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Perspective

Issues and Trends in the Teaching of Process and Product Design

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Introduction

This article presents an overview of basic concepts, major textbooks, issues and trends in the teaching of process and product design. We argue that these courses are both fundamental and key to the education of chemical engineering students, and are highly relevant for exposing students to energy, sustainability and innovation challenges.

Process design is a core body of knowledge of chemical engineering that deals with conceiving processes based on chemical, physical and/or biological transformations of raw materials into products. These processes are typically for large-scale production (e.g., fuels, petrochemicals, bulk chemicals), but also include smaller batch manufacturing facilities (e.g., specialties, pharmaceuticals, food), as well as microsystems (e.g., medical diagnosis). Furthermore, the important goal in process design is to accomplish this objective by optimizing multiple objectives such as profit maximization, and minimizing energy consumption and environmental impact so as to meet product and market specifications (see also Grossmann and Westerberg, 2005).

Product design on the other hand is a more recent area that has emerged as a result of the increasing importance for developing new and novel products, and the increasing employment of chemical engineers in product oriented industries (e.g., consumer products, specialties, materials). Important objectives in product design are to determine the needs of a chemical product; identify candidate chemicals and/or mixtures of chemicals and quickly evaluate key economic, market and process design issues in order to support decisions in the early stages of product development. As opposed to process design, major objectives are often time to market (e.g., for new molecules) and performance of a given function (e.g., nanostructured materials) (Westerberg and Subrahmanian, 2000; Cussler and Moggridge, 2001).

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In this article, we discuss key issues related to the teaching of process and product design. However, to provide a broader context to the discussions, we start with a brief review of recent research trends in these areas.

Research Trends in Process Systems Engineering

Both process design and product design formally belong to the wide body of knowledge known as process systems engineering (PSE). As discussed in Grossmann and Westerberg (2005), a major trend in the recent past has been to expand the scope of PSE from the macroscopic level (e.g., unit or plant level), down to the molecular level on the one hand, and on the other hand up to the supply chain level. The trend toward the molecular level has promoted the creation of the area known as computer-aided design modeling (CADM), which is one of the useful emerging tools for product design. The trend toward the molecular level has also been promoted by systems biology, a multidisciplinary area where chemical engineers have increasingly been playing a major role. The trend toward the supply chain level has promoted the creation of the emerging area known as enterprise-wide optimization (EWO). In addition to these broadening trends for PSE, energy and sustainability have emerged as new major drivers for the PSE research. Again, these have refocused the attention to the unit and process level since these are key in the development of sustainable renewable energy sources.

In order to support the aforementioned research trends in PSE, some of the major challenges that are currently being addressed include design of sustainable energy systems, integration of product and process design, integration of planning, scheduling and control for enterprise-wide optimization, and robust fast algorithms for large-scale differential/algebraic models, global and mixed-integer optimization, and optimization under uncertainty.

The aforementioned research outlined has not yet fully impacted the teaching of design at the undergraduate level. Nevertheless, some of the topics cited previously are being taught in graduate level courses by faculty in the PSE area. We should note that major advances in PSE over the last 2-3 decades have trickled down to the curriculum through textbooks and educational resources, as discussed in the next sections.

Teaching of Process Design

Process design has been the traditional capstone course for chemical engineering, in which material learned in previous semesters is integrated and is applied to a major design project where students work in groups. A major component of this course is *decision-making* since students have to select the process technology, the flowsheet and its operating parameters. In contrast to traditional approaches to design, which focus more on the detailed aspects of equipment design, modern trends emphasize process invention (i.e., synthesis of flow sheets) and the teaching of systematic techniques for design. These include synthesis strategies (e.g., hierarchical decomposition, separation synthesis, heat exchanger networks, energy integration, and water networks), process simulation tools to perform the mass and energy balances, as well as more detailed modeling tools for chemical reactors and separators. It should be noted that the major developments that are now taught in process synthesis and process simulation and modeling took place in the 1970s and 80s.

