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Model Based Operation of Polymer Processes – What has to be Done?

Jens Bausa

Summary: 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 chemical engineering problems on the basis of rigorous process models at every office workplace. However, although in many cases process models are available from the process design step, model based operation of production plants can only be found rarely. Changing this situation would significantly contribute to the cost effectiveness of many production plants.This contribution focuses on the model based operation of polymer processes which are for some reasons not perfectly suited for model application: Polymer process models tend to be complex, meaningful online measurements are expensive and not always reliable, many polymer processes are performed in batch instead of steady-state and for most polymer plants, due to the smaller throughput, the economic impact of model application is much smaller than compared to for instance a steam cracker.When model based operation is considered, it has to be recognized that there is not one single approach but many different alternatives of which maybe only a single one will lead to a sustainable economical improvement of the process. From many successfully applied concepts for model based plant operation it can be clearly identified that always trying to implement the most complex solution (e.g. nonlinear closed-loop online optimization) is neither possible nor reasonable but that plant specific tailor-made solutions are necessary.

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

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 conceptual process design, detailed steady-state design of unit operations and dynamic process simulation for the development of control strategies.[1] From these tasks many process models are available and the next logical step is to use these process models for model based control concepts.

BASF AG, Ludwigshafen, Germany
E-mail: jens.bausa@basf.com

However, although there are numerous academic papers demonstrating the capabilities of model based methods and the potential economic benefit, these kinds of techniques cannot be found widely spread in the industry.[2] In fact, the level of application decreases drastically along the value chain of the chemical production processes: Almost all refineries are applying model predictive controllers (MPC), the set-points of many steam crackers are optimized with elaborated rigorous steady-state online-optimizers, but there are not too many polymer plants in which these kinds of techniques are applied.[3–7] A closer look on polymer processes reveals that the level of application also decreases from high throughput continuously operated processes to lower throughput batch-processes. As a matter of fact the percentage of model-based operated non-commodity batch-processes is almost zero.

If we believe that model based methods can significantly contribute to the profitability of our plants, it has to be asked, why the level of application is still that low and what has to be done to overcome this situation. Since this is a very complex question, the answer is not a simple one but starts with an analysis of the current situation: The following section presents the manifoldness of model based methods and the subsequent section discusses the application of nonlinear Model Predictive Control (nMPC) as the highest level of model based process operation from the industrial perspective. These sections can be understood as the first answer to the question, namely how the available methods and tools can be applied successfully. A second answer is given in the last but one section: What is still missing in our toolbox and has to be developed by academia and solution providers in close cooperation with the industrial end-users.

What Does Model Based Operation Mean?

Considering the whole life cycle of a chemical production process, ‘‘model based operation’’ means to apply process models during the production phase to improve the process. From this definition it is not fixed what kind of models are applied, where these models come from, what methods are applied, what the objective is, and if the application works online or off-line. Therefore, some clarifications seem to be necessary to categorize the broad range of model based methods.

What Kind of Models Can be Applied for Model Based Operation?

It has to be distinguished between rigorous process models and empirical, data-driven models. The advantage of rigorous process models is that they consist of physically meaningful balance equations (mass, energy, momentum) and algebraic equations describing the necessary physical and chemical phenomena (reaction kinetics, phase equilibrium, mass and heat transfer, diffusion, pressure drop, etc.). These kinds of equations incorporate the available process knowledge and can be applied to predict the process behavior even for process states at which the process has never been operated. However, the big disadvantage is the effort that has to be made to develop high quality rigorous models. For many processes this effort and the associated costs are prohibitive for operation concepts involving models.

The situation is the other way round for the empirical data driven approach. The effort to develop data driven models is small and is facilitated by modern Process Information Management Systems which allow to access process data from every office PC. Of course black box models do not allow to extrapolate the process behavior beyond the observed states and also do not provide insight into the cause-effect relationship.

A very promising approach is to combine these two classes in an hybrid model: Mass and energy balances are described by mechanistic equations and all phenomena which are too difficult to describe or not yet fully understood are described by means of data driven modeling techniques.[8] There are already commercial tools available on the market applying these techniques.

Does Model Based Operation Always Mean to Apply Dynamic Process Models?

