MODELING TECHNIQUES FOR INTEGRATION OF PROCESS SYSTEMS

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KEYWORDS
Process Systems Engineering, Hybrid modeling,
integration paradox, optimization.

ABSTRACT
Increasing social, economic and environmental pressure force the process industry to look for new ways to improve the overall operation of their process systems.Since these systems are operated at different levels of decision (apparatus, plant, enterprise, etc.) integration of the different levels is expected to lead to significant improvements in system efficiency (energy, waste, costs, quality, product distribution, logistics, etc). Integration also results in increased mathematical
complexity that can not be handled with the current numerical methods. This leads inevitably to a paradox:
the integrated problem needs to be decomposed again
into simpler sub-problems that are solved independently providing sub-optimal solutions. This paper will discuss why integration fails and which steps are needed to break the paradox. Focus will be on new modeling techniques for the different decision levels.

INTRODUCTION

The process industry (petrochemical-, pharmaceuticaland consumer goods industries) is an economic key sector in the world. During the last ten years, the process industry sensed an increasing pressure to reduce costs and inventories as a result of environmental, social and economic changes. The overall optimization of R&D, manufacturing and supply chain is seen as the 'holy grail' and as a complete solution to deal with these emerging changes (Grossmann (2005), Varma *et al.* (2007)). In the past, such process systems were relatively simple and straightforward models could be used for the optimization of the process efficiency. However, in the last decades processes became increasingly complex and are continuously subject to changes. The integration of various levels in company functions (purchasing, manufacturing, distribution and sales), distributions (markets, facilities, vendors) and decisions (strategic tactical and operational) is crucial to realize overall optimization resulting in dramatic increases in operating efficiency.

At this moment modeling and optimization at each of the levels is mostly done sequentially and this leads to the obvious question whether the optimal solutions of the individual levels are the same as the optimal solutions of the overall problem (Harjunkoski *et al.* (2008)). For the overall optimization, integration of the different levels into a monolithic structure is applied. Integration could mean that targets are closer to their global optima, but it also encompasses the increasing complexity of the overall optimization problem. Most of these monolithic structures are NP complete problems, i.e. there is no known way to locate the solution. This conclusion leads to the integration paradox: for most industrially scaled optimization cases, the integrated problem is too complex to be solved and needs to be decomposed again into sub-problems that can be handled with the available methodologies. The integration paradox can only be broken by resolving four fundamental flaws in the integration process:

1. Different levels speak different languages (the models used for each of the layers differ structurally) (Wang *et al.* (2007))
2. There is no proper interface to communicate information between the levels (Stehphanoupoulos & Han (1996))
3. Methods for active re-optimization and experimental validation are not incorporated in the integrated optimization problem, making the solution insensitive to external changes (Shobrys & White (2002)) and
4. Numerical algorithms to deal with complex problems are far from perfect (large computational times and/or sub-optimal solutions). (Klatt & Marquardt (2008))

In this proceeding we will address the first flaw in the integration process: modeling issues. We will identify a modeling technique that is suitable for process systems integration and on the basis of two examples we will project what the capabilities of the envisaged modelin technique should be.

PROCESS MODELING

Fig. 1 shows schematically how a process system can be described by models at several levels.

At this moment, each of the levels uses different models with distinction in: mechanistic/black-box, deterministic /stochastic, distributed/lumped, discrete/continuous, linear/nonlinear, event/data-driven, etc.

The development of a modeling technique that captures the essence of each of the decision levels adequately is of crucial importance to solve the integration paradox.

Proceedings 23rd European Conference on Modelling and Simulation ©ECMS Javier Otamendi, Andrzej Bargiela, José Luis Montes, Luis Miguel Doncel Pedrera (Editors)
ISBN: 978-0-9553018-8-9 / ISBN: 978-0-9553018-9-6 (CD)

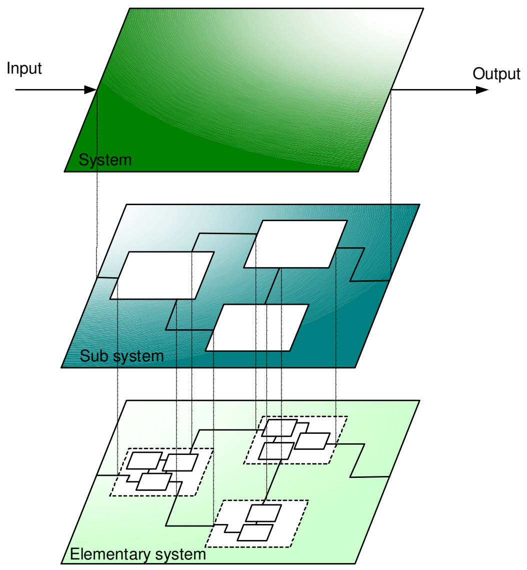

Figure 1: Decomposition of a process system into several sub problems and levels, after Marquardt (Klatt & Marquardt (2008))

