



Optimization of Process Operation Strategies by Combining Process Models with Plant Operating Data

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Competition, cost pressure, and market fluctuations lead to a persistent increase in complexity and degree of integration of chemical plants. The utilization of accurate process models facilitate plant efficiency optimization in real-time and improve process transparency for the plant personnel. To reduce development time and costs, existing models from the process development phase of the chemical plant can be used. Next to the general availability of a plant model and plant operating data, a systematic strategy is helpful to successfully implement a validated process model into the process control system of a chemical plant.

This contribution presents a strategy to develop a technology platform with a validated process model containing the following steps: analysis of the economic potential, software selection, process analysis, steady-state detection, parameter identification, and process optimization. The presented strategy is applied to an industrial plant of BASF SE in Ludwigshafen, Germany. The application of this platform exposes great economic potential. Firstly, a significant cost reduction can be achieved by reusing existing models during the development phase. Secondly, with the help of the technology platform soft-sensors are created, bottlenecks identified, and an optimization of process operating strategies is undertaken.

1. Motivation and Problem Statement

Over the last decades an increase of complexity and degree of integration of chemical plants has occurred. This has happened – among other things – due to the consistent rise of overall cost pressure as well as market fluctuations with regards to resource availability, resource costs, and retail prices. In order to cope with the increased cost pressure, greater plant efficiency is required, while on the other hand, market fluctuations demand higher plant flexibility. One possibility to assist the plant operator in achieving these two goals is by implementing a validated process model. With such a model plant transparency can be increased and optimization studies realized.

Real-time optimization has become an established technology for the optimization of steam cracker operation. For regular chemical plants on the other hand, few real-time optimizers have been realized, mainly due to the high cost-benefit-ratio. One of the main effort and cost factors, according to Wozny and Jeromin (2004), is the modelling of the chemical plant. Marquardt (1996) as well as Wozny and Arellano-Garcia (2009) emphasize that great cost and development time reduction can be achieved through the reuse of existing models from the process development phase of the chemical plant. In the

following a systematic strategy for the development, implementation and utilization of a validated process model on a real chemical process of BASF SE is presented.

2. A Systematic Strategy for Utilizing a Validated Process Model in Real-Time

The main aspects for developing, implementing and utilizing a validated process model are described in the following from an industrial viewpoint. A more detailed discussion can be found in Müller (2011).

2.1 Economic Potential and Software Selection

Before deciding to implement such a model-based application it is important to estimate its economic potential. For process monitoring for example, the number of necessary measurement instruments can be reduced and efficiency losses such as fouling can be identified early on, thus leading to an economic improvement. Comparisons between historic process data and optimized values can reveal model deficiency but also potential improvements of the operating strategy. If enough economic potential is identified, the software system is designed and selected. Factors such as licence costs, data storage and modelling capabilities as well as available optimization algorithms are considered.

2.2 Process Analysis

The process is analyzed with respect to its degrees of freedom (DoF) and its disturbance variables, which is done in this paper by the method of Konda et al. (2006). The DoF is the maximum number of variables which can be manipulated in the process optimization.

The disturbance analysis reveals which process variables influence the operating point and have to be checked for steady-state behaviour prior to evaluating the steady-state process model. If a defined set of disturbance variables are at steady-state, the process can be regarded as being in steady state, whereas a change in a disturbance variable results in a non-steady-state. Examples for disturbance variables are feed streams, feed concentrations, feed temperatures, heat streams, or fouling. The disturbance variables can generally be divided into two groups: measurable and non-measurable variables. For the non-measurable ones measurable substitutes need to be found.

2.3 Steady-State Detection

When using stationary process models, steady-state detection is essential. If the model parameters are fitted to a process which is not in steady state, incorrect results could be received, inter alia, the conclusion of mass balances is no longer possible and thus model prediction errors are increased (Baht et al., 2004). There are various methods to detect quasi steady-state points, such as those presented by Savitzky and Golay (1964) or Schladt and Hu (2007). If the process is at steady state the model parameter identification can begin.

2.4 Parameter Identification

According to Schuler (1995) an identification of varying model parameters such as fouling and efficiency factors has to be undertaken to fit the process model to the current steady-state operating point. The model parameters are estimated using the method of least squares. In an simplified version the least squares problem is

$$\min_{p_j} \sum_{i=1}^n \frac{(\tilde{x}_i - x_i(p_j))^2}{\sigma_i^2} \cdot w_i \quad i \in \{1, 2, \dots, n\} \text{ and } j \in \{1, 2, \dots, m\}, \quad (1)$$

wherein \tilde{x}_i are the measured and x_i the model variables, p_j the model parameters, and σ_i^2 a fixed estimate of the measurement error variance. Yip and Marlin (2004) highlight the necessity of high model accuracy at relevant plant operating points to allow for reliable decisions later on.

