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Integrated Chemical Product-Process Design: CAPE Perspectives

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Abstract
In chemical product design, we try to find a (chemical) product that exhibits certain desirable or specified behaviour. This can be a single chemical, a mixture, or a formulation, where an additive is added to the original chemical product (molecule or mixture) to significantly enhance its desirable functional properties. Examples of chemical products, such as functional chemicals (solvents, refrigerants, lubricants, etc.), agrochemicals (pesticides, insecticides, etc.), pharmaceuticals & drugs, cosmetics & personal care products, home and office products, etc., can be found everywhere. An important criterion for development of many chemical products is to achieve "*first time right*" by establishing critical scientific and regulatory parameters early on and eliminating errors early in the design and development processes. There are chemical products where the reliability of the manufactured chemical product is more important than the cost of manufacture, while there are those where the cost of manufacture of the product is at least as important as the reliability of the product. Thus, product-centred process design is also very important. Identifying a feasible chemical product, however, is not enough, it needs to be produced through a sustainable process. The objective of this presentation will be first to define the general integrated chemical product-process design problem, to identify the important issues and needs with respect to their solution and to illustrate through examples, the challenges and opportunities for CAPE/PSE methods and tools. Integrated product-process design where modelling and supply chain issues play an important role will also be highlighted.

Keywords: Chemical product, chemical process, design, process-product integration

1. Introduction

Chemical process design typically starts with a general problem statement with respect to the chemical product that needs to be produced, its specifications that need to be matched, and the chemicals (raw materials) that may be used to produce it. Based on this information, a series of decisions and calculations are made at various stages of the design process to obtain first a conceptual process design, which is then further developed to obtain a final design, satisfying at the same time, a set of economic and process constraints. The important point to note here is that the identity of the chemical product and its desired qualities are known at the start but the process (flowsheet/operations) and its details are unknown.
Chemical product design typically starts with a problem statement with respect to the desired product qualities, needs and properties. Based on this information, alternatives are generated, which are then tested and evaluated to identify the chemicals and/or their

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mixtures that satisfy the desired product specifications (qualities, needs and properties). The next step is to select one of the product alternatives and design a process that can manufacture the product. The final step involves the analysis and test of the product and its corresponding process. The important points to note here are that a) the identity of the chemical product is not known at the start but the desired product specifications are known, and b) process design can be considered as an internal sub-problem of the total product design problem in the sense that once the identity of the chemical product has been established, the process and/or the sequence of operations that can produce it, is determined. Note also that after a process that can manufacture the desired chemical product has been found, it may be necessary to evaluate not only the product but also the process in terms of environmental impact, life cycle assessment and/or sustainability.

From the above descriptions of the product and process design problems, it is clear that an integration of the product and process design problems is possible and that such an integration could be beneficial in many ways. For example, in chemical product design involving high value products where the reliability of the chemical product is more important than the cost of production, product specifications and process operations are very closely linked. In pharmaceutical products, there is a better chance to achieve first time right with respect to their manufacture by considering the product-process relations. In the case of bulk chemicals or low value products, the use of product-process relations may be able to help obtain economically feasible process designs. In all cases, issues related to sustainability and environmental constraints (life cycle assessment) may also be incorporated.

As pointed out by Gani (2004a), integration of the product and process design problems can be achieved by broadening the typical process design problem to include at the beginning, a sub-problem related to chemical product identification and to include at the end, sub-problems related to product and process evaluation, including, lifecycle and/or sustainability assessments. Once the chemical product identity has been established, Harjo et al. (2004) proposes the use of a product centric integrated approach for process design. Giovanoglou et al. (2003), Linke and Kokossis (2002) and Hostrup et al. (1999) have developed simultaneous solution strategies for product-process design involving manufacture of bulk chemicals, while Sune et al. (2004) have highlighted the integration of chemical product identification and its performance evaluation. In all cases, integration is achieved by solving simultaneously some aspects of the individual product and process design problems. Recently, Cordiner (2004) and Hill (2004) have highlighted issues related to product-process design with respect to agrochemical products and structured products, respectively. Issues related to multi-scale and chemical supply chain have been highlighted by Grossmann (2004) and Ng (2001).

The objective of this paper is to provide an overview of some of the important issues with respect to integrated product-process design, to highlight the need for a framework for integrated product-process design by employing computer-aided methods and tools, and to highlight the perspectives, challenges, issues, needs and future directions with respect to CAPE/PSE related research in this area.