Several attempts were made to develop some form of uniform modeling. *CAPE and standards* Romero *et al.* (2002) used ISA standards to realize some form of uniform modeling at the higher levels and Klatt & Marquardt (2008) and Morales-Rodriguez *et al.* (2008) developed CAPE (Computer Aided Process Engineering) tools for automatic model generation for some of the levels. Their approaches, however, do not offer the possibility of integration because these models operate as stand-alone items and do not have the possibility to be connected.

Hybrid modeling

A hybrid modeling technique will do because hybrid models are constructed in such way that the structure of the model at each of the decision levels is similar, which provides the required capabilities for integration and overall optimization. The first step in a hybrid model design is to establish an Input-Output structure that describes the key variables of the process. With a basic modeling approach the process can be analyzed and a model structure can be designed on the basis of physical knowledge and process expertise. The analysis will reveal which parts are mechanistic, black-box, continuous, discrete, etc. After the analysis, the unknown parameters in the model have to be identified. Once analysis and identification are done, the model can be re-assembled into a hybrid structure (See fig. 2).

The model blocks can be connected in several ways combining parallel and serial structures. In fig. 3, a parallel and a serial two block model are shown. In a serial hybrid model, process states and fixed parameters are interchanged between the blocks while in a parallel hybrid model the blocks all require the same information.

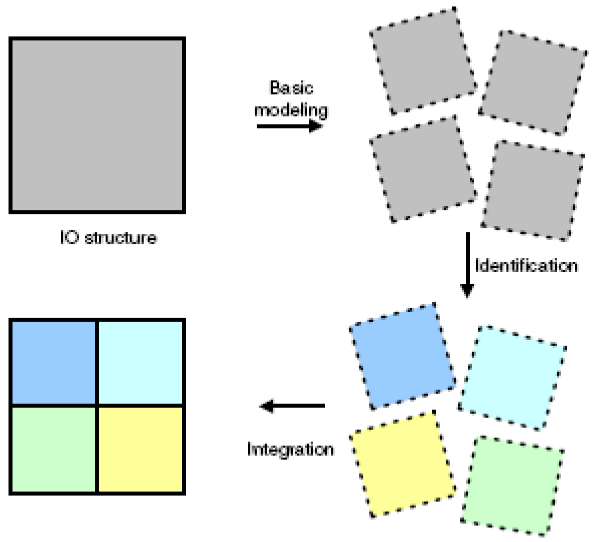

Figure 2: Hybrid model design

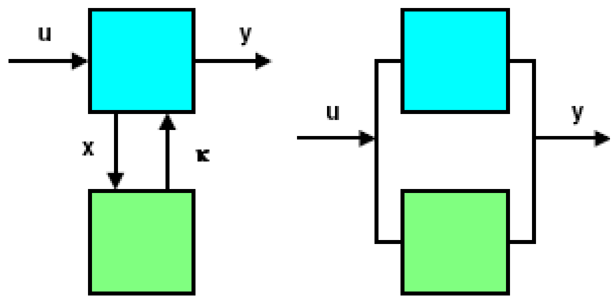

Figure 3: Two-block hybrid model (left) serial model, (right) parallel model.

A hybrid modeling framework is universally applicable to each of the decision levels making integration much easier. Hybrid modeling techniques are already around for a while, but are limited to combining discrete with continuous or phenomenological- with first-principle models. The insence for hybrid models that combine multiple representations is clearly present. *Continuous versus discrete.* We noted earlier that process systems (and control methods) are modeled in the continuous time domain as well as in the discrete event domain. The combination of these domains is called the hybrid domain. In extensive work by Baeten *et al.* (2008) a single formalism is developed that captures discrete and continuous behavior in a single modeling language. Several cases were tested, i.e. a bottle filling line, where bottles on a conveyer belt are fed from a storage tank (discrete event) while the storage tank is filled with product (continuous time domain).

Phenomenological versus first-principles

The work of van Lith *et al.* (2002) describes the development and analysis of dynamic hybrid fuzzy first principles models for process engineering applications. Such hybrid models consist of a framework of dynamic mass and energy balances (first principles) that are supplemented with fuzzy models (black-box).

EXAMPLES

In the chemical process industry are many cases that could benefit from a systematic integration of the decision levels using an extended hybrid modeling technique.