2.5 Applications of the Validated Process Model

The validated process model can be used as a technology platform for different model-based applications, such as soft-sensors, bottle-neck analysis or key-performance-indicator monitoring. Furthermore, the process model can be used for applications which require additional calculations, such as offline optimization studies and real-time optimization.

3. Industrial Application

The presented strategy is applied to an industrial plant of BASF SE in Ludwigshafen, Germany.

3.1 Investigated Process

The process produces and purifies a base chemical. It consists of a reactor part, in which mainly the product *B* and one byproduct *C* are produced, a rectification column for byproduct removal, and two heat integrated columns for product purification. Product and byproduct form an azeotropic mixture, which is then separated in a two pressure distillation system. The figure below depicts the general structure of the plant.

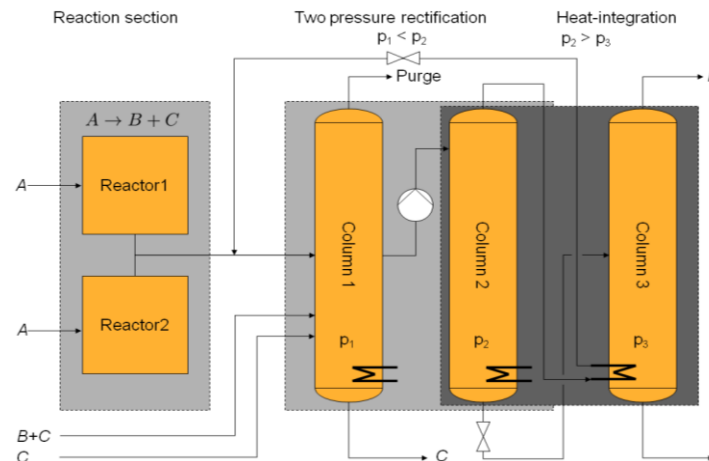


Figure 1: Simplified flow diagram of the industrial process of the BASF SE in Ludwigshafen, Germany

3.2 Process Model Development

In order to model this process, the BASF in-house process simulation program CHEMASIM is used, which is described by Hasse et al. (2006). To keep development time low, an existing process model is used. The process model consists of 35 process units, 72 process streams, and 18 heat streams. In total, 19 different components are considered. To determine whether the actual process is in steady state at the current operating point, a t-test is employed as an indicative method. When an operating point has been detected as quasi-steady state, parameter identification is started. Using a combination of a Gauß-Newton and a sequential quadratic programming (SQP) algorithm, presented by Schittkowski (2009), the parameters of the stationary process model are fitted to the measurement data of the current plant operating point. The required operating data is obtained from the BASF process information management system. For the additional calculations regarding optimization of the current operating point, an SQP method is used.

4. Results

In the following the results regarding the soft-sensor analysis and the process optimization are discussed. A detailed discussion on the accuracy of the reused model can be found in Müller (2011). The differences between model parameters and measurement values were generally below 0.5 %, which indicates that model predictions will be reliable.

4.1 Process Monitoring

With the help of the validated process model, non-measurable plant parameters are estimated. Among others are the fluid dynamics within column one and three. The goal of the analysis is to determine, if the current operating point is within the normal operating area and how far away the boundaries are located. The operating area with its boundaries for each tray is modeled using BASF's own equations based on theories presented by Mersmann et al. (2005) and Stichlmair and Fair (1998). Figure 2 is an

example of the operating area and displays the modeled F-factor of several operating points in which the process could be identified as being in steady state.

