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PSE for problem solving excellence in industrial R&D

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ABSTRACT

PSE, process systems engineering, is about the development and application of systematic methods for process studies by the chemical engineer. By means of software tools, the application of these methods is facilitated. Over the last about half a century, CAPE (computer aided process engineering) tools have found their way into process engineering. For example it is unthinkable nowadays to design a plant without a simulation through a process simulator. But there are many more applications of PSE in industry.

The aim of this paper is to provide a taste of the meaning of PSE within the industrial R&D environment. The intention is not to provide a complete overview but to give a flavour of what is perceived as the benefits of PSE during process development, and, in which areas PSE should be extended to render further benefits. The combined approach of experiments and modelling offers a very (cost-)effective strategy in industrial R&D. Further improvements are desired in the areas related to process intensification (PI) and (conceptual) product design. It is believed that the current methods would be more beneficial and have a stronger applicability in industry by inclusion of semi-predictive models and uncertainty considerations.

1. Introduction

In 1830 Auguste Comte wrote that “every attempt to employ mathematical methods in the study of chemical questions must be considered profoundly irrational and contrary to the spirit of chemistry. If mathematical analysis should ever hold a prominent place in chemistry (an aberration which is happily almost impossible) it would occasion a rapid and widespread degeneration of that science” (Sathyamurthy, 2004).

Since Auguste Comte published his opinion, chemical science has seen major changes and strong developments such as the establishment of chemical engineering as a separate and crucial discipline. The prophetic words of Comte have been proven wrong, not the least exemplified by the important role of PSE in the field.

Traditionally PSE is concerned with the understanding and development of systematic procedures that assists the engineer to design, operate and control the production facilities. The procedures are automated in software tools, enabling computer aided process engineering (CAPE) (Gani and Grossmann, 2007). They find their use in many application areas: production, engineering, R&D, education to name a few.

The typical engineering work-flow for the chemical engineer comprises the development of (conceptual) process design, mass and energy balances, equipment selection and sizing, control strategies, techno-economic evaluations and so on. CAPE tools are applied in all of the steps of this work-flow. These are typical activities for most chemical engineers, whether working at the plant, in an engineering unit or in process R&D. Yet, obviously the focus in R&D is more on the ‘unknown’ than it is at the plant or in engineering, where the focus is more on existing knowledge to troubleshoot, debottleneck or design the plant.

PSE offers the methodological approach to unravel the unknown and optimize the known, and moreover the software tools needed in that approach. In this paper the focus is on industrial R&D. In the following sections, the rationale behind industrial R&D, the software tools and the role of PSE in industrial R&D, paradigm shifts that PSE could deliver and finally, outlining of a structured approach in product and process R&D are discussed.

2. PSE for new (process for) product introduction

The costs precede the benefit as they say and this is also true for a new process or product. In the early stages from idea to market there are only costs: expenditures made for developing and marketing the new process or product. Then, at the moment of time-to-market, production and sales begin generating an inflow of money. After some time, at the moment of time-to-profit, the cumulative earnings and costs balance out, indicating the turning point from net losses to profit. From that moment onwards the owner makes profits with the new process or product, until it

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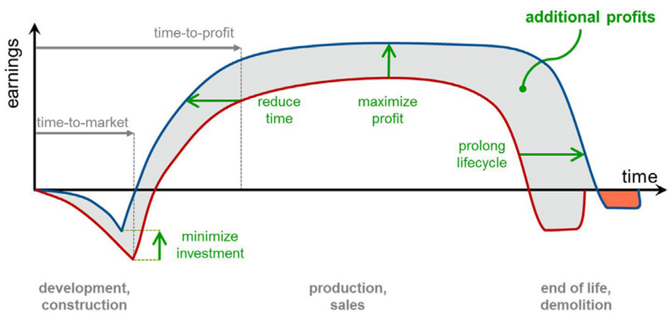

Fig. 1. Schematic profile for earnings during the timeline of a process or product, including options to shift from the less profitable scenario (red curve) to the most profitable scenario (blue curve); the additional profits are indicated by the grey surface minus the red area. (For interpretation of the references to color in figure legend, the reader is referred to the web version of the article.)

Adapted from Gerdemann et al. (2012).