2. Design Problem Formulations

In principle, many different chemical product-process design problems can be formulated. Some of the most common among these are described in this section together with a brief overview of how they can be solved.

2.1 Design of molecule or mixture for a desired chemical product

These design problems are typically formulated as, given the specifications of a desired product, determine the molecular structures of the chemicals that satisfy the desired product specifications, or, determine the mixtures that satisfy the desired product specifications (see Figure 1).

In the case of molecules, techniques known as computer-aided molecular design (CAMD) can be employed, while in the case of mixtures, techniques known as computer aided mixture-blend design (CAM^bD) can be employed. More details on CAMD and CAM^bD can be found in Achenie et al. (2002) and Gani (2004a-b). These two problems are also typically known as the reverse of property prediction as product specifications defined in terms of properties need to be evaluated and matched to identify the feasible alternatives (molecules and/or mixtures). This can be done in an iterative manner by generating an alternative molecule or mixture and testing (evaluating) its properties through property estimation. This problem (molecule design) is mainly employed in identifying process additions such as solvents, refrigerants and lubricants that may be used by the process to manufacture a chemical product. In the case of mixture design, petroleum blends and solvent mixtures are two examples where the product is designed without process constraints.

2.2 Design of a process

These design problems are typically formulated as, given the identity of a chemical product plus its specifications in terms of purity and amount and the raw materials that should be used, determine the process (flowsheet, condition of operations, etc.) that can produce the product (see Figure 1).

This is a typical process design problem, which now can be routinely solved (see for example, textbooks on chemical process design) with CAPE methods/tools when the chemical product is a low-value (in terms of price) bulk chemical. The optimal process design for these chemical products is usually obtained through optimization and process/operation integration (heat and mass integration) in terms of minimization of a single or multiparametric performance function. These problems can also now be routinely solved (see for example textbooks on process design). For high value chemical products, however, a more product centric approach is beneficial, as pointed out by Harjo et al. (2004), Fung and Ng (2003) and Wibowo and Ng (2001).

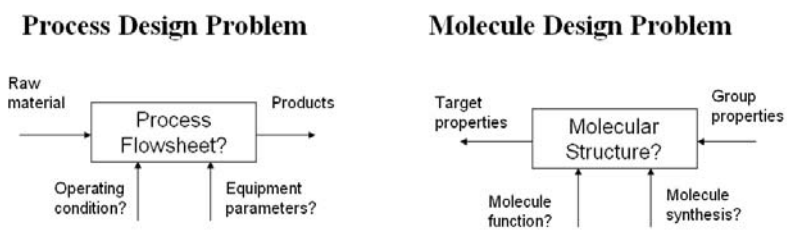

Figure 1. Differences between process design and molecule design problems. The "?" indicate what are unknown (needs to be determined) at the start of the design problem solution

2.3 Total design of a new chemical product

In these design problems, given, the specifications (qualities, needs and properties) of a desired product, the objective is to identify the chemicals and/or mixtures that satisfy the given product specifications, the raw materials that can be converted to the

identified chemicals and a process (flowsheet/operations) that can manufacture them sustainably, while satisfying the economic, environmental and operational constraints.
As illustrated in Figure 2, solution of this problem could be broken down into three sub-problems, a chemical product design problem that only identifies the chemicals (typically formulated as a molecule or mixture design problem), a process design part that determines a process that can manufacture the identified chemical or mixture (typically formulated as a process design problem) and a product-process evaluation part (typically formulated as product analysis and/or process analysis problems). In principle, mathematical programming problems can be formulated and solved to simultaneously identify the product and its corresponding optimal sustainable process. The solution of these problems are however not easy, even if the necessary models are available (Gani, 2004a). Cordiner (2004) and Hill (2004) also provide examples of problems (formulations and structured products) of this type and the inability of current CAPE methods and tools to handle them.