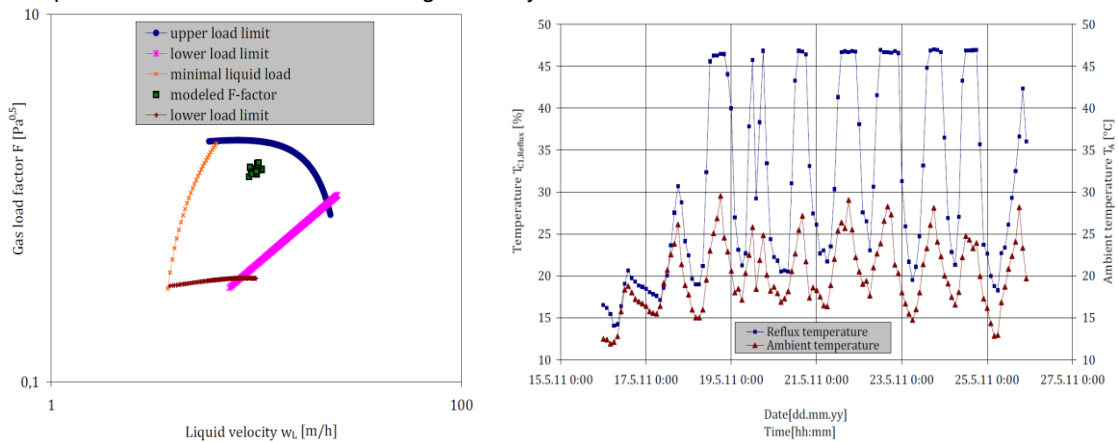


Figure 2: Operating area of the 72nd tray of column one with the modeled F-factor (left). Comparison of the temperature of the reflux stream at the top of column one with the ambient temperature (right).

Furthermore, the cooling capacity of the air coolers at the top of column one are investigated. The right-hand plot in Figure 2 compares the ambient temperature with the temperature of the reflux stream at the top of column one. Results show that the cooling capacity is a bottleneck for increased production on days with an ambient temperature greater than 25 °C, which becomes obvious by the temperature plateau of the reflux. Furthermore, it is also apparent that the ambient temperature is not the only influence parameter on the cooling capacity.

4.2 Process Optimization: Product Maximization

The first analyzed objective function is product maximization. Therefore, two questions are to be answered for the existing plant. Firstly, is it possible to produce a higher amount of product at the top of column 3 with the same amount of reactor feed? Secondly, if the reactor feed is implemented as an optimization variable, what are the boundaries of the system?

The main process optimization variables for the first analysis are the pressure at the top of column one, the boiler duty of column one, the side stream from column one to column two, and the reflux streams at the top of columns one and three. For the second analysis, the decision variables are the same as in the first analysis with the addition of the two feed streams to the reactors. The optimization results for the first analysis show that it is not possible to increase the product stream in a sensible way. The reason for this is that the specifications of the purities of the substances are very high. These specifications are already met by the actual plant. The second analysis on the other hand proves that the boundary for the goal of maximum production lies in the capacity of the reactors. These could be used to their full extent, thus enabling the possibility to produce more product. This result refutes the assumption that the fluid dynamics inside the columns are the boundaries for product maximization.

4.3 Process Optimization: Energy Cost Reduction

The second objective function is the energy cost reduction. The goal is to modify the operating point towards minimal cumulative steam costs. The decision variables are the reflux ratio of the side-stream of column one, the reflux stream at the top of column one, the tray temperature above the reboiler of column one as well as the temperature at a middle tray of column two.

The optimization is realized for various operating points from low to high production loads. The results show that if the operation of the plant is slightly changed, a maximum amount of about 14.5 % of energy could be saved. In order to achieve this performance, the optimizer first suggests to increase the reflux ratio at the side stream of column one. This can be seen in the left diagram of Figure 3. This automatically forces the reboiler in column one to increase its duty.