Textbooks in Process Design. There are several textbooks in process design that cover the topics outlined previously. Traditional books which emphasize the practical aspects of process design and economic evaluation include the textbooks by Baasel (1990), and Peters and Timmerhaus (1968, 1990). The modern approach to process design was first introduced by Dale Rudd and Charles Watson in 1968 with their seminal book "Strategy of Process Engineering" that introduced systematic approaches including optimization to process design. This book was followed by another pioneering book by Rudd, Powers and Siirola (1973) that covered for the first time the topic of process synthesis that deals with the problem of developing structures of process flowsheets. This book was written so that it could be taught to sophomore students to introduce the idea of design early in the curriculum. A monograph by Linnhoff et al. (1982) introduced the concept of pinch analysis in order to predict targets for minimizing energy consumption ahead of detailed design of heat exchanger networks. Next, the book by Douglas (1988) followed on the theme of process synthesis by emphasizing hierarchical decomposition as a way to systematically generate alternatives for conceptual designs. That book also emphasized the idea of short-cut models as a way to perform more effectively screening of process alternatives. The book by Robin Smith (2005) is also along somewhat similar lines except that the emphasis is more on the idea of targeting for design. The book by Biegler, Grossmann, and Westerberg (1996) presents a comprehensive treatment at both undergraduate and graduate levels of preliminary design, process modeling, conceptual design and optimization approaches for synthesis. The part on preliminary design is based on an approach for developing linear mass balances, and includes an introduction to the design and scheduling of batch processes. The part of process modeling covers the basics of process simulation and nonlinear optimization; the part on conceptual design emphasizes the synthesis of separation systems and their heat integration; the part on optimization approaches emphasizes superstructure optimization, batch processes and process flexibility. The recent book by Seider et al. (2009) also presents a comprehensive overview of design by emphasizing process simulation with ASPEN Plus, and includes the topics of process operability and product design, which is discussed in the following section. Finally, the recent books by Turton et al. (2002) and Towler and Sinnot (2007) present a somewhat more traditional approach to process design, while incorporating some of the modern design concepts as well.

Issues and Trends in Process Design. In contrast to the traditional approach in project design that deals with a large commodity chemical process, the recent trend is to assign projects related to energy. There is currently great interest on how best to design biomass processes, coal gasification processes, fuel cells and solar energy systems. Therefore, the process design course has become an ideal vehicle for exposing students to energy and sustainability topics. Needless to say, students have been highly motivated with design projects that focus on these areas. Moreover, a good part of the emerging interests in energy and sustainability can naturally be addressed in the process design course. This is an extremely important point given the ever increasing reduction of fundamental courses in chemical engineering, along with the introduction of new courses, especially related to biological engineering.

Another important issue in the teaching of process design is that the course is increasingly being taught either by adjunct faculty from industry (often retired), or by lecturers, with little or no involvement from tenure-track faculty. Commonly it is only those departments who have faculty in process systems engineering that the design course is taught by a regular faculty member. In fact, less than 50% of the top 25 departments have regular faculty teaching the design course. While there is obviously value in having people from industry teach the design course, we believe that this is a worrying trend because it means that the faculty is increasingly unable to teach this core course in chemical engineering.

We believe some of the reasons for this trend are the following: (a) process design is a time-consuming course to teach, especially since it involves an open ended project and supervision of groups; (b) the strong move toward science vs. engineering that has taken place in chemical engineering in the least a decade has made topics like process design to be relegated to a second level, and (c) increasingly many faculty in chemical engineering departments do not have an undergraduate chemical engineering degree, and, therefore, do not have the background for teaching this course.

It is interesting to note that the trend of not having regular faculty teach design is particular to the US and has not been observed in other countries (Europe, Asia, Canada, Latin America). We believe that while practicing engineers should be involved in the process design course, it is very important that regular faculty also participate, especially since this course is an ideal vehicle for addressing energy and sustainability issues, which have clearly become major challenges and a source of opportunities for chemical engineers.

Teaching of Product Design

Design considers two major questions: what to make (product design) and how to make it (process design). While process design has so far been the emphasis of this article, and we have prided ourselves on the process discipline, the past two decades have seen many of our graduates deeply involved in the design of products. These include beautiful but tough new cases for cell phones, new films, facial products, small portable kidney machines, vascular stents, removable sticky tape, rocket fuel, medicines, time-release medicines, and new refrigerants. In addition to introducing our students to the design of processes required for these projects, we also must establish the product characteristics. Here we need to find the question before looking for the answer. As such, this is related to the thinking required to do a PhD research project.

Westerberg and Subrahmanian (2000) outlined the differences between the design of processes, as we have typically taught it, and the design of products. Products typically have short lifetimes (often only months before a new product appears), and have trade-offs involving such things as appearance, usability, durability, safety, disposability, and getting to market now. Manufacturing is often in revamped equipment rather than in all new processing equipment. The design process for products involves establishing all the stakeholders, their widely divergent requirements ranging from "will it stick on the wall for two years while holding a two pound picture" to "does it smell and look right when the customer is looking to buy it." Designers have to establish ways they are going to assess how well a proposed design actually will fulfill these requirements when looking among the design alternatives. They have to discover and set limits on the variety of technical and nontechnical ways one can deliver the functionalities desired, and may even have to think through the business plan and its impact on the design. They could find themselves having to prepare a sales pitch to get the venture capital needed, etc.

