Application of integrated process and control system model for simulation and improvement of an operating technology
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Application of integrated process and control system model for simulation and improvement of an operating technology

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Abstract

According to costumers' expectations and market challenge, chemical industry of the immediate future needs to have the ability to operate complex, highly interconnected plants that are profitable and that meet quality, safety, environmental and other standards. Approaches to fulfill these expectations are under continuous development, they 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. A main disadvantage of these tools is that they are independently developed for particular solutions and mostly the models applied in the design phase of the technology are not re-used for process analysis or improvement but particular models are used.
The methodology proposed in this paper integrates production systems, where integration means information, location, application and time integrity. Models of process and control systems are integrated to a process Data Warehouse. This structure support engineering tasks related to analysis of system performance, process optimization, operator training (OTS), reverse engineering, and form decision support (DSS) systems.
The aim of this work is to present the effective usability of such framework in an operating polymerization process to emphasize how integrated modeling and simulation of process and control systems and information flow among the production units can improve the overall performance of complex process systems. The case study used for this purpose deals with the development of a new soft-sensor used for the estimation of the product quality.

Keywords: model-based optimization, offline simulator, process analysis

1. Introduction

Costumers' satisfaction and the economical challenge of modern technologies claim for a continuous optimization 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. 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]. Leading chemical product companies, like DuPont and Dow Chemical Co., stand for life-cycle modeling, where an overall model is applied at every level of a plant, i.e. "the model integrates the whole organization" [2].
The application of process models is typical in planning areas of chemical engineering, where steady-state process design and dynamic control strategy development are the main tasks [3], but at the operational level the recycled usage of models in automation and control is not widely realized, thus it might be concluded that the profitability of life-cycle-modeling and model re-usage is not widely recognized. [4]. Concluded from the above statements, the integrated design of processes and their model based control system had its attention in the literature based on economical analysis [5,6,7] or operability indicators [8].
Unfortunately, process models that have been applied in planning phase, for instance in model predictive control, are not re-applied during process analysis and improvement because the process knowledge is already distributed: process models owned by process and control system designers, laboratory and plant experience of plant engineers is not incorporated into an integrated framework. But re-usage of process models in steady-state simulation analysis is efficiently applicable in developing of new bias points, sensitivity functions between product quality measures and state variables or in reverse engineering. Dynamic process models are additionally capable to analyze the transitions between these steady states and their control strategies that lead a state into another.
From the above described phenomena comes the conclusion that there is always need for systematic tools that help improve the control level of not only the process but the products based on modeling and simulation, hence these tools can model product properties and estimate product quality with respect to the controlled process states. Application of such tools is known in soft sensors, monitoring tools, operator support systems (OSS) decision support systems (DSS) but these areas are separate and are improved independently. For all these purposes, an integrated process methodology was developed. This methodology integrates the system, where integration means information, location, application and time integrity. Recently there is a good innovation on this topic at Bayer Technology Services.
Obviously, the solutions are rather system-specific but the systematic methodology can be generally applied to handle the complexity and get relevant knowledge. Section 2 gives a detailed description of a data-driven process improvement methodology while section 3 deals with its implementation and application as a case study on a Hungarian polymerization plant.

2. General methodology for process analysis and improvement

Optimization tasks of complex operating systems generally begin with a detailed process and process control investigation. If it is possible to collect sufficiently large amount of data from the process, also Knowledge Discovery in Databases (KDD) technique can be applied to achieve information focused on the maintenance or control operation problems to get production more efficient [9].
Figure 1 shows our methodology scheme for process analysis. At process (operation) level, the distributed control system (DCS) assures locally the secure and safety operating of the technology. The measurements serve the values of the process variables (PV's) to DCS which forwards the information to the graphical user interface (GUI). The operators of the

technology can get information about the system via the GUI and (if it is necessary) they control the process by changing the set points (SP's). An advanced model based process control (Process Computer) computer calculates among others the operation set points (OP's) to DCS.
The data stored by DCS definitely have the potential to provide information for product and process design, monitoring and control, but these data have limited access in time on the process control computers, since they are archived retrospectively, they can be unreliable because of measurement failure and are stored inconsistently. Process Data Warehouse (DW) is a data analysis-decision support and information process unit, which operates separately from the databases of the DCS. It is an information environment in contrast the data transfer-oriented environment, which contains trusted, processed and collected data for historic data analysis.

