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Process Modeling and Simulation for Optimization of Operating Processes

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Abstract

During the last decade, a major shift has begun in chemical industry, since there is an urgent need for new tools that are able to support the optimization of operating technologies. This trend is driven by the new tools of information technology. Approaches of this shift differ from company to company but one common feature is that communication between design, manufacturing, marketing and management is centered on modeling and simulation, which integrates not only the whole product and process development chains, but all the process units, plants, and subdivisions of the company. These approaches are under continuous development. Among the wide range of possible improvements, this paper focuses to two frequent imperfections: (i) developed and refined process models are used only in advanced process control system (APC) integrated into distributed control system (DCS) and operator training systems (OTS), and not for detailed analysis and optimization, and (ii) optimal process operating points of these chemical plants are adjusted only at the design and test phase of a new technology, but optima moves with time, new catalyst system, lower price of reactants, claim for new or higher purity products, etc.
The aim of this paper is to review, how to manage process optimization, and to show our process simulator based on the chemical engineering model of the technology. This paper will present a case study to demonstrate the technological and ecological benefits of the analysis and optimization of an

operating multi-product polymerization plant. The models of advanced process control system (APC) and reactor cascade were implemented in MATLAB® Simulink® environment, as a powerful and popular dynamic simulator.

Keywords: integrated modeling and simulation, polymerization plant

1. Introduction

Costumers' satisfaction and the economical challenge of modern technologies claim for a continuous optimalization in every field of life. In chemical industry, products with precise quality values have to be produced while specific costs have to be on a minimal level. To fulfill these expectations, chemical process industries are renewed, redesigned, and rebuilt, i.e. modernized continuously to have the ability to operate complex, highly interconnected plants that are profitable and that meet quality, safety, environmental and other standards. Towards this goal, process modeling, simulation and optimization tools are increasingly being used industrially besides of the design process at every level of subsequent plant operations [1].

During designing new technologies, several works have been done on connecting the process and its control system and design them as one entity. Narraway et al [2] used a model that permits of the estimation of economical benefits for a given control scheme with specified disturbance regime. Perkins et al. worked out a simultaneous process and control design methodology where process operability is analyzed by mixed integer dynamic optimization (MIDO) [3][4]. During design phase, several works report the importance of calculating operability indicators [5][6], but these are generally limited to linear systems.

In contrast to the numerous scientific results of optimally designing technologies, optimization techniques of existing, operating processes are unnoticed. Although lot of existing plants and technologies are reviewed for cleaner production forced by the environmental defense, only few articles deal with simulation and analysis as tools of optimization, like the one of Turon et al [8], that proposes the simulation of a paper mill process and its optimization by the application of genetic algorithm for reducing water consumption and material losses. Reasons of this phenomenon, namely the lack of articles reporting process modeling and simulation, may be that researchers hold an operating technology not to be "science" anymore and they consider that scientific research only belongs to the design phase, "engineering research", like analysis and fine-tuning of operating processes, should be done by experts of the current technology. Process model is already integrated into the model predictive control system, and is thought to be useless for further aims. On the contrary, engineers and directors of leading chemical product companies, e.g. DuPont and Dow Chemical, think that *"model integrates the whole organization"*. It is the way that data, information, and knowledge are conveyed

from research to engineering to manufacturing and on to the business team[9]. According to that, modeling and simulation will have a much greater part in chemical engineering, it is prognosticated as a key feature of modern process maintenance in the future. Officials of AspenTech and other companies dealing with simulation technologies talk about "*life-cycle modeling*" and integrated modeling technology, i.e. a model that is applied at every level of a technology. The hardware side of the problem already exists, process computer systems commonly have the data saving and storing sub-functions besides their basic process control functions, thus these industrial, economical etc. data time series can be used to adjust model parameters and to evaluate the models. The process analysis can result in product life-time analysis, sensibility function of product quality to the process variables, optimal product change strategies, product quality and quantity maximization, catalyst activity analysis. Our methodology consists of two main parts: (i) black-box and statistical modeling, which was introduced in our previous work [10], and (ii) a priori modeling and simulation, whereto a priori engineering knowledge is integrated.
Section 2 deals with the detailed description of our system performance analysis: our methodology, the analyzed system and a case study to demonstrate the technological and ecological benefits of the analyisis and optimization of an operating multi-product polymerization plant. Section 3 introduces our conclusions and future plans.

2. System performance analysis

2.1. The proposed methodology

Optimalization tasks of complex systems generally begin with a detailed process and process control investigation, called *knowledge discovery*, to get focused on the maintenance or control operation problems where to intervent to

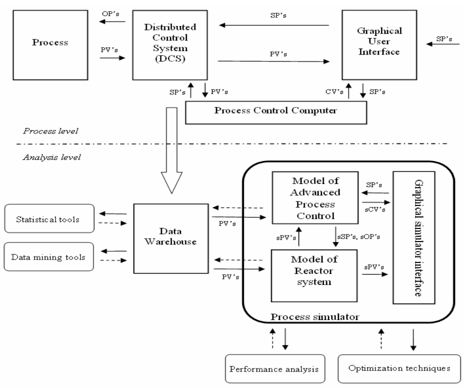

Figure 1.**:** the methodology of process analysis

get production more efficient.