Since 2000 three books in chemical engineering have directed their attention to product design: Cussler and Moggridge (2001), sections in Seider et al. (2nd Ed, 2003 and much more in their 3rd Ed., 2008), and Wei (2006). These books stress course material suitable for teaching to classes comprising chemical engineers only. Moreover, product design is a long-time mainstay in other disciplines, and two interesting books useful for giving undergraduates in all disciplines a set of simple tools for product design are by Ulrich and Eppinger (2008) and Dym and Little (2009). Another book with a twist on discovering breakthrough products is by Cagan and Vogel (2001).

The product design course can be included in our undergraduate curriculum in a number of ways. One could have the students design a product instead of a process as "the project" for the senior design course. However, as the only course, students will not see all the technology elucidated earlier on process synthesis, simulation and optimization, and we believe that these are important technologies that must be included. In the second option, one could add another undergraduate course specifically aimed at product design, an option that we have at Carnegie Mellon (see the appendix). A third option, that we also have at Carnegie Mellon (Wesner et al., 2004), and which is also described in the appendix, is to have a university-wide course, wherein students mix with peers from other disciplines to carry out a product design. New courses, of course, take space in an already overcrowded curriculum. However, all three options emphasize the very important "what should we design" aspect that is an integral part of product design. The interesting exercise to putting this material into the curriculum is itself a product design problem.

Fundamentals Concepts in Process and Product Design

Process and product design courses can be been viewed from a number of perspectives. They usually contain a synthesis of engineering content and professional practice and include activities that mimic the real-world workplace in process and product engineering. Often they involve the social process of working in teams that leverage diverse personalities and skills. Moreover, as mentioned previously, there is an emerging and important trend to evolve to new products and processes. Underlying all of these perspectives is teaching the task of decision-making based on engineering experience and domain knowledge. A systematic approach toward this is to transform ill-defined problems to a set of well-defined problem formulations — and then to develop effective and efficient solution strategies that can solve them. To accomplish these objectives, having good and interesting design projects is clearly essential (e.g., Dimian and Bildea, 2008; Ng et al., 2007).

In the case of *process design*, development of chemical processes, i.e., the *process synthesis* task, one needs to define this strategy in terms of three general elements. First, metrics must be defined to compare design alternatives, and these include safety, environmental impact, energy efficiency and, of course, economics. Second, the space of design alternatives must be represented in such a way as to easily evaluate these metrics and compare alternatives. Last, a fast search strategy is needed to determine good solutions from this space of alternatives. Research in PSE has focused on these issues over the past four decades and has evolved into systematic approaches that have led to the efficient, safe and profitable processes that operate today. To develop the future generation of chemical engineers, we believe that these approaches are essential features of process design course.

The *Basics* of such a process design course include the following. First, *how should a flowsheet be constructed*? Methods accessible to undergraduates include systematic rule-based decision hierarchies, based on the textbooks by Rudd, Powers, Siirola (1970) and Douglas (1980). These can be demonstrated to reflect decisions that lead to state-of-the-art continuous processes. Next, *how should a flowsheet be evaluated*? This task includes decisions that lead to *technical feasibility* and *economic feasibility*. For the former, we consider how it produces desired products from given feedstocks. For this task shortcut models and linear mass balances are used for quick performance evaluations and to explore flow sheet interactions. These simple models lead to a natural evolution to detailed process simulation models. For *economic feasibility* we consider profitability for the company. This task naturally leads to evaluation of capital and operating costs, time value of money, net present values (NPV) vs. rates of return, and economic evaluation. Once the basics are understood, *process simulation and modeling tools* can be better appreciated and used with a purpose-driven perspective for process evaluation. Computer simulation has experienced a speedup of four to six orders over the past two decades, with roughly three-orders of magnitude due to better numerical methods and simulation algorithms. Since they can be installed on any laptop, they are ubiquitous tools in process engineering and essential components for process engineering education.

Moreover, *process synthesis concepts* have also evolved from research topics to accessible elements for undergraduates. Important components include *energy integration* with the introduction of pinch technology to design heat exchanger networks and networks of heat and power systems. In addition, *separation synthesis* focuses on the sequencing of near-sharp distillation separations. In addition, triangular phase diagrams allow insightful understanding of complex, nonideal and azeotropic distillation operations. Finally, *reactor networks*, through attainable regions, take students beyond the design and analysis of single reactors to deal with the interplay of complex networks for real-world reactive systems. While covering all these topics in detail is more appropriate for a graduate level course (e.g., Biegler, Grossmann and Westerberg (1997) text), covering basic concepts and insights allows students to understand the trade-offs between capital and operating costs, as well as the interactions of these process subsystems. These skills should be established in the undergraduate design course.