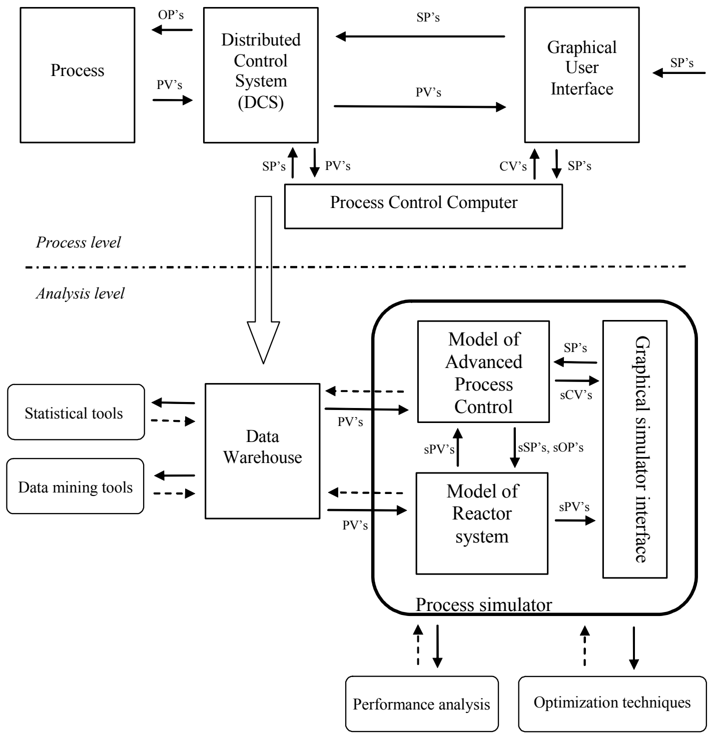

Figure 1: the integrated methodology of process analysis

The data collected into DW directly provide input for different data mining, statistical tools, like classification, clustering, association rules, etc., and visualization techniques, e.g. quantile-quantile plots, box plots, histograms, etc. Besides these tools and techniques DW indirectly creates a basis for optimization and system performance analysis techniques through a process simulator of the process and its advanced local control system, since models are validated based on the historic data stored in DW.
In order to achieve such an offline process simulator, process model and its model based control system should be created in a dynamic environment. One needs to integrate the existing models and information of the system or re-create them if they do not exist anymore. The following components are needed to build such a dynamic environment:

- *Technology model*: an integrated application of laboratory kinetics and experiments with plant scale-up parameters embedded into different hydrodynamic reactor models;
- *Control system model*: uses the designed structure of regulatory process control system, information about the controlled and the perturbed variables, possible states, and operation ranges;

- (Graphical) *Interface*: it handles the input-output connections between process model, control model, data warehouse and the user;
- *Visualization and analysis tools*: that convert raw outputs into valuable information.

For particular analysis, the applied components decide whether the result is a soft sensor, process monitoring, reasoning or reverse engineering tool, operator training/qualification or decision support system application.
Moreover, if the simulator outputs are stored in the DW for further analysis, comparison of the analyzed simulated outputs to the real industrial data can provide further information for simulation based optimization and that results in a DW-centered continuous process improvement cycle.
Generally, the advantage of having 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.
The following section details the applicability of such methodology on a Hungarian polymerization plant.

3. Case Study

The proposed methodology was applied as a theoretical basis for a research project in a polymerization plant of Tisza Chemical Group Plc., Hungary. This section presents a case study of the DW-based modeling part in order to mine the potential in re-using or – if these models are not present anymore – re-building a technology simulator.