At this level, a large amount of data is needed to create a data warehouse from the process values, operation points and set points collected and stored by the DCS, to apply statistical and data mining tools AND modeling and simulation to get useful information. In order to achieve an offline process simulator, process model and its model based control system should be created in a dynamic environment. For this purpose, Matlab's Simulink software was applied, which can handle the calculations of a highly complex integro-differential equation system during transitions of the technology.

The main advantage of having such an offline simulator of the system is that it can be used to predict product quality, estimate the state of the system and find new optimal operating points in a multi-objective environment, results of operability tests, effects of e.g. new recipes or catalyst can be investigated without any cost attachment or system failure, and it is easily expansible for system performance analysis tools and optimization techniques. Figure 1. shows our scheme for process analysis.

To shortly summarize, the application of first principle (a priori) modeling is suggested as an equal part of process analysis besides black-box modeling and statistical data mining tools, such as fuzzy decision rules and classification.

2.2. The system: a polymer technology

This paper proposes the simulation and optimization of a polypropylene polimerization plant, localized in Hungary. It uses the Spheripol® technological license of Himont Inc. (Japan), the advanced process control system was developed by Honeywell Inc. This technology produces propylene homopolymer in two loop reactors in series, and propylene-ethylene copolymer in a gas phase reactor. Nevertheless, copolymer production needs also homopolymer production in the loop reactor section. Technology description can be found in [10]. Eight different homopolymer products are produced with different calculated quality measures (melting flow index (MFI) and cold xylene solubility (CXS)), hence, there is a clear need to minimize the time of changeover because off-specification product is produced during transition.

2.3. Case study

Currently, our process simulator handles homopolymer production. The reactor model system runs based on a mass balance, the advanced process control model (as in the reality) is based on an energy balance. Figure 2. shows the model validation on a 44-hour-simulation period with a product change at 19th hour to verify that model dynamics correspond to the real production system. One can recognize that during product change, production rate is significantly lowered to minimize off-grade product, our model follows this trend based on mass and energy balance as well.

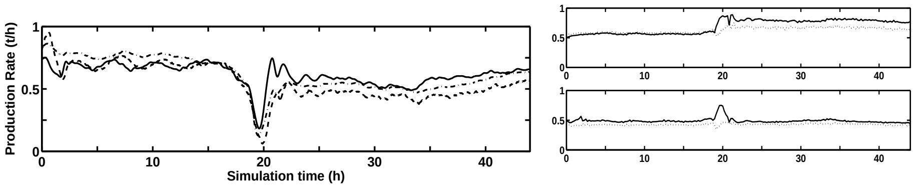

Figure 2.: production rates as outputs of the system (dash-dotted), the model (cont.) and the APC model (dotted line); and residence times by model (cont.) and system(dotted line) in the first (upper) and second (lower) reactors

Possible application of the simulator is answering "what if"-type questions. Our case study shows a simple, trivial analysis: the effect of bad control or valve malfunction. For example, the monomer flow increases rapidly (i.e. step-wise) and hydrogene flow control does not follow the new bias point to keep the hydrogene to monomer ratio, so product quality changes from its nominal value. This type of correlations can be easily achieved already with this test-phase simulator.

Simulation parameters are as follows: the experiment lasts for 10 hours, a monomer flow step of 10 % occurs at the 5^{th} hour, other variables are kept constant. Results are presented in Figure 3.

2.4. Results & discussions

As expected, production rate would follow the increase, but without the increase of the catalyst flow, it cannot be carried out. Slurry density decreases caused by the excess fluid in the reactor, and melting index increases because it is highly correlated with the lower hydrogene concentration: lower hydrogene content in the reactor results in longer polymer chains and higher melting index values. For a 10 percent disturbance in the inlet flow without hydrogene to monomer

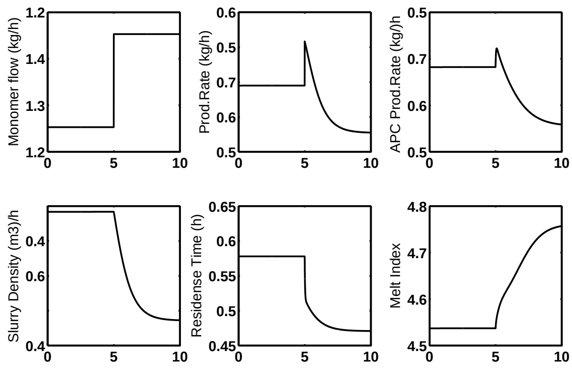

Figure 3.: simulator outputs as an answer to a monomer flow step function

ratio percent, MI increases by 5 percent.

3. Conclusions and future work

In this paper a novel approach has been presented for the analysis and the optimization of operating technologies based on the integration of models of complex production processes and their control system. This new tool has been validated and fine-tuned by historical process data. Future work will concentrate on performance analysis and optimization techniques that rely on the presented simulator.

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