If continuous plants are to be considered, steady state models can be applied to predict the plant performance and to optimize the operating point of the plant. The advantage of steady-state models is that they can be much more complex than dynamic models because the numerical effort is smaller compared to dynamic models. For example the steady-state online optimization of a steam cracker means to optimize a system consisting of about 150.000[6,9] equations whereas the optimization problem that has to be solved should not involve more than about 100 equations if nonlinear model predictive control is performed on a semi-batch polymer plant.

Where Do the Process Models Come From?

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.[10,11] In practice, the integrated use of models in automation and control, as illustrated in Figure 1, can only be found rarely so far. The reuse of existing models for process operation is restricted for several reasons. Existing models from process design are too complex and there is no model available with the necessary level of detail. So far there is no product on the market that generates simple models from detailed models. Another reason is the incompatibility of model representations between different software packages for online and off-line applications. All these obstacles lead to a situation in which models have to be developed individually for each online-application.[2,12]

How Can These Models be Applied?

There is a bandwidth from simple to very complex model applications. The most complex application is nonlinear model predictive control (nMPC) of polymer plants.[7] An nMPC application mainly consists of a nonlinear dynamic process model, a state observer and a dynamic optimization solver (Figure 2). Starting from the observed state of the system, a dynamic optimization is conducted that provides time profiles of one or more manipulated variables. From these time profiles only the first values are applied to the process and after a short time interval (e.g. about 10 seconds) the procedure starts again with new measurements. The advantage of nMPC is that highly coupled systems with multiple inputs and multiple outputs can be controlled under consideration of

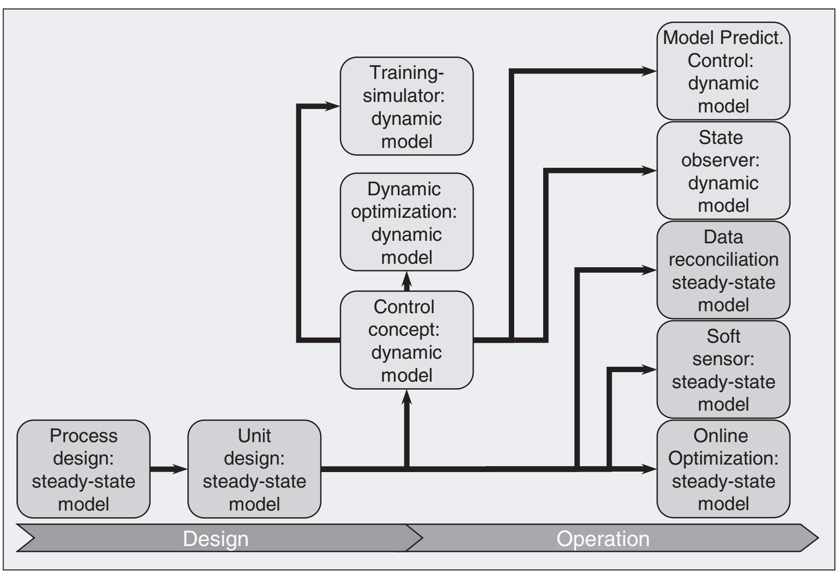

Figure 1.
Possible paths for the reuse of process models.