3.1. The polymerization technology

The analyzed technology uses the Spheripol® technological license of Himont Inc. (Japan), the advanced process control (APC) system was developed by Honeywell Inc. This technology produces propylene homopolymer in three 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. The homopolymer production is split i.e. distributed between the two main loop reactors and this split ratio is product-dependent.
A three-component-catalyst is used for polymerization. It is very important to maintain their ratios within the preset range because of the product quality and productivity of catalyst system.
The hydrogen feed is used to control the intrinsic viscosity of the polymer acting on the length of the polymer chains thus on the melt flow index, the main empirical quality indicator value of polymerization. Additionally, productivity of the catalyst system highly depends on hydrogen content of the reactors. To maximize productivity and catalyst yield, reactor slurry densities (i.e. residence times) are operated at the maximum while reactor temperatures are kept constant. A more detailed technology description can be found in [10].
The above mentioned effects conclude that the control of production rate by catalyst feed and by temperature and the control of product quality by hydrogen feed are related, hence there are several ways to drive the technology from a steady state of a product to another one. Product transitions are managed frequently because of the wide-quality product range: in a production cycle 6-8 homopolymers are produced with increasing MFI values, then 10-11 decreasing MFI copolymers, so the technology runs steady for only 2-3 days.
That means that there is a clear need to optimize grade transitions because of off-specification product and transition time minimization.

3.2. Implementation of the proposed methodology

The implemented integrated process methodology consists of a process DW collected from the operating process, the corresponding rule-based knowledge discovery tools and the process simulator with its graphical interface.
The process Data Warehouse is implemented in MySQL Database Server and it consists of the following data sources:

- Measured data: selected variables of the technology measured and stored by the DCS;
- Silo changes: reasons and dates of changing the storage drums that have the information of product transitions;
- Production parameters of every product type;
- Off-line laboratory MFI measurements: for polymer powder and granulate with different sampling frequency;

Data Warehouse is reached via ODBC driver through MATLAB® wherein every tool and interface was programmed, the dynamic environment for process models is MATLAB® Simulink®.
As an experimental tool, only the bulk polymerization subsystem was modeled and implemented: (i) hybrid models of the three loop reactors (ii) a copy of the original indirect control performance calculation system of the Advanced Process Control by Honeywell Inc. The model was achieved by hybrid modeling technique: where first principle models were not available because of confidentiality or unavailability, black box models were applied, which parameters were identified based on the process DW collected from industrial data.
Regulatory control is based on the calculations of this APC system that is responsible for steady state operation. Since APC does not have originally implemented transition strategy, transitions are managed by plant operators.
To handle this problem, our process simulator has besides the re-simulation with real valued data input downloaded from DW the dynamic simulation capabilities as well to freely choose transition trajectories as set points between steady state values of process variables, thus it is an adequate basis for multi-objective optimization. The following local control loops were implemented and tuned:

- Production rate control by catalyst inlet flow rate;
- Reactor density control by propylene monomer inlet flow rate;
- Product quality control by hydrogen inlet flow rate with respect to monomer flow rate;
- Reactor temperature control by necessary inlet cooling water temperature;
- Catalyst composition ratio control by inlet flow rates of catalyst components;

These regulatory control loops can separate the simulator from DW or make it use only the set points of the controlled variables to re-simulate operators' transition strategy

3.3. Application examples

As mentioned above, we implemented the homopolymer production subsystem of the technology; gas phase copolymer production subsystems, separation and cleaning subsystems were out of the range of this project.
In Figure 2-4 the validation of the applied separate models and the integrated model can be seen that were validated on production rate, production split and residence times in reactor. Two product transitions were managed in a two days period (productions are separated by vertical lines).
As seen on the Figure 2, the model describes some productions very well while others are loaded with errors. Production rate has negative or positive excess in the simulated cases while production split and residence times follow the trend of original data (Figure 3 and 4). The basic cause of this phenomenon is that an average model was implemented, and these positive or negative error rates can create a basis for reasoning about e.g. catalyst productivities that can cause such anomalies. The technology model based APC performance

calculation gives the same results as the technology model, which means that it is a good approximation based on heat balance for the mass balance based technology or technology model.