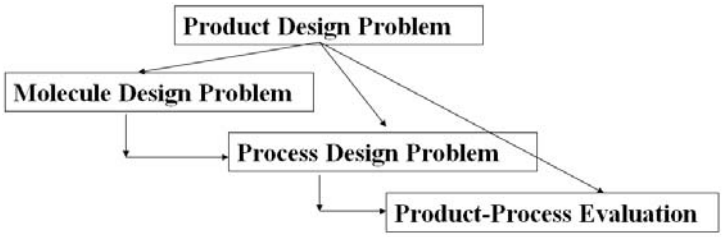

Figure 2. Product design problem includes the molecule design and the process design problems

2.4 Chemical product evaluation

In these problems, given a list of feasible candidates, the objective is to identify/select the most appropriate product based on a set of product performance criteria.
This problem is similar to CAMD or CAM^{b}D except for the step for generation of feasible alternatives. Also, usually the product specifications (quality, needs, and properties) can be sub-divided into those that can be used in the generation of feasible alternatives and those that can be used in the evaluation of performance. A typical example is the design of formulated products (also known as formulations) where a solvent (or a solvent mixture) is added to a chemical product to enhance its performance. Here, the feasible alternatives are generated using solvent properties while the final selection is made through the evaluation of the product performance during its application. Consider the following problem formulations:

- Select the optimal solvent mixture and the paint to which it must be added by evaluating the evaporation rate of the solvent when a paint product is applied
- Select the pesticide and the surfactants that may be added by evaluating the uptake of the pesticide when solution droplets are sprayed on a plant leaf
- Select the active ingredient (AI) or drug/pesticide product and the microcapsule encapsulating it by evaluating the controlled release of the AI.

In all the above design problems, the manufacturing process is not included but instead, the application process is included and evaluated to identify the optimal product.

2.5. Chemical process evaluation

These problems are formulated typically as, given the details of a chemical product and its corresponding process, perform a process evaluation to improve its sustainability.

To perform such analysis, it is necessary to have a complete design of the process (mass balance, energy balance, condition of operations, stream flows, etc.) as the starting point and new alternatives are considered only if the sustainability indices are improved. Here, the design (process evaluation) problem should also include retrofit design. Uerdignen (2003) and Jensen et al. (2003) provide examples of how such analysis can be incorporated into an integrated approach by exploiting product-process relations. Note that the choice of the product and its specifications, the raw materials, the process fluids (for example, solvents and heating/cooling fluids), the by-products, conditions of operation, etc., affect the sustainability indices.

3. Issues & Needs

Three issues and needs with respect to integrated product-process design are considered in this paper, namely, the issue of models and the understanding of the associated product-process complexities, the issue of integration and the issue of problem definition.

3.1 The need for models

According to Charpentier (2003), over fourteen million different molecular compounds have been synthesized and about one hundred thousand can be found on the market. Since however, only a small fraction is found in nature, most of them will be deliberately conceived, designed, synthesized and manufactured to meet the human needs, to test an idea or to satisfy our quest for knowledge. The issue/need here is the availability of sufficient data to enable a systematic study leading to the development of appropriate mathematical models. This is particularly true in the case of structured products where the key to success could be to first identify the desired end-use properties of a product and then to control product quality by controlling microstructure formation. Another feature among product-process design problems is the question of systems with different scales of time and size. Any CAPE method/tools will need to organize the scales and complexity levels so that the events at different scales can be described and understood.

3.2 The need for integration

Another issue/need is the increasing complexity of new chemical products and their corresponding technologies, which provide opportunities for the CAPE community to develop/employ concurrent, multi-disciplinary optimization of products and processes. Through these methods and tools, the necessary collaborative interaction between product designers and manufacturing process designers early in the product realization cycle can be accomplished. Few collaborative (design) tools are available to help turn ideas into marketable products, and those that are available are technology- and product-specific. Optimizing a product design to meet a set of requirements or the needs of the different production disciplines remains a manually intensive, iterative process whose success is entirely dependent on the people involved.

According to IMTI (2000), integrated product/process development is the concurrent and collaborative process by which products are designed with appropriate consideration for all factors associated with producing the product. To make product right the first time and every time, product and process modelling must support, and be totally integrated with, the design function – from requirements capture through prototyping, validation and verification, and translation to manufacture.

3.3 Definition of product needs

Good understanding of the needs (target properties) of the product is essential to achieve *first product correct*, even though it may be difficult to identify the product needs in sufficient details to provide the knowledge needed to design, evaluate and manufacture the product.

3.4 Challenges and opportunities

Based on the above discussion, a number of opportunities have been identified by IMTI (2000), which are summarized below.

Definition of product-process needs (design targets)

- Provide knowledge management capability that captures stakeholder requirements in a complete and unambiguous manner.
- Provide modeling and simulation techniques to directly translate product goals to producibility requirements for application to product designs.

Methods/tools for product-process synthesis/design

- Provide a first principles understanding of materials and processes to assure that process designs will achieve intended results.
- Provide the capability to automatically create designs from the requirements data and from the characterization of manufacturing processes.
- Provide the capability to automatically build the process plan as the product is being designed, consistent with product attributes, processing capabilities, and enterprise resources.
- Create and extend product feasibility modeling techniques to include financial representations of the product as an integral part of the total product model.