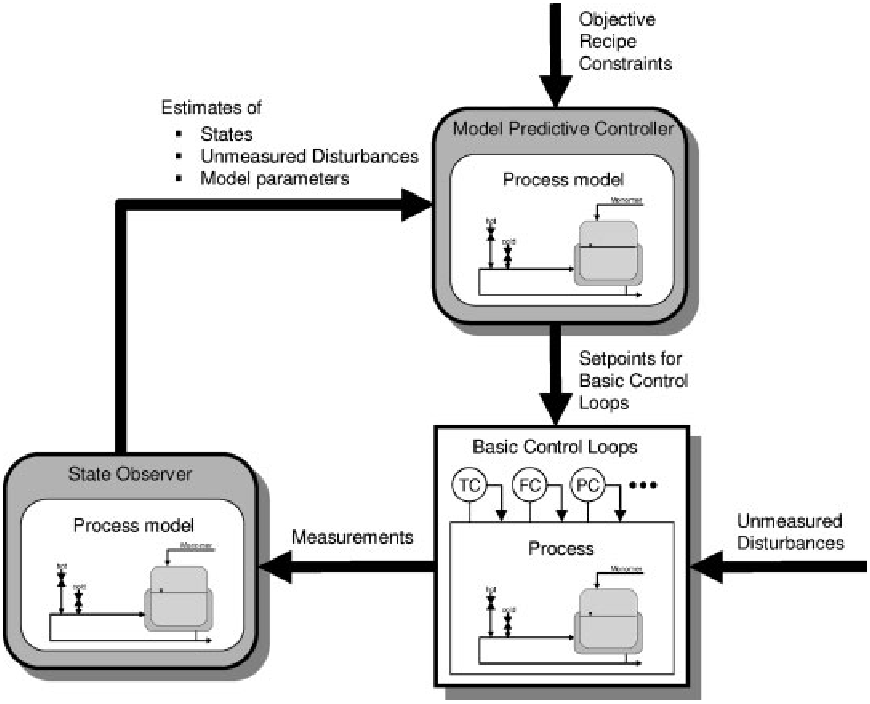

Figure 2.
Basic structure of a MPC application.

several constraints (e.g. restricted cooling capacity, plant safety considerations). However, the disadvantage is the big effort that has to be made to develop a model and to build an nMPC application. In particular for small processes the economic potential of the possible improvement is too low to justify the necessary capital spending.

If nMPC is not an option, it does not mean that model based operation methods are not applicable at all. For example it is very often possible to apply the observer which is always part of an nMPC as a stand-alone application. The observer consists of a process model that is simulated in parallel to the real process. Deviations between model output and measurements are fed into the model in a feedback manner to let model output and measurements converge. An observer gives information about the process that cannot be measured directly or that is too expensive to be measured. The additional information of the observer can be used in many ways: Estimations of heat transfer coefficients and instantaneous reaction heat rate can be introduced in the process control scheme as disturbance feedforward information to improve the control performance.[13–16] There are different observer methods available. Typically, the classical linear methods (e.g. Luenberger, Kalman Filter) are not applicable if the nonlinear characteristics of polymer processes have to be taken into account. Thus, modern nonlinear techniques like Extended Kalman Filter (EKF) and Moving Horizon Estimation should be considered for these tasks.[17,18] The advantage of the EKF method is that the calculations often can be directly implemented inside the Distributed Control System (DCS) of the plant without a need to couple a dedicated PC to the DCS. However, a major obstacle in the application of observers is that interesting process variables are not observable with the available measurements in the sense of control theory. Sometimes this leads to a situation in which additional (quality) measurements are needed but these measurements are either too expensive or already provide the information the observer was intended to deliver.

Online calorimetry is another interesting model application that gives access to the conversion ratio of a reaction system.[19–22] In the case calorimetry is applied by closing the energy balance (in contrast to heat flow calorimetry) then this method needs very accurate measurements but is relatively simple to implement for example in the DCS or a Programmable Logic Controller (PLC). Online calorimetry can also be applied to detect unsafe process conditions due to accumulated monomers and the danger of a runaway reaction. In the past, plant safety had to be guaranteed by pressure relief systems. Nowadays, model based safety systems are another option for safeguarding a plant.[23,24] In most cases the model based safety systems are not applied to increase plant safety, but aim for allowing to operate new types of processes with increased cost efficiency compared to conventional designs with the same, well established very high level of plant safety.

Does Operation Always Mean Online?

Process operation means how the existing plant equipment and the involved chemicals work together. For batch processes a large part of the operation of the process is determined by the recipe. Typically, recipes are not strictly fixed but have a certain degree of freedom that can be exploited to improve the cost effectiveness of the process. Applying dynamic optimization methods e.g. to minimize the cycle time by generating optimal trajectories for manipulated variables like feed flow rate and cooling water temperature should therefore be understood as an operation oriented model application. There are several simulation packages on the market that directly allow for dynamic optimization of polymer reaction systems. With general purpose process simulators (e.g. gPROMS, Aspen Custom Modeler) polymer systems typically are described with the method of moments, whereas PREDICI gives direct access to the molecular weight distribution.

Another promising approach is to improve processes from batch to batch.[25–27] Often it is much easier to find a correlation that relates some key measurements or measurement profiles to the final product quality than to develop a rigorous model for that purpose. In such a setup the model has access to lab results after the batch is finished and the correlations are applied to improve the recipe from batch to batch.

Nonlinear Model Predictive Control

Since almost two decades linear MPC solutions are available and applied in particular in the refinery and petrochemical industries.[5] In these linear MPC controllers most often the process dynamics are represented by Finite Impulse Response (FIR) or state space models. These models can be identified empirically by step-testing the plant behavior without any need to develop rigorous equations. An important property of linear MPC algorithms is that during the dynamic optimization step only a linear quadratic optimization problem has to be solved. The generally applied numerical algorithms always find a solution with a preliminarily known computational effort. The extension of linear MPC methods to be applicable to processes that cannot be described with linear models took several years and led to different types of nMPC algorithms.

