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Process Systems Engineering and CAPE – What Next?

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1. Extended Abstract

Process systems engineering (PSE) has been traditionally concerned with the understanding and development of systematic procedures for the design, control, and operation of chemical process systems (Sargent, 1991). Computer aided process engineering (CAPE), like PSE, has been traditionally concerned with the development and solution of problems related to chemical process design, control and operation through systematic computer aided techniques. Both emphasize the development and use of a systematic approach to problem solution understanding. The oil & gas industry, the petrochemical industry and to some extent, the chemical industry have been the traditional users of methods and tools, including software, from the PSE/CAPE community. Indeed, it is routine these days to perform a detailed mass and energy balance for a process through one of several process simulators that have been developed by the PSE/CAPE community.
Problems related to process optimization, process integration and process synthesis/design are currently routinely solved through knowledge based techniques as well as mathematical optimization techniques. Also, systematic methods and tools have been developed and applied to solve industrial problems in the area of planning and scheduling, on-line optimization, solvent selection/design and many more.
The above developments have been possible because of the availability of sufficient knowledge and data related to the relevant process engineering

problems and an interest from the industry for collaboration with academia for their solution. This encouraged the development of reliable process simulation models that together with the available knowledge and data lead to the development of systematic (and/or computer aided) methods and tools for a wide range of problems for the chemical process industries. Examples of such methods and tools are the development, to name a few, MINLP based process synthesis, design, integration; computer-aided molecular design; generation of optimal heat and mass exchange networks; planning and scheduling optimization models; model identification and data reconciliation techniques; real-time optimization; model predictive control, to name a few.

Most of the above developments can be linked to chemical processes involved with the manufacture of high volume bulk chemicals and the related industries (such as the oil and gas, petrochemical and chemical industries). To a lesser extent, these methods and tools have also been applied to the manufacture of low volume specialty chemicals. CAPE/PSE has contributed by providing systematic, reliable and efficient methods and tools that have now become standard for the chemical process industries as well as in chemical engineering education.

The question therefore arises, what next? Where the new challenges are for CAPE/PSE and what could be the new directions for research and education? In this paper, we will try to answer these questions by looking at the current trends and the future needs with respect to chemical products and the processes that manufacture them. Some these issues have been discussed previously by Grossmann & Westerberg (2000), Grossmann (2004) and Gani (2004). The main issues that are emerging and that can be viewed as new opportunities for CAPE/PSE include the areas of chemical based products, energy, sustainability, biosystems engineering, and enterprise-wide optimization.

To satisfy the needs of the modern society, we need to continuously develop better and significantly improved chemicals based products. Within chemical products, we include bulk chemicals as well as low volume specialty chemicals covering thereby a wide range of industries (oil & gas, petrochemical, chemical, pharmaceutical, food, agrochemical, bio, etc.) as they all have important roles. For example, the bulk chemicals act as raw materials, solvents, process fluids, etc., needed in the manufacture of specialty chemicals that may become an active ingredient for a pharmaceutical and/or drug product. Therefore improved designs of continuous processes (needed for the manufacture of bulk chemicals) are as important as designs of batch operations (needed for the manufacture of specialty chemicals). Here, as Grossmann (2004) notes, while it has become trendy over the last few years to question the future of chemical engineering and the process industry, it is important to note that the latter still remains a major sector of the economy. It is true that globalization of the industry has opened new markets and with it, new demands. However, how does one identify the chemicals and their synthesis routes that will help to meet these demands, taking into account, also the questions of sustainability and protection of the environment? The sources for many of the raw materials used, especially those derived from oil, gas, and some plants and animals continue to be depleted and may soon be economically infeasible to use. Also, how does one find their replacements and the processes to manufacture them? Will it be possible for the CAPE/PSE community to provide the methods and tools to address these problems?

Analyzing the problems successfully addressed by the CAPE/PSE and the new challenges, one can be noted that while the processes (continuous versus batch), chemicals (simple/small versus complex/large), performance criteria (single versus multiple criteria), factors (economic versus economic-social), etc., for the current and future problems are different, the problem definition and basic methods and tools needed to solve them, may actually be the same. For example, the design of a formulated chemical product can be defined as a computer-aided mixture design and is similar to design of petroleum blends (Gani 2004). The important difference is that the mixture model for the formulated chemical product may not be available, while that for the petroleum blend may be available. Similarly, the synthesis of batch operations needed to produce a new chemical can be formulated and solved in the same way as the synthesis of a continuous process flowsheet. Again, different models (with different objectives) are needed but the solutions steps are similar.