Modelling systems and tools

- Provide a standard modeling environment for integration of complex product models using components and designs from multiple sources/disciplines, where any model is completely interoperable and plug compatible with any other model.

Integration

- Provide the capability to create and manipulate product/process models by direct communication with the design workstation, enabling visualization and creation of virtual and real-time prototyped product.
- Provide simulation techniques and supporting processing technologies that enable complex simulations of product performance to run orders of magnitude faster and more cost-effectively than today.
- Provide the capability to simulate and evaluate many design alternatives in parallel to perform fast tradeoff evaluations, including automated background tradeoffs based on enterprise knowledge (i.e., enterprise experience base).
- Provide integrated, plug & play toolset for modeling and simulation of all life-cycle factors for generic product types (e.g., mechanical, electrical, chemical).

4. Framework for Integrated Approach

The first step to addressing the issues/needs listed above could be to define a framework through which the development of the needed methods and tools and their application in

product-process design can be facilitated. Integration is achieved by incorporating the stages/steps of the two (product & process) design problems into one integrated design process through a framework for integration. This framework should be able to cover various product-process design problem formulations, be able to point to the needed stages/steps of the design process, identify the methods and tools needed for each stage/step of the design process and finally, provide efficient data storage and retrieval features. In an integrated system, data storage and retrieval are very important because one of the objectives for integration is to avoid duplication of data generation and storage. The design problems and their connections are illustrated through Figure 3. The various types of design problems described above can be handled by this framework by plugging into it, the necessary methods and tools. One of the principal objectives of the integration of product-process design is to enable the designer to make decisions and calculations that affect design issues related to the product as well as the process. The models and the types of models needed in integrated product-process design are also highlighted in Figure 3. In the sections below, the issues of models and data-flow and work-flow in an integrated system are briefly discussed.

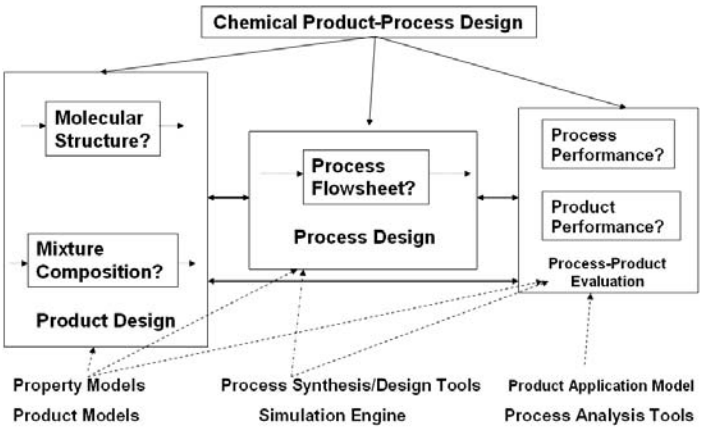

Figure 3. Integration of product-process design (see Table 1 for data-flow details)

4.1 Models

One of the most important issue and need related to the development of systematic computer-aided solution (design) methodologies is models. For integrated product-process design, in addition to the traditional process and equipment model, product models and product-process performance models are also needed. A product model characterizes all the attributes of the product while a product performance model simulates the function of the product during a specific application. Figure 4 illustrates the contents and differences among the process, product and product-performance models. Constitutive (phenomena) models usually have a central role in all model types.

4.2 Data-Flow and Work-Flow

The data-flow related to the framework for integrated product-process design is highlighted through Table 1, where the input-data and output data for each design (sub-) problem is given.

