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Life Cycle Modelling in the chemical industries: Is there any reuse of models in automation and control?

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Abstract

In the last two decades, simulation technology had a large influence on process industries. Today, modern numerical methods, powerful personal computers and convenient software packages facilitate the solution of complex engineering problems at every office workplace.
The concept of model re-usage in the chemical industries and the supporting methods and tools are subject to current research and can be found in numerous publications. In practice, the integrated use of models for different applications, in particular in automation and control, can be found only rarely so far.
This contribution concentrates on these applications in process optimisation and advanced control. By considering the different viewpoints of (academic) researchers, software providers and industrial users, the authors discuss potential reasons for the gap between the positions of these three groups.
This contribution demonstrates the current state of industrial applications, the problems and limitations occurring therein, and the fact that these problems are no insurmountable obstacles for the application of model based methods in automation and control.

Keywords: model based control, advanced process control, dynamic simulation, life cycle modelling.

1. Introduction

Today, modern numerical methods, powerful personal computers and convenient software packages facilitate the solution of complex engineering problems at every office workplace. Typical tasks in the chemical industries are steady-state process design, dynamic process simulation for the development of control strategies and the design of model based control concepts [1,5,13].
In principle, existing models could be applied comprehensively to make use of the already available process knowledge. For instance, this aspect comprises the usage of steady state design process models for controller design based on dynamic models. The general concept of model re-usage and the supporting methods and tools are subject to current research and can be found in numerous publications. In practice, the integrated use of models in automation and control, as illustrated in figure 1, can be found only rarely so far. Since the main driver for application is not availability of a technology but the profitability, it might be concluded that the profitability of life-cycle-modelling and model re-use is at least not widely recognized.
This contribution concentrates on integrated use of models in process optimisation and advanced control. By considering the different viewpoints of **(academic) researchers**,

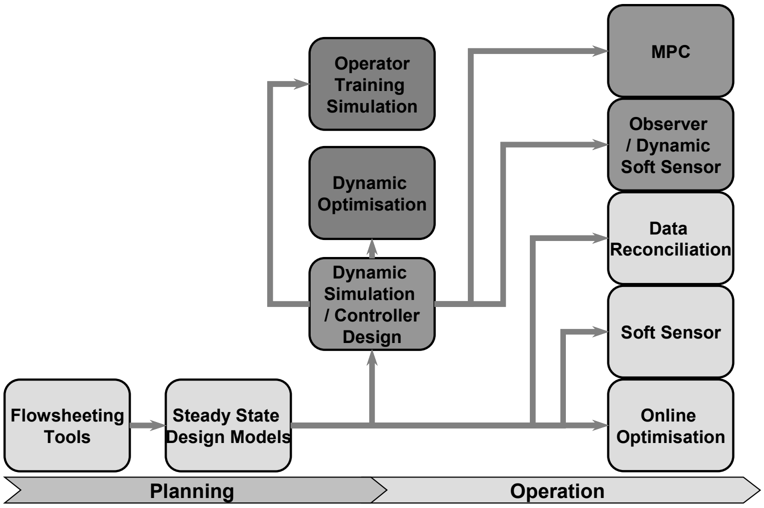

Fig. 0: Model reuse in automation and control

software providers and **industrial** users in sections 2 to 4, the authors discuss potential reasons for the gap between the positions of these three groups. Specifically, it is remarkable that after a wave of projects using dynamic simulation in the 1990s, the integrated use of models for automation and control has not become widely accepted in chemical industries yet.

The mayor part of this contribution is a collection of industrial applications in chemical industry, both “historical” in section 5 and current in section 6, to illustrate the capabilities of the technology.

The following discussion is, besides the references cited, based on the professional experience of the members of the NAMUR working group “Advanced Process Control”, representing a wide range of the German process industries.

2. Academic Perspective

From the academic perspective, modelling and simulation in the chemical engineering field is widely accepted as technological mature and research is currently conducted mainly in very specialised areas. Recent research focuses on the integration of different simulation tools through standard interfaces (CAPE OPEN, which is already an established technology for physical properties,[7]), and software independent model repositories (ROME, [6]). Some even more specialised aspects are model reduction, efficient initialisation and efficient algorithms for dynamic optimisation.

One possible summary for the academic perspective could be: A numerous amount of methods has been developed over the last decades, which theoretically allow the solution of most problems occurring in industrial reality for “classical” chemical processes. Methods for model re-use are developed and even the applicability has been demonstrated. The current research is addressing several application driven open issues, like solid and biological processes, and modelling of product properties (instead of processes), to mention a few aspects only. Some lessons might also be learned from the automotive industry where issues of model reusability and platform indepence for control applications has been addressed for quite a while (see eg. [22] for an overview).

3. Software Provider Perspective

The integration of steady state and dynamic simulation in a single product or a product family became a standard in many cases, and several common simulation tools offer the possibility to export process models in a general mathematical form to be used in other applications. Supplier independent model libraries should gain larger impact in the future, but economical interests of in particular the large suppliers in the market and the lack of power to effectively define standards retard this process.
Current developments concentrate on application areas with high profitability, e.g. large continuous (e.g. petrochemical) processes. The extension to small scale applications ("keep it smart and simple") is not visible. However, it has to be addressed that the process industry does not provide a clear wish list or roadmap to the software providers. Customer needs are hard to guess, if the discussion with different people from one company (e.g. plant manager, service provider automation, conceptual process deigner) does not lead to a consistent picture.