Starting with continuously operated large scale refinery or petrochemical plants it seems natural to further develop the methods for the application on large continuously operated polymer plants: The continuous operation causes a system behavior with much less nonlinear characteristic than batch processes and the large throughput makes it much easier to set up an economically successful application compared to plants with less turnover. The nonlinearities that have to be considered mainly occur during grade change: A model that was identified for a special grade typically does not predict the correct process gains (ratio between input step height and process step response) when some other quality is produced. Thus, it is a logical step to extend the linear MPC algorithms gradually by slightly adding nonlinear model characteristics. This can be done by multiplying the linear model inputs with a nonlinear function (Hammerstein model) or to multiply the linear model outputs with a nonlinear function (Wiener model). The nonlinear functions often are neural nets that are trained with process data obtained by step-testing.

Nonlinearly extended linear MPC algorithms have already been successfully applied to polyolefin plants (LDPE, HDPE, PP). The tighter control on the process allows for higher throughput. Moreover, the improved control enables the plant personnel to change much faster from one grade to another grade minimizing the off-spec production in between. There are several commercial products on the market (e.g., Pavillion Process Perfecter, Aspen Tech. Apollo) and solutions for these kind of plants can be purchased as turnkey projects.

The situation is much more complex when it comes to batch or semi-batch processes.[4,7,28,29] In fact, there is no way to apply the methods described in the previous paragraph because the processes behave much more nonlinear and there is no steady-state in which some linear part of the dynamics could be identified by step testing. Therefore, the process model must have a completely different foundation which must be partially or completely mechanistic. The complexity of the underlying numerical optimization problem increases drastically. The nonlinear process model leads to a nonlinear programming problem which has much less favorable convergence properties: There might be more than one extremum, if the optimizer converges, it is not known how long it takes and the optimizer might not converge at all. Many extensions to standard algorithms are necessary to achieve a high level of robustness which is mandatory for an online application.[30,31]

In spite of the complexity, recently some commercial implementations have become available that are applicable in an industrial environment (IPCOS INC A for Batch, Cybernetica Cenit, Honeywell Profit NLC (formerly PAS)). The products are able to handle nonlinear process models that are based partly or completely on first principles. To facilitate the application of nMPC controllers on reaction systems without known kinetics, it is possible to implement hybrid models:[8] All easily describable phenomena (e.g., mass & energy balances, heat transfer) are implemented in the mechanistic part, whereas the complex reaction kinetics are modeled in a data driven manner. Since end user suitable modeling tools are missing and expert knowledge is necessary, applying these nMPC controllers always means to conduct a turnkey project with the service providers. The main advantages of applying nMPC to batch processes are that the variance of the process parameters and accordingly the variance of product quality can be decreased and that the process can be operated closer to the operation limits (e.g. maximum cooling capacity) resulting in higher throughput. Although these techniques are quite new, it is likely that many of the larger polymer batch plants will be equipped with nMPC controllers in the near future.

Obstacles to be Overcome

Although there are several different options for model based operation, many plants are still operated conventionally. Obviously, some difficulties have to be resolved to enable a broader level of application.

Availability of a Process Model

If no process model is available, then the project costs will increase, the time to conduct the project will increase and also the risk of being unsuccessful will increase because it is not always clear if the process characteristics can be modeled with the necessary accuracy. A promising approach are hybrid models that combine first principles models with data driven elements to accelerate the modeling step.[8]

Even if a process model is available, it can not be taken for granted that the existing model can be applied in the planned framework. The reduction of a very complex polymer reaction model providing a two dimensional molecular weight distribution to a simple method of moments model is almost as time-consuming as to start from scratch. What is still missing are modeling tools, that allow to handle different levels details and to export these different model representations, for instance in a generic equation format that can be implemented inside a DCS. Many of these unresolved issues have already been addressed almost 10 years ago.[32]

Profitability

It is essential to conduct a detailed analysis of the expected economic benefit. Modern Process Information Management Systems (PIMS) largely facilitate such studies by providing the necessary plant data. For the decision makers it must be evident, that there will be a fast payback of the capital expenditure. The payback time should not be much longer than one year, otherwise proposed projects tend to be canceled. Fortunately, many model based operation concepts are highly profitable and have typical payback times of less than one year.