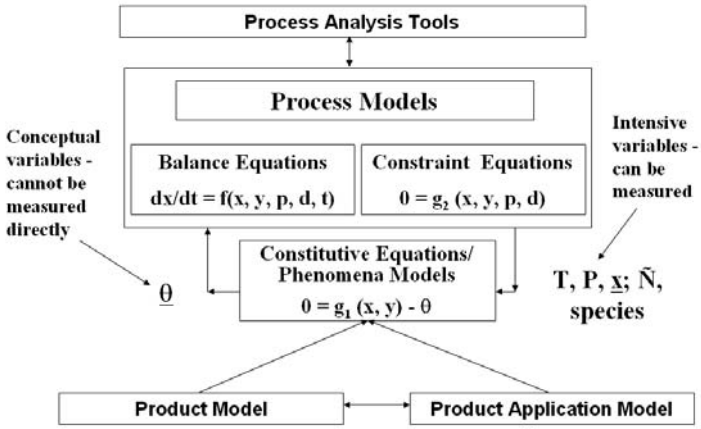

Figure 4. Different types of models and their connection to each other

Table 1. Data-flow for each design problem

Input Data	**Problem Type**	**Output Data**
Building blocks for molecules; target properties and their upper/lower bounds and/or goal values	Molecular Design (CAMD)	Feasible molecular structures and their corresponding properties
List of candidate compounds to be used in the mixture, target properties and their upper/lower bounds and/or goal values at specified conditions of temperature and/or pressure	Mixture Design (CAM^bD)	List of feasible mixtures (compounds and their compositions) and their corresponding properties
Desired process specifications (input streams, product specifications, process constraints, etc.)	Process Design/Synthesis (PD)	Process flowsheet (list of operations, equipments, their sequence and their design parameters)
Desired separation process specifications (input streams, product specifications, process constraints, etc.) and desired (target) solvent properties	Process-Solvent Design	Process flowsheet (list of operations, equipments, their sequence and their design parameters) plus list of candidate solvents
Details of the molecular or formulated product (molecular structure or list of molecules and their composition and their state) and their expected function	Product Evaluation	Performance criteria
Details of the process flowsheet and the process (design) specifications	Process Evaluation	Performance criteria, sustainability metrics

As highlighted in the problem formulation section, the work-flow for various types of design problems is different and needs to be identified. In general terms, however, the

following main steps can be considered (note that, as discussed above, some of these steps may be solved simultaneously),

- Define product needs in terms of target (design) properties
- Generate product (molecule, mixture, formulation, etc.) alternatives
- Determine if process considerations are important
    - If yes, define the process design problem and solve it
    - If no, go directly to the product evaluation (analysis) step
- Analyse the process in terms of a defined set of performance criteria
- Analyse the product in terms of a defined set of performance criteria

In Table 2, the methods/algorithms and their corresponding tools/software are listed. Under tools/software, only tools developed by the author and coworkers have been listed (see the tools & tutorial pages at http://www.capec.kt.dtu.dk/Software/).

Table 2. List of methods/algorithms and tools/software that may be used for each problem (design) type.

Problem Type	**Method/Algorithm**	**Tools/Software**
Molecular & Mixture Design (CAMD)	Molecular structure generation; Property prediction & database; Screening and/or optimization	ProCAMD
Process Design/Synthesis (PD)	Process synthesis/design Process simulation/optimization Process analysis	ICAS (PDS, ICAS-sim, PA)
Process-Solvent Design	CAMD-methods/tools; Process synthesis/design; Process simulation/optimization Process analysis	ICAS (ProPred, ProCAMD, PDS, ICAS-sim, PA)
Product Evaluation	Property prediction & database; Product performance evaluation model Model equation solver	ICAS (ProPred, ICAS-utility, MoT)
Process Evaluation	Process synthesis/design; Process simulation/optimization Process analysis	ICAS (ICAS-sim, ICAS-utility; MoT, PA)

Examples of application of the tools listed above are not given in this paper but can be found in several of the referenced papers.

5. Conclusion

As pointed out by Cordiner (2004), Hill (2004), and the referenced papers by Ng, even though the primary economic driver for a successful chemical product is speed to market, this does not mean that process design is not strategically important to these products. The important questions to ask (to list a few) are which chemical product, how they will be manufactured, how sensitive is product quality related to cost and production, where they will be used or applied, how their performance will be evaluated and, how long a period will they be sustainable? Obviously, the answers to these questions would be different for different products and consequently, the methods and tools to be used during problem solution will also be different. Many opportunities exist for the CAPE/PSE community to develop systematic model-based solution approaches

that can be applied to a wide range of products and their corresponding processes. It is the study through these model-based solution approaches that will point out under what conditions the process or operational issues become important in the development, manufacture and use of a chemical product. Successful development of model-based approaches will be able to reduce the time to market for one type of products, reduce the cost of production for another type of product, reduce the time and cost to evaluate another type of product. The models, however, need to be developed through a systematic data collection and analysis effort, before any model-based integrated product-process tools of wide application range can be developed. Finally, it should be noted that to find the magic chemical product, these computer aided model-based tools will need to be part of a multidisciplinary effort where experimental verification will have an important role and the methods/tools could be used to design the experiments.

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