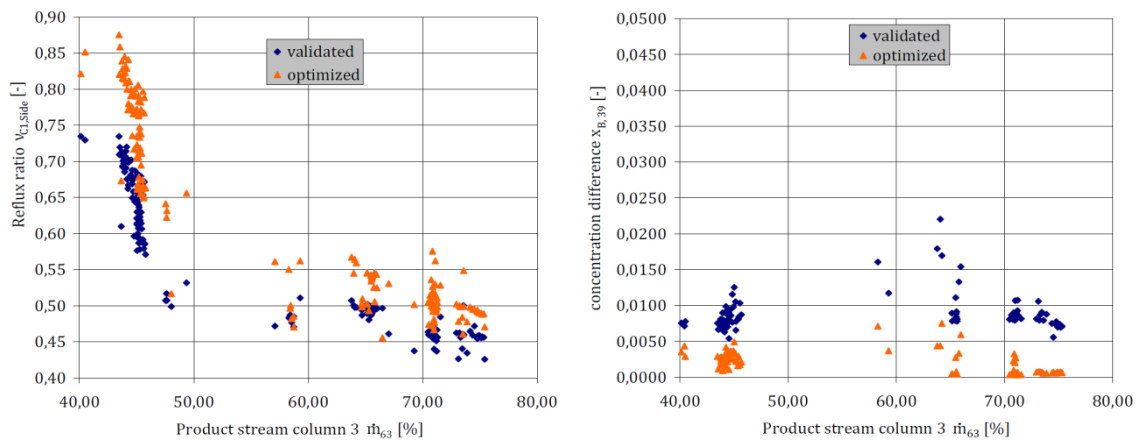


Figure 3: Increase of the reflux ratio of the side stream of column one (left). Difference in concentration between the azeotropic concentration and side stream concentration (right).

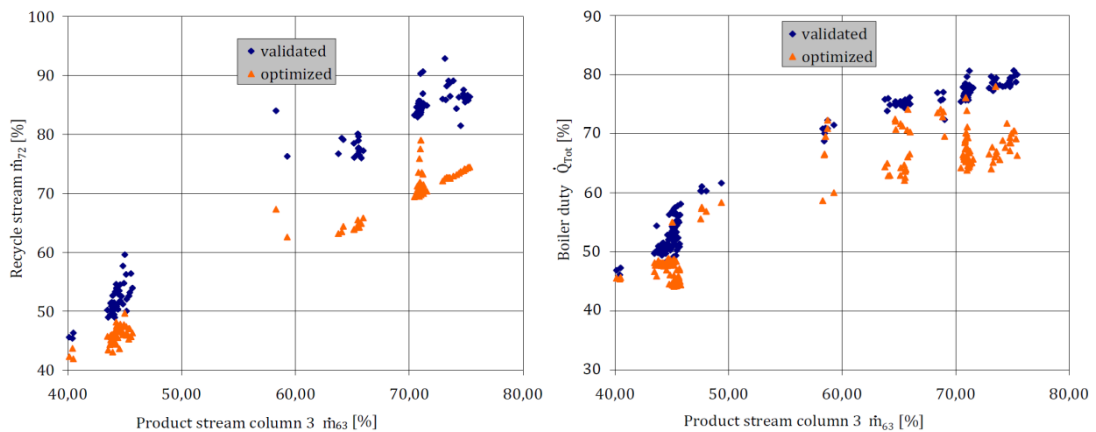


Figure 4: Plots of the reduction of the recycle stream for all operating points (left). Diagram of the reduction of the cumulative reboiler duty (right).

The concentration of product B at the side stream is then higher than in the operating point and the composition of the mixture closer to that of the azeotropic point. The right diagram of Figure 3 shows the difference in concentration between that of the side stream and the azeotropic concentration. With an increase in concentration of product B in the side-stream less of substance C flows to column two, thus reducing the reboiler duty in column two. Since the pressure in column two is higher than in column one, the energy of the reboiler duty is higher. That way, reducing the reboiler duty in column two leads to greater energy savings. Furthermore, as less of substance C is reboiled in column two, the recycle stream to column one is reduced. This decreases the reboiler duty in column one slightly. The left-hand plot in Figure 4 shows the reduction of the recycle stream. In total, this reduction leads to a decrease of reboiler duty of column one and two. The right-hand plot of Figure 4 depicts the cumulative energy for different product amounts. Depending on the production load of the chemical plant, 9.5 to 14.5 % of reboiler duty could be saved if the plant is operated according to the optimizers suggestions.

5. Conclusion

By reusing an existing model and applying a systematic strategy it was possible to effectively develop a validated online model for a chemical plant of the BASF SE in Ludwigshafen, Germany. The

technology platform was successfully applied for several investigations: process monitoring by a soft-sensor and real-time optimization. The fluid dynamics in the columns could be analyzed and it was possible to expose the cooling capacity of the air coolers as a bottleneck for increased production on hot days. Regarding the goal of process optimization, two different objective functions were investigated, namely: product maximization and energy cost reduction. Recent results have confirmed the success of the suggested operating points.

The application of this technology platform in the form of a validated process model poses great economic potential. On the one hand a significant cost reduction can be achieved by reusing existing models during the development phase and on the other hand soft-sensors are created, plant specific bottlenecks can be identified, and optimization of the operating strategies can be undertaken. Since the technology is quite new and few of these applications are existent for regular chemical plants, mainly heuristics exist to determine their economic potential beforehand. Therefore, the authors would like to motivate research in the preliminary determination of the economic potential of such a technology platform.

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