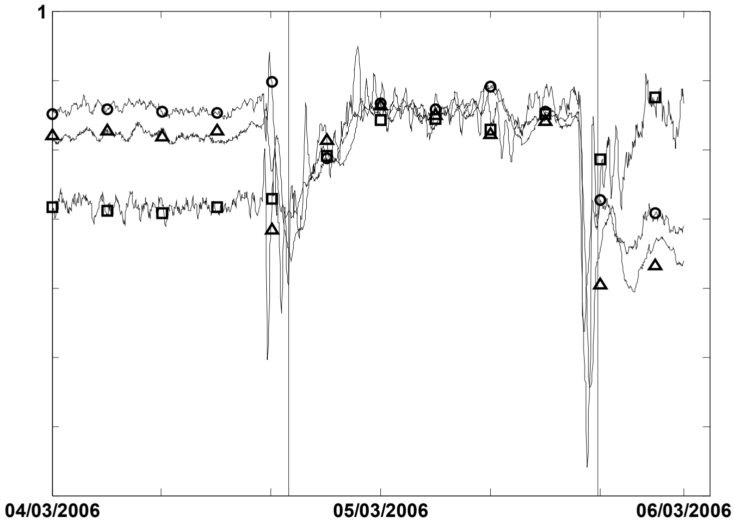

Figure 2: Validation of the applied models for production rate (original APC data with 'o' markers, calculated APC output with 'Δ' markers, technology model output with '□' markers).

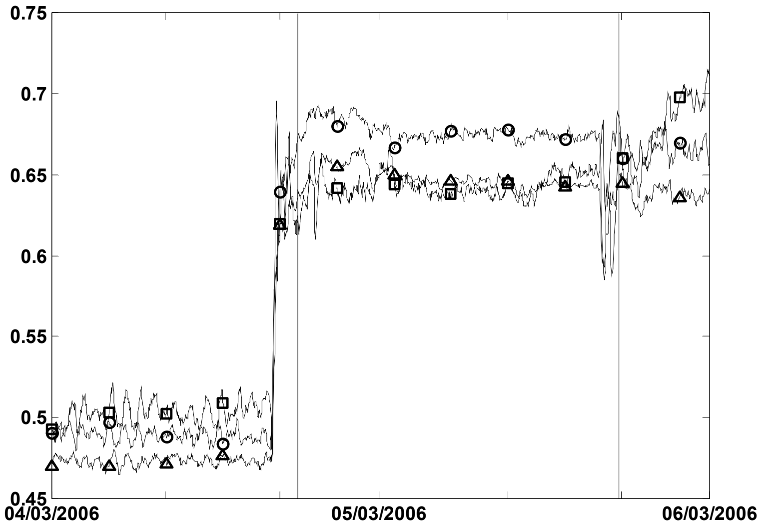

Figure 3: Validation of the applied models for production split (original APC data with 'o' markers, calculated APC output with 'Δ' markers, technology model output with '□' markers).

Based on several validating simulations, it can be stated that productions differ from each other, so to get useful information sensitivity analysis techniques need to be done either in a steady or a dynamic manner. Steady simulations can lead to e.g. estimation of catalyst activity but another even more important application is that based on steady state values of state variables and the corresponding product quality (melt flow index - MFI) measures, a sensitivity function of quality with respect to state variables can be identified which can be easily visualized by e.g. Self-Organizing Map (SOM) [11]. The SOM facilitates visual understanding of processes so that several variables and their interactions may be inspected simultaneously. Once a SOM model is trained by transition-free data, it can predict product quality from state variables hence it can work as an online product quality estimator. We applied the original SOM Toolbox developed by Vesanto et. al [12].

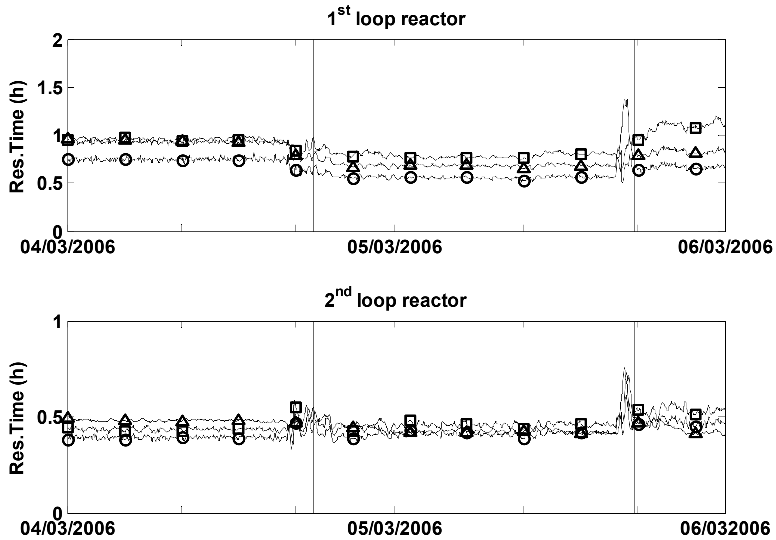

Figure 4: Validation of the applied models for reactor residence times of first (upper) and second (lower) loop reactor (original APC data with 'o' markers, calculated APC output with 'Δ' markers, technology model output with '□' markers).