Model Platform and Connection to DCS

For high-end online applications like nMPC, commercial turnkey solutions are available. The dedicated PCs that run the application are typically connected to the DCS via OLE for Process Control (OPC). If smaller applications are to be implemented, it is the first choice to run the model on the DCS because no additional equipment has to be connected and to be maintained. As soon as an implicit equation has to be solved iteratively, an external PC becomes necessary. Many modern DCS systems have a built-in OPC interface for this task. However, if a PC has to be connected to an older, not yet OPC-capable DCS, the costs for the interface of up to 50.000 Euro can be prohibitive in terms of project profitability.

It is also a problem that there is no general modeling and runtime environment with the necessary interfaces for small online model applications. Thus, such applications tend to be individual, single copy pieces of software that are much more costly to maintain than necessary.

Robustness

Chemical production plants cannot be simply switched off if some computer application does not work anymore or delivers useless results. This is in particular important for model based operation strategies that are much more complex than conventional PID-control loops. During the development phase a great effort has to be made to ensure the robustness of the application under any circumstances. It is always necessary to implement a fallback strategy that activates the conventional operation mode in case of a failure of the model, the connected PC, or the interface. Several high end model application projects failed because of robustness issues that caused the plant personnel to loose trust in the new technology.

Maintenance

Taking into account that production plants are modified frequently and models must be adjusted to correctly predict the process behavior, a maintenance concept for sustainable model application over several years must be developed. In case of a high-end online optimization project, maintenance is usually provided by the turnkey service provider delivering the application. Smaller model applications often are implemented by employees in research departments that frequently change to other positions in the company. Thus, for a successful project it has to be ensured that throughout the whole lifespan, the number of employees knowing about all technical details does not fall below a critical number.

Industrial Applications

Model Based Recipe Optimization

The task was to increase the production capacity for a product that is produced worldwide at different BASF sites. Some plants are equipped with modern DCS whereas other plants still have conventional panel mounted compact controllers. Although plants are located on different continents and differ in equipment, any new process operation strategy must be established at every plant in the same way to ensure the same product quality. This is a significant limitation and makes it unrealistic to propose the application of e.g. nMPC since the mandatory retrofitting of each old plant with a modern DCS would lead to an uneconomical overall project.

Fortunately, the process has a high level of reproducibility and there are no dominant disturbances. Thus, it is possible to perform an offline recipe optimization. The optimized trajectories (e.g. for reactor temperature) are then passed as set-point profiles to the conventional PID controllers. The less modern equipment is again a restriction that prohibits the implementation of complex trajectories. Only a sequence of different ramps is allowed.

The dynamic optimization was performed with gPROMS (molecular weight distribution modelled with momentum method) and PREDICI taking restrictions on the cooling capacity into account and enforcing that the molecular weight distribution must be identical to the base case. The results are displayed in Figure 3 and demonstrate that a reduction of the batch time by 25% was achieved. Of course it was not possible to apply the optimized recipes directly without validation by laboratory experiments, but even with considering the effort for validation the costs of the project were negligible compared to the economic benefit.

Model Based Safety System

Due to the economy of scale, competitive production plants are becoming larger and larger. For an exothermic batch or semi batch polymerization process the reactor size directly causes an increased accumulation of monomer and, as a consequence, a higher risk during a runaway situation. Traditionally, reactors are safeguarded by safety valves to ensure that the pressure does not reach values beyond the specification. However, for large-scale reactors the design calculations for safety valves suggest valves with a diameter larger than the reactor which is for obvious reasons not practical.

To operate these large-scale reactors safely, model based safety concepts can be applied. If the state of the system is directly related to one simple measurement (e.g. reactor pressure is a function of vapor pressure and molefraction of key component), only a moderate effort has to be made for implementing a model based safety system. Unfortunately, there are