The teaching of *product design* is still relatively young in chemical engineering, but a number of essential concepts and approaches have already emerged (Hill, 2009; Seider et al., 2009). Students must first be sensitized to the different avenues that can lead to innovation in product design. The best way to do this is to provide a historical overview of successful product designs and the impact they have had in the marketplace. This would include market pull, technology push and accidental discovery cases. Once a particular product has been established as the design goal, along with detailed property targets, product designers must be able to quantitatively assess how molecular structure, morphology, rheology, and other factors affect product performance. Here, group contribution techniques (Kontogeorgis and Gani, 2004) complemented by data base searches and design of experiments are useful for predicting the performance of new molecular structures. While quantum mechanics or molecular simulation models for property predication are normally beyond the scope of an undergraduate course, teaching molecular design and related subjects provides an opportunity to cover systematic methods for design of experiments, especially if the course is accompanied by an actual experimental component.

The second key issue in product design is the concept of life cycle analysis (Guinée et al., 2002). A major objective here is to expose students to the evaluation of a given sustainability index that factors all the elements involved in the design of a product, from cradle to grave. Coverage of this topic, of course, brings up an understanding that product and process design must be viewed concurrently, as a great product concept has no future unless it is accompanied by an economically feasible, environmentally friendly and sustainable process. Finally, another important aspect in the product design course is to expose students to issues related to intellectual property, particularly on patents.

In addition, process models, process synthesis and molecular design models can be incorporated into systematic decision-making tools through the formulation of optimization models that generally involve discrete and continuous variables. The solution of such models with advanced tools allows the engineer the systematic evaluation of alternatives to identify optimal designs. These tools also lead to more effective analysis of different scenarios and the treatment of uncertainty. Moreover, large-scale optimization models provide a natural way to integrate design aspects and subsystems, and to balance economics (capital vs. operating costs vs. environment). Finally, the impact of optimization models in practice has led to shorter design cycles (e.g., 1 h to perform two weeks of case studies), significantly better and more consistent performance in work processes, improved *nonintuitive* results that lead to increased process understanding. While a comprehensive exposure to optimization can only be accomplished in a graduate level course, the teaching of optimization concepts in the process and product design courses has been aided by the availability of powerful optimization platforms including GAMS, AIMMS and AMPL, along with integrated optimization algorithms within simulators (ASPEN, ProII, Prosys) and modeling tools (Excel, MATLAB). Moreover, the power and easy access to these tools requires students to develop a qualitative understanding of the algorithms that are the engine of the modeling platforms, to diagnose problems for failed simulations and to assess the usefulness of the final answer through conceptual knowledge of the process problem.

Conclusions

Process and product design continue to be key subjects in chemical engineering education and provide the vehicle to integrate engineering fundamentals to engineering practice. Based on the previous sections we draw the following major conclusions:

- Process design offers a unique opportunity to expose students to energy and sustainability issues. Moreover, the benefits of incorporating strategies for systematic decision-making extend to further integration of multiple objectives, subsystems and modeling platforms, and application to emerging areas including energy, bioprocessing and advanced materials. Finally, the modeling, simulation and optimization tools extends to multi-scale modeling and simulation in order to link time and length scales to cover the full spectrum of system behavior — ultimately from *ab initio* calculations to the modeling of multiprocess networks and supply chains.
- While it is desirable to involve industrial expertise and resources, faculty must be involved in the teaching of design courses. Otherwise there is the risk that chemical engineering education will become increasingly out of touch with the real world and with engineering practice. There are a significant number of textbooks on process design that tenure track faculty will find accessible.
- The teaching of product design should be embraced by departments as a complement to the process design course. This can be done either as a specific departmental course, or as a multidisciplinary course involving students from different departments, including non-engineering students. Although there is not a large selection of textbooks, it might be easier to involve faculty who are not chemical engineers in a product design course, since one can envisage projects that for

instance highlight applications in biotechnology and nanotechnology.

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Appendix: Process and Product Design Courses at Carnegie Mellon University

Departmental Process and Product Design Courses

At Carnegie Mellon University the undergraduate design sequence is as follows. In the fall of senior year we teach process design (06-421 Chemical Process System Design, a four credit course). In the spring, we teach first a two credit mini-course on optimization (06-462 Optimization Modeling and Algorithms), followed by a two credit mini-course 06-463 Chemical Product Design.

