undergraduate curricula. As pointed out by Villadsen,[32] it would be a major mistake to exclude chemical engineers from their potential competitive advantage in chemical products due to inappropriate design of their curricula.

In recent years, significant efforts have been made to effectively teach chemical product engineering topics. Cussler and Moggridge[17] published the first textbook specifically addressing chemical product design, and some recent editions of traditional process design books include this topic as a chapter.[53,54] A number of different universities now offer chemical product engineering-related courses. A recent survey over the World Wide Web identified more than 25 departments of chemical engineering in which this type of course is taught, and more that a hundred with some kind of chemical product engineering activity being carried out.[36] Without being exhaustive, a number of pioneering courses deserve note. A course focusing on the history and organization of new product inno-

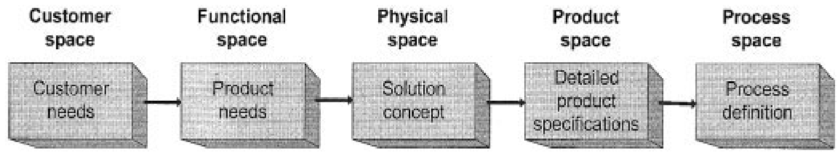


**Figure 7. Chemical product design as a translation of information between different representational spaces.**

vations, molecular structure and property relations, and recent case studies of chemical product design has been taught for several years in Princeton University.[31] According to Westerberg and Subrahmanian,[33] Carnegie Mellon University has been offering for a number of years a cross disciplinary course on the design of engineered products. Chemical product design is part of the required undergraduate curriculum at the University of Minnesota.[21] Wei[55] referred to teaching efforts in the field at other leading American universities (including MIT and Columbia University). European chemical engineering departments have also been implementing chemical product engineering-related courses. At the University of Cambridge, a chemical product design course is taught for final year students.[21] Other U.K. universities have also introduced this topic into their courses.[56,57] Wesselingh[10] presented a chemical product engineering course, provided as a joint effort between the University of Groningen, the University of Oldenburg and Deutsches Institut für Lebensmitteltechnik (DIL), a German food processing research center. The University of Karlsruhe, the Technical University of Denmark and ENSIC-Nancy (part of the Institut National Polytechnique de Lorraine) have initiated teaching activities in this field.[58-60] A chemical product design course incorporating principles of quality management and quality engineering is offered at the University of Coimbra.[52] Taking such efforts one step further, the Hong Kong University of Science and Technology provides a Chemical and Bioproduct Engineering degree that emphasizes the application of engineering to the design of chemical and bioproducts, in what seems to be the first undergraduate training dedicated primarily to this topic.

Despite the importance of such courses specifically addressing chemical product engineering, it needs to be stressed that to effectively teach this discipline these courses must be accompanied by a redefinition of the way chemical engineering is taught in general. In addition to a broadening of the body of knowledge and the adoption of a multifaceted approach (Figure 1), process design courses and the introduction of chemical engineering fundamentals should also be revised appropriately. Even though chemical engineers play an increasingly important role in the chemical product business, process design will continue to be central to the curricula. However, traditional courses can be expanded and adapted to cover processes appropriate for the manufacture of chemical products, which are in many respects different to those commonly used for the production of commodities. For example, courses on separation processes, which currently strongly emphasise distillation, might give greater attention to adsorption, liquid-liquid extraction and recrystallization. The issue of the integration of chemical product and process design also needs attention. As pointed out by Cussler and Wei,[23] Hill[39] and Villadsen,[32] it would be helpful to explicitly teach concepts such as property function and process function and their applications, as well as to illustrate process analysis with examples of chemical products. For example, principles of fluid mechanics and rheology can be used to analyze the flow of a toothpaste from a tube under an applied force. The Engineering Subject Centre in Loughborough, U.K. has recently sponsored a project aimed at producing such product oriented examples for teaching in chemical engineering.

Some textbooks on chemical product design exist,[17,53,54] but a general reference addressing the field of chemical product engineering does not: what Smith and van Ness, and Hougen and Watson did for applied thermodynamics, and what Bird, Lightfoot and Stewart did for mathematical modeling of transport phenomena has yet to be done for product engineering.

## Research Challenges and Opportunities in Chemical Product Engineering

The scope of chemical product engineering is large. The research challenges currently faced are diverse and can be organized in terms of five generic objectives covering the development of: (1) tools to convert problem representation spaces from customer needs to technical specifications; (2) modeling and optimization approaches for chemical product design; (3) predictive capabilities for physical properties; (4) systematic approaches supporting chemical product design, and (5) frameworks to effectively link product discovery to R&D efforts.

### *Development of tools to convert problem representation spaces from customer needs to technical specifications.*

The development of a new chemical product requires the conversion of customer requirements into a completely specified product and its manufacturing process, and, hence, necessitates the translation of information between different spaces of representation (Figure 7). The property, process and usage functions are three of the main pillars supporting this translation process.