The areas of energy and sustainability clearly provide new challenges and opportunities to the CAPE/PSE community. The shift towards renewable resources for energy, most notably through biomass, requires addressing processes that have quite different characteristics than the traditional petrochemical processes in that reactions are biochemical in nature, mildly exothermic and take place at relatively moderate temperatures. Furthermore, the separations tend to involve highly diluted systems which again are different in nature from the ones encountered in more traditional processes. Although mot likely not trivial, there should clearly be significant scope for improving the design and operation of these processes, which have been largely designed in an ad-hoc manner, very often by biochemists. Another area in energy includes clean-coal processing making use of CO_2 sequestration, development of Integrated Gas Combined Cycles integrated with chemical processes with syngas. Then of course there is the potential of hydrogen and solar energy that pose formidable challenges for energy storage, and designs that can greatly reduce the cost of fuel and photovoltaic cells. Finally, although oil and gas are presumably not going to last for more than 30-50 years, the fact remains that there are huge reserves in the form of oil shale that can still be exploited to satisfy energy needs. Of course the area of energy is closely tied to the area of sustainability in which the broader challenges include developing process systems that are sustainable in the long term. Furthermore, the other important aspect is the environmental one in which the effective use of resources like water is paramount, and the negative impact to the air quality is minimized.

An area that has also been receiving increasing attention is bioengineering systems that ranges all the way from protein design to biomass processing going through metabolic networks. A major issue here for the CAPE/PSE is how to provide meaningful and useful simulation and optimization tools for modelling these complex systems that in turn require integration with data-intensive experimentation. Then there is the added dimension of biomedical applications in which design of drug delivery or therapeutic treatment can in principle benefit from quantitative simulation and control models that the CAPE/PSE community has been so successful in developing.

The area of Enterprise-wide Optimization has also emerged as a new opportunity for the CAPE/PSE community given the increasing need for integrating the functions of R&D, manufacturing and supply in the chemical industry (see Grossmann, 2005). This trend, which is due to the need of making industry more competitive, the chemical has in large part been driven by advances in Information Technologies that allows the access of data across an entire supply chain. A major challenge here is the use of these data in models for the integration of planning, scheduling and control activities across geographically distributed sites, which in turn gives rise to very large-scale optimization models, which presently are unsolvable.

From the above trends it is clear that current and future problems require a multidisciplinary approach because the model development (including data) comes from different sources and the performance criteria, factors, etc., involve other communities besides the CAPE/PSE community. The advantage for the CAPE/PSE community, however, is that it can play the role of the "integrator" or "glue". That is, develop the systematic solution approaches that combine methods and tools from different sources into a single, flexible, reliable and efficient system. That is, the CAPE/PSE community provides the framework as well as some of the methods and tools needed to solve the problems and challenges of the future. This can be done through the development and adaptation of current systems, and where necessary, to also develop new systems. It can be seen that in many cases, models, methods and tools used for one chemical product-process can easily be adapted for use for another chemical product-process. However, for the CAPE/PSE to meet the challenges for the future, computer aided frameworks for generation and use of multiscale models, methods for design of experiments to collect and analyze data, methods and tools for process-product monitoring systems (and their design), techniques for optimization of the enterprise and its supply chain, systematic methods for product discovery would need to be developed, and validated through interesting (industrial) case studies. These case studies will also need to highlight the scope and significance of the new methods and tools in terms of satisfying the technological, economic and social issues.

The presentation will start with a brief overview of the current status of CAPE/PSE, highlight the current trends and needs of the chemical process industry, and highlight some of the challenges for the future and some opportunities for the CAPE/PSE as outlined above. A major conclusion is that it is not necessary to redefine the scope and significance of CAPE/PSE. What is necessary is to redefine the chemical process-product engineering problems in the context of energy, sustainability, bioengineering systems and enterprise-wide optimization to define the scope-significance of the new systematic methods and tools that are able to solve them.

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