The main objectives of the course are 06-421 Chemical Process System Design are the following:

- to learn systematic techniques for the conceptual design of chemical processes;
- to perform preliminary process calculations systematically and efficiently,
- to learn systematic methods for process synthesis and energy recovery,
- to perform economic evaluations of competing processes,
- to learn the fundamentals of flowsheet simulation and batch processing,
- to gain an appreciation of energy and CO_2 issues,
- to learn how to work in teams of 3-4 students in a preliminary design project.

The main topics covered in the course include hierarchical decomposition of process flow sheets, linear mass balances, equipment sizing and cost estimation, synthesis of distillation sequences, heat integration, process optimization and heat integration, economics (time value money, net present value, project comparisons), process simulation (i.e., Aspen) and batch processing. We basically follow the first six chapters of the Biegler, Grossmann and Westerberg (1997) textbook, and selected parts of the more advanced chapters.

The course involves a major project which in the last few years has been related to energy (e.g., production lignocellulosic bioethanol, polygeneration of methanol in IGGC plants, conversion of glycerol into liquid fuels). Students have to submit three memos on the project: (1) Literature search and selection of initial flowsheet; (2) mass and energy balance, and (3) economic evaluation. The emphasis in the memos is that students revise their designs in order to hopefully obtain novel and efficient process flowsheets. The students work in groups of 3-4, and give an oral presentation at the end of the course that is attended by several industry people who in turn normally give throughout the semester lectures on topics like process innovation, simulation and safety. Students are given eight homework assignments to review the material covered. Also, there are two exams, each before the second and third memo so that students have the required background to work on in order to perform the material and energy balances and economic evaluations while applying some of the ideas on process synthesis.

The main objectives of 06-462 Optimization Modeling and Algorithms are the presentation and description of modern optimization algorithms, as well as optimization modeling tools and strategies that relate to process engineering. The emphasis is on modeling as opposed to detailed description of the algorithms. Topics covered in this course include modeling problems as mathematical programs, use of GAMS as a modeling tool for optimization, and overview of methods for unconstrained optimization, linear and nonlinear programming, mixed-integer programming and derivative-free optimization. An important component of the course is a group project where students implement an optimization model from an article reported in the literature.

As the final course in the sequence, 06-463 Chemical Product Design is a project-based course that requires students to work in groups of ~5, assigned by the instructor. In this course, students are asked to identify a market need and design a chemical product to meet this need. The course requires students to submit two versions of their product selection reports and slides, and to present their selection to the class. With student permission, the final student presentations and reports are made publicly available through future publications or web sites. In addition, course lectures introduce the area of chemical product design and discuss approaches and history of innovations in product design. Each year, particular product design cases are presented that describe innovations and methodologies related to the design of new projects. Each case study includes a problem statement, formulation of design objectives, physical property prediction via group contribution methods and structural feasibility constraints of target molecules. Two example case studies are:

- Design of automotive and secondary refrigerants with emphasis on determining target properties through group contribution techniques.
- Solvent design with emphasis on solubility, bioconcentration factors, LC50, flash points, and ozone depletion potential.

Additional topics in the course include database searches, methods for property prediction, design of experiments, as well as issues of intellectual property and technology transfer.

A University-wide Product Design Course

In 1999 at Carnegie Mellon, one of the authors (Westerberg) along with E. Subrahmanian and a partner from industry, C. Buenzli, designed and initiated a project-oriented course on engineering product design open to all juniors, seniors and graduate students throughout the university. This course (see Wesner et al., 2004) continues today and is taught every semester. The course quickly evolved into our creating each team so it had no two people from the same discipline on it. A typical team might have a chemical engineer, a computer scientist, an English major, an industrial designer (from our School of Fine Arts), and a business major on it. A volunteer faculty member directed each project, and each had an industrial sponsor who provided the initial word description of the desired product, one or more actively participating consultants and funding. As the course was in our engineering college, products required engineering input, and a few typical projects have been the creating of a web-based tool to teach about air separation, the designing a laser tape measure that one might buy at Sears to replace a 32 ft tape measure, and designing a medical stent. Almost always students entered the course either thinking they would be the most important discipline for the project or seriously wondering what they were to contribute. They almost always left with an awakening as to the value all bring to the table. They quickly appreciated that, should they lose a member, they lost a whole discipline. We always felt the course was an excellent capstone to a university education as it brought together concepts the students should be learning outside engineering as well as within. We electronically captured and still have all materials developed in the course, making it a valuable searchable and augmentable resource for both students and faculty in all subsequent semesters.