A fertile and rapidly developing area of chemical product engineering research is the improved understanding of the relationship between product performance, product composition, product ingredients' properties, processing variables and usage variables for systems of relevance to chemical products. This is a difficult and interesting problem for multiphase and metastable systems with developed microstructures, such as foams, colloids and gels, which are of particular importance in chemical products.

### *Development of modeling and optimization approaches for chemical product design.*

Chemical engineering has focused on the development of models and optimization formulations for manufacturing processes. The background of knowledge available in this field has to be adapted and extended to address chemical product design and the integration of chemical product and process design.

Computer-aided molecular/mixture design (CAMD) is a promising topic of research in this field. Essentially, it is the optimization-based solution of the inverse problem of finding a compound or a mixture of compounds possessing a set of previously specified properties. Much research work has been done in this area and a large number of references in this topic can be found, among which is the book by Achenie et al.,[61] which provides one of the first extended reviews on the subject. However, many challenges and opportunities remain unaddressed in this area. Gani[62] recently listed some such.

Global optimization approaches in which the objective function is formulated to address product and process performance and consider not only economic considerations, but also risk analysis, uncertainty,[63] environmental impacts,[64] quality costs[46] and health, safety and social concerns over the entire chemical product life cycle also constitutes an interesting research area in chemical product engineering.

### *Development of predictive capabilities for physical properties.*

Closely related to CAMD is the need to develop capabilities to accurately predict the physical properties for compounds and mixtures.[65] In fact, the effective resolution of the inverse problem of finding a compound or mixture matching a set of prespecified functionalities involves the prediction of the properties associated with candidate solutions. There is a serious gap between current thermodynamic modeling capabilities to describe commodity chemicals and the understanding of more complex chemical products, such as formulated products.[66] Thus, applied thermodynamics is a promising research area in the context of chemical product engineering.[67]

### *Development of systematic approaches supporting chemical product design*

The chemical process industries have been launching successful chemical products for a long time. However, such products have traditionally been developed through costly and time-consuming trial-and-error design procedures. The development of a systematic and integrated framework based on identified tools, methodologies, workflow and data-flow for the inter-related activities involved in the design of new products has been recognized as one of the main research challenges in the context of chemical product engineering.[13,62] Such a framework would not only have potential industrial application, but would also provide a significant contribution to the effective teaching of chemical product engineering.

### *Development of frameworks to effectively link product discovery with R&D efforts*

The optimal planning of R&D efforts and scheduling approaches aimed at a better coordination of the pipeline of new products have been emerging as an interesting research field supporting effective product discovery.[13,68-70]

## Concluding Remarks

In view of the dynamic and demanding markets chemical process companies have to deal with, there is a need for systematizing the design of chemical products. As a result, the concept of chemical product engineering has been emerging in the vocabulary and practice of chemical engineering.

In this article, chemical product engineering is defined as the whole science and art of creating new chemical products, and a structure for organizing this emerging area is proposed.

Central to this structure is the concept of chemical product design, which refers to the systematic procedure employed to develop new chemical products meeting market needs. However, it is important that chemical product design is not seen as synonymous with chemical product engineering. Chemical product engineering is a much broader field, incorporating the range of knowledge, tools and approaches that are essential for, and support the central activity of chemical product design.

The performance and end-use properties of a chemical product depend on its composition, ingredients' properties, microstructure and the circumstances under which it is used. Its microstructure is determined not only by the product recipe, but also by the process conditions used in its manufacture. For this reason, understanding the product pyramid, whose vertices are occupied by the materials, process, usage and product spaces, is crucial for chemical product design. The connections between the different spaces represented in the product pyramid are established by property, process and usage functions.

While the growing emphasis on chemical products is undoubtedly changing chemical engineering as a discipline, their design should not be seen as distinct from the process engineering traditionally associated with it. Process design is essential in supporting and guiding chemical product design.

The development of a chemical product spans many length and time scales, from the molecular level to the macrolevel of production plants and megalevel of distribution networks. Effective integration between all these scales is a major challenge of chemical product engineering. Achieving such integration involves many disciplines, both scientific and commercial, which must be effectively interfaced with core chemical engineering.

The emergence of chemical product engineering in the context of chemical engineering has significant implications for both teaching and research.

Some textbooks discussing chemical product design have been published, but no general reference addressing the whole field exists. Many leading universities around the world have begun to include this discipline in chemical engineering curricula. At a time when much work remains before chemical product engineering becomes widely taught, collaboration and sharing of experiences are essential. The model for chemical product engineering proposed in this article provides a systematized view of the scope of the discipline, which can be helpful as a framework for those starting courses on this subject.

The research challenges and opportunities posed by chemical product engineering can be organized in terms of five generic objectives concerning the development of: (1) tools to convert problem representation spaces from customer needs to technical specifications; (2) modeling and optimization approaches for chemical product design; (3) predictive capabilities for physical properties; (4) systematic approaches supporting chemical product design, and (5) frameworks to effectively link product discovery to R&D efforts.

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