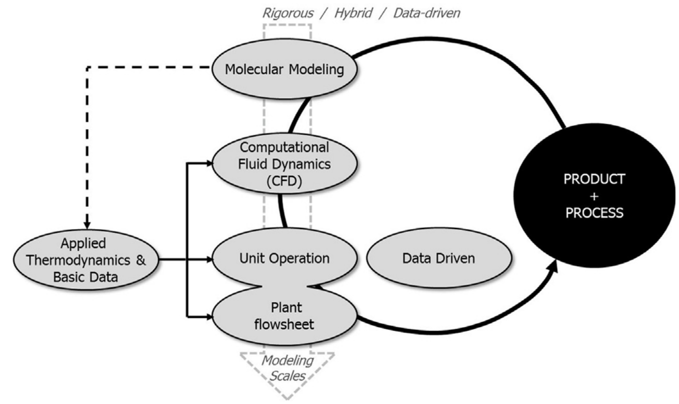

Fig. 2. Chemical engineering modelling platforms at the various scales.

declines at the end of the lifetime of the process or product. This typical profile for earnings during the timeline of a process or product is schematically illustrated through Fig. 1.

There are a number of options to maximize the earnings:

- Minimizing the investment
- Reducing the time-to-profit
- Maximizing the profit
- Prolonging the lifecycle

All of these options can be considered making use of PSE methods and CAPE tools, whether it is at the development stage in R&D, the design stage in engineering or debottlenecking and optimization stage in plant operation and maintenance.

The focus in this paper is on R&D and the role PSE methods and CAPE tools play in that arena.

3. Providing software to exploration

When applying CAPE tools, the usual objective in industry is to provide a (semi-)quantitative description of at least a part of the process or product of concern. A variety of CAPE modelling tools is available for R&D purposes, for different scales in dimensions and time:

- At the smallest scale molecular modelling tools are available. They provide an alternative, preferably integrated, approach to experiments for gaining insight into reaction mechanism, crystallization behaviour, emulsion stability and so on.
- At a somewhat larger scale, CFD (computational fluid dynamics) provides insight into flow characteristics in systems that otherwise are hard to investigate, e.g. at high temperature or harsh corrosive conditions. CFD has long outgrown its infancy state of 'colors for directors' as e.g. it is capable to describe multi-phase reactive systems.
- The heart of process engineering modelling remains the simulation of single and integrated unit operations up to the entire plant. Aspen Engineering Suite, ChemCAD, Hysis, Pro/II, ProSim and gProms are software platforms that offer flow sheeting capabilities for steady state and dynamic simulation (Fig. 2).

Even larger scale models exist like manufacturing execution system (MES) and enterprise resource planning (ERP). These models and related CAPE tools are very useful for manufacturing purposes, but typically they are less applicable in the industrial R&D environment.

Basic data, comprising chemical and physical properties, are crucial for plant and unit operation models and CFD models. In general the basic data models used in unit operation and plant modelling are more sophisticated than those in CFD applications.

The time and effort for building the model is typically larger than for running the model and the interpretation of the simulation results. Likewise it takes more time and effort to set up an experiment than performing the experiment and interpreting the results:

model:	computation time $\ll$ interpretation time $\ll$ model synthesis time
experiment:	interpretation time $\ll$ experimental time $\ll$ preparation time

It typically takes a much shorter time to simulate the effect of a certain event than to perform an experiment if the model is available. However, if not available, the model needs first to be developed and just doing an experiment may be much more efficient.

On top of that, the experiment may reveal certain aspects not covered by the model, e.g. unforeseen side reactions. A balanced choice between modelling and experimentation should be made.

The remarks made above should not be interpreted as a plea to strive for 'universal models', i.e. models that include everything. The strength of models lies in the fact that they are an abstraction of reality. The model should be fit for its purpose. In that sense, the purpose affects the shape of the model (similar to the experiment that is also shaped by its purpose, amongst other things). For example, the vapour pressure does not have to be included in the kinetic model of a liquid phase reaction. Vice versa, the user should not expect this model to represent the vapour pressure of the reaction mixture.

Hence, a pragmatic choice should be made between models and experiments or the combination of those. In industrial practice, one strives for the latter: where models serve as quantitative input for the hypothesis based research and where experiments serve as quantitative input for building and validating the models. This is further exemplified in the next sections.

4. PSE of R&D function

In essence, the R&D function can be seen as a business activity to quantify and reduce uncertainty when introducing a new product or process:

- **P**urpose: (enabling the) introduction of new or improved products and processes