4. Industrial (End-) User Perspective

Model centred technologies are most consequently applied in the large scale (petro-) chemical processes. Model predictive control [2,3], online optimisation and training simulation projects are executed by external engineering companies with dedicated software products, and supplier decisions are driven mainly by (short-term) economic consideration and not by model reusability.
Due to the dynamic development of simulation technology, version and even product cycles are short. The disability of many software tools to easily import old model files often leads to the reimplementation.. A common, standardized simulation language would definitely help the software end-user to deal with tools of different vendors and to overcome the fast release cycles. However, current commercial simulation software became very efficient for standard unit operations, such that the reimplementation of models in different tools does not cause significant costs.
To establish a company wide model library is a challenging task. Most often the units responsible for conceptual process design, equipment design and process automation are widely spread over the organization. To bring these units to complete agreement about the benefit of a common model library and to find a funding for these long-term activities often fails. Thus, company-wide model libraries have only been introduced in a few exceptional cases. To promote the implementation of model based methods in the future, the consciousness for the long-term value of process model needs to be raised significantly.
The main challenge is to overcome the gap between the long-term benefit of concepts for the re-use of models on the one hand side and the short-term difficulties like the lack of continuity of simulation tools on the other hand side.

5. Historical Examples

In the sequel, we refer to a set of previously published "historical" application examples mainly collected within Bayer and BASF to document the industrial research focus and implementations some ten or more years ago:
Dating from already more than 40 years back, an online optimisation example for an oxo plant at BASF is documented. This application used an early digital computer, a process model derived by regression using 7 inputs and 5 outputs and a gradient based optimisation algorithm [15]. Considering the very limited capabilities of digital computers at this time, and the non-existence of comfortable programming helps, not to

speak of modelling tools, this implementation was extremely ambitious and far ahead of times.
Dating from approximately 10 years later, a data reconciliation application for the selectivity calculation of an ethylene oxide reactor is reported [16]. Model and optimisation algorithm are of similar complexity and the digital computer was certainly slightly more advanced using FORTRAN as programming language than in the previous example, but basically the methodological approach remained unchanged for more than 10 years and probably was still ahead of its time. The latter application has been extended recently and is still running today [17].
The peak of dynamic simulation research and development in the 1990's is illustrated be the cooperation between Bayer and Cray to implement a dynamic simulation of a whole distillation train using supercomputers [18,19]. Even though models of comparable complexity now run on a PC and are much easier to engineer, applications with such ambitious scope today are only frequently reported in the operator training simulation area.
The model usage along the lifecycle has never been a real topic until then, first attempts from industry to reuse dynamic simulation model for controller design are documented in academic collaboration in the mid 1990's [20].

6. Recent Applications

This section briefly lists some recent examples for applications and pilot projects collected in the NAMUR working group "*Advanced Process Control*", mainly focusing on the reusability of process models along the lifecycle and towards automation and control applications.
Operator Training Simulation to Advanced Control: The integration of operator training simulation and advanced process control support the start-up of a Bayer monomer plant to full load in automatic mode in two weeks only [14].
Steady State Design Model to Advanced Control: To derive a control concept of two coupled distillation columns, BASF compared the efforts needed for two different approaches, first to start from a steady state design model, and second, only reuse the physical property configuration and reimplement the remaining process model with a detail level tailored for the purpose [9]. Due to the high level of comfort and efficiency of commercial software products for this type of standard equipment, the usage of the existing model has proven to be the more expensive case here, which is mainly due to the fact of the different assumptions and details in the design model.
Online Optimisation: Steam crackers are the most common application for online optimisation. In the BASF example, there was no existing process model for the old steam crackers which lead to a new implementation in a dedicated tool [10,11]. But even for units with existing design models, the direct transfer of existing models was nearly impossible due to new developments in the optimisation software.
Dynamic Optimisation to Model Predictive Control: The integration of dynamic optimisation and model predictive control for a polymerisation process using an existing design model was one application within the INCOOP research project [4,12]. The feasibility and economic potential could be shown in simulations and plant experiments, but an online implementation could not be achieved during the project duration. This is certainly due to the fact that neither the developed technology nor the mindset of the responsible operating personnel is yet ready for a sustainable application.
Dynamic Simulation to Model Predictive Control: A similar application was used in the POLYPROMS research project [8], whilst the design model available here had to be

transferred manually since it was implemented in a software package dating back from the 1990's. In this case, the model is being used for model predictive control, and the transfer to a modern software environment should only be considered as a little break in the lifecycle usage of the model towards automation and control.
Some of the conclusions which can be drawn from this set of representative applications are:

a) Model based methods today are indispensable in process automation. Many of these applications have proven to be profitable and reliable. However, process models typically are developed uniquely without making use of already available process models.

b) Many achievements of academic research do not yet reach the industrial end-user, sometimes due to necessary extensions or refinements of the methods, but mostly due to the lack of a commercially available and affordable software implementations that are in line with the already company wide applied tools

c) The economic break-even for model based application using the currently available methods and tools is still relatively high, tailor-made approaches for smaller processes and those extending the "classical" gas-liquid systems (e.g. batch/multipurpose units, solid processes, biotechnology, smaller life science processes) are urgently needed to promote the technology more widely.

7. Summary and Conclusions

The discussion of the historical development and the perspectives of the three different interest groups shows (not surprisingly) partly different perspectives, which are, amongst others, driven by economic interests on the supplier side and organisational constraints on behalf of the end users. These conflicts in some case limit the technical developments. Research issues driven by industrial needs are towards small scale processes and those involving not only gas and liquid systems.
Nevertheless, the list of examples shows the feasibility and the economic potential of model centred application in automation and control. Even in the far future, not every technically feasible solution will lead to economical applications, but the applicability of the methods needs to be extended by close cooperation between academic researchers, software providers and industrial end users.
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