Modeling of oil refinery operations

As other heavy industries, the crude oil processing industry can be identified as an area where small increases in efficiency have a large economic impact Moulijn *et al.* (2006). The available global reserves of oil show that the available reserves for 'easy' crudes are estimated at 50 years, while the 'difficult' or shale oil reserves could supply the world for maybe 350 more years. As the easy oil becomes scarce, the need for better processing techniques becomes more urgent. World-wide research attention is drawn to new processing techniques to increase the overall efficiency of the crude oil processing steps. Oil refinery operations are modeled and optimized at different level of decision, and in that respect the oil refining industry is a perfect test case for an integrated hybrid modeling methodology. Fig. 4 shows an example of an oil refinery supply chain.

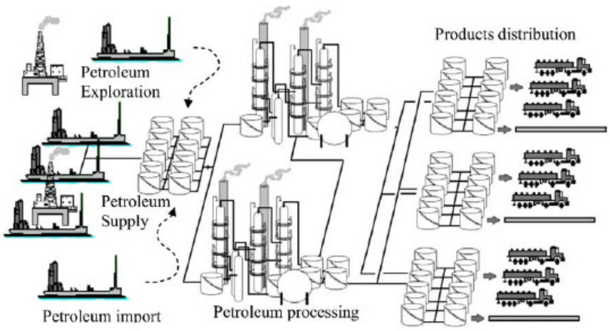

Figure 4: Supply chain of an oil refinery

At nano- and micro level, physical intereactions are described (mechanistic, continuous). At meso level the temperatures, pressures, flows and compositions are modeled (mechanistic, continuous). At meso-macro level, scheduling tasks are normally evaluated: division of tasks, storage and crudes, deliveries of crudes, distribution of products, etc (discrete, linear). And at macro level, strategic decisions have to be made (heuristics). At all levels uncertainty plays a dominant role in the outcomes of the optimization.

Modeling of multi-product reactive distillation.

Reactive distillation (RD) is a successful example of process intensification. Traditionally, products where produced in reaction vessels and the products were subsequently purified in separation devices (e.g. distillation columns). Reactive distillation combines both processing steps into a single piece of equipment (See fig. 5). The advantages are numerous: smaller spaces required for the setup, reduced energy requirements, larger conversions (as removal of products shifts chemical equilibrium to the product side). Current research explores possibilities for the use of RD in a multi-product setting; a single unit is used to produce several products (depending on the market). This poses new challenges as descriptions of such systems also require hybrid models at all levels of decision, from process control to scheduling, planning and long term strategic decisions.

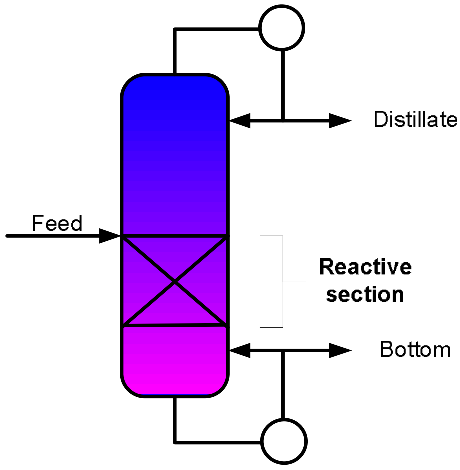

Figure 5: Reactive distillation setup

In the lowest level of a multi-product reactive distillation system models that describe mass transfer, kinetics, thermodynamics and hydrodynamics are required (mechanistic, continuous, and nonlinear). These models can be used to find optimized settings for temperatures, flows, pressures, concentrations, etc (i.e. minimization of operational costs in terms of energy). At the medium levels production- and maintenance models are required that can be used to optimize production, storage and distribution of reactants and products (linear or nonlinear mixed integer models). In the higher level long-term economic models and protocols are required to optimize long-term performance of the plant, e.g. market effects (linear, stochastic and heuristics). For each level currently different model structures are used and different optimization objectives hold.

CONCLUSIONS

In this proceeding we have identified the flaws that cause the so called integration paradox. One of the flaws is the result of inconsistency in the models for each of the decision levels. Ergo, a universal modeling technique that is applicable to all the levels could enhance the integration process significantly. Such modeling technique should incorporate process features such as mechanistic/black-box, deterministic /stochastic, distributed/lumped, discrete/continuous, linear /nonlinear, event/data driven. Hybrid modeling is such a technique. 2-Block hybrid models are currently derived for discrete/continuous systems and mechanistic/blackbox models. Extending hybrid modeling frameworks to multiple blocks, incorporating more features is a major research challenge that deserves attention.

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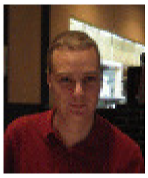

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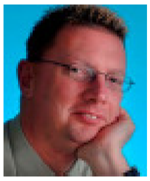

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