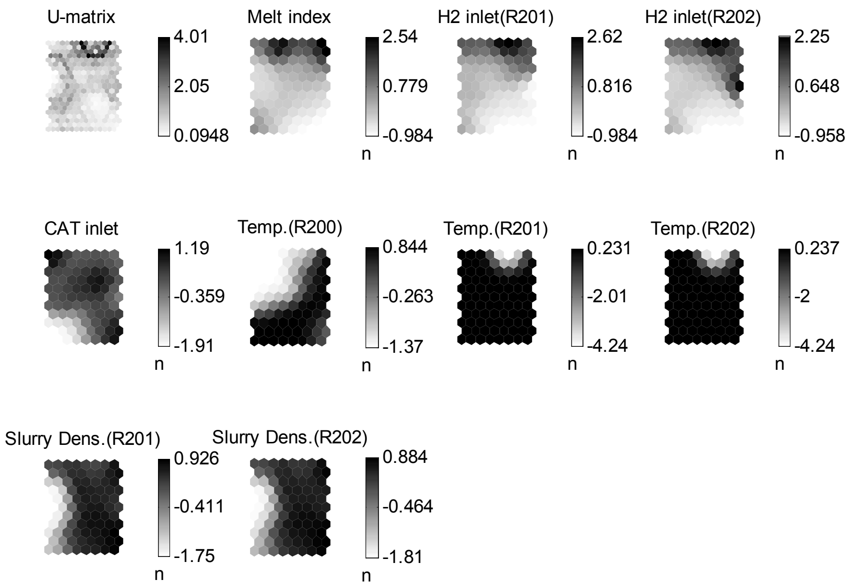

Figure 5: Component planes of polymer production map generated by SOM Toolbox.

Results are shown in Figure 5, where it can be univocally seen that hydrogen feeds are the perturbing input variables for melt flow index. From a SOM model a soft sensor can be built as an MFI estimator based hydrogen feed to the reactors.
Other experiments showed that hydrogen concentration in the reactors, hence hydrogen as state variable, is a more accurate in estimating MFI. Though it cannot be directly measured in the technology it has to be calculated by the APC model.

Several process state variables have the effect on the estimated outcome of production, and the regulatory control loops are not independent, currently there is no perfect solution how to manage product transitions.
To handle this problem, the simulator extended by local controls has the capability either to qualify operators' transition strategy based on their adjusted set points collected from the process DW or to analyze the effect of particular transition trajectories on melt flow index. This latter task deals with how one can optimize a complex transition strategy. All these functions are available through a graphical user interface programmed also in MATLAB.
Since the implemented simulator generally has all the mentioned application possibilities, the applied components of models and outputs depend on the current application and purposes.

4. Summary

In this article a process and product analysis approach methodology was introduced with a particular solution for highly complex system, a polymerization production subsystem of a Hungarian plant. This methodology is applicable for general purposes as well where a large amount of disorganized data is present. Besides direct data mining applications, engineering modeling has a large potential in data driven process and product optimization and reasoning. The presented case study has presented a brief overview under a research project in a Hungarian polymerization plant: a historical process data warehouse was built to store relevant information about the production in a coherent format. Based on this data warehouse it was shown that re-application of process models in process and product improvement analysis has a great potential and process modeling and simulation need to incorporated into simple statistical tools to better manage complex systems. In this sense, our tool is very useful not only for operator training systems (OTS) or decision support systems (DSS), but for product/process development as well because of its structural variability.
Future work will concentrate on the application of this DW-based process simulator for optimal operation during product transitions.

5. Acknowledgement

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