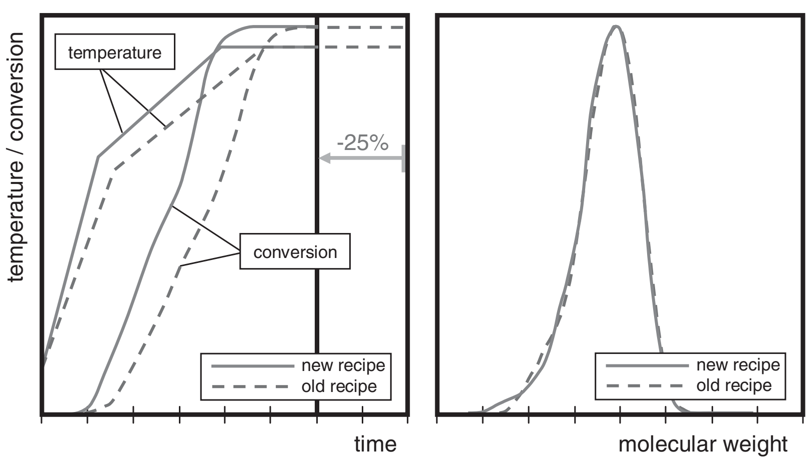

Figure 3.
Comparison of old recipe and results of dynamic optimization.

many relevant chemical reaction systems that do not allow the calculation of significant state information on the basis of simple measurements. In these cases the standard approach is online reaction calorimetry providing the instantaneous conversion ratio followed by a subsequent runaway calculation resulting in the adiabatic temperature and pressure.[23,24]

Although calorimetry as a method is very simple to understand and well established in research laboratories, it is a challenge to apply it in an industrial production environment if the plant safety has to be guaranteed in any circumstance 24 hours a day and 7 days a week. The main issue with calorimetry in an industrial production environment is to handle the extremely high requirements concerning the accuracy of measurement.

Figure 4 indicates the remarkable sensitivity of the calculated runaway pressure with respect to measurement errors. In this example, the calorimetry and adiabatic runaway pressure calculations were performed for three different scenarios: The plant measurements have been applied directly ($p_{\text{adiabatic}}$), measurements of cooling water temperatures and flow rate have been disturbed simultaneously in worst case direction to underestimate the adiabatic pressure ($p_{\text{adiabatic,min}}$) or in best case direction to overestimate the adiabatic pressure ($p_{\text{adiabatic,max}}$). Although high accuracy temperature sensors (PT100, class A, accuracy ±0.15 K) and flowmeters (accuracy ±0.9%) have been applied, in the worst case the adiabatic pressure is underestimated by about 25% at the end of the batch. Due to the integrating character of the method the measurement errors accumulate during the batch.

As a consequence of the high reliability requirements, in a project dealing with model-based safety systems only marginal effort is spent on developing the model and the basic calculation formulas. It is much more demanding to analyze the sensitivities, to design a reliable and self-monitoring instrumentation and to develop a comprehensive documentation of the safety concept that is needed for requesting an operating license at the concerned authorities. It is also obvious that the effort does not end with the implementation of the safety concept: Specially skilled personnel must be available in case of problems and when recipes are changed. However, the effort is worthwhile and necessary for achieving a competitive advantage compared to operating smaller plants safeguarded with conventional safety-systems.

Nonlinear Model Predictive Control of a Semi-batch Reactor

nMPC is by far the most complex application of process models. There are high demands regarding algorithms, software

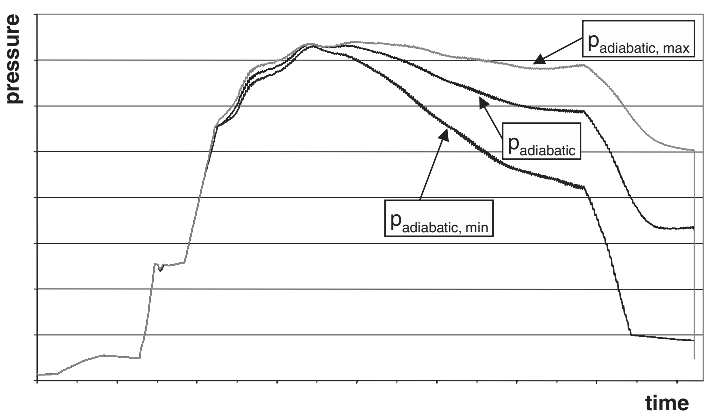

Figure 4.
Sensitivity analysis of the model based safety-system.

implementation, process model and process understanding. Since nMPC is a new technology it is very important to achieve a success with the first application. Otherwise in a big company it will be difficult to find any plant manager who is willing to give a technology a second chance that has proven to be unsuccessful or at least risky. Considering these facts it is the usual approach to apply new technologies in the lab scale first. At BASF nMPC has been successfully applied in pilot plant scale on a 0.1 m^2 reactor during an academic research cooperation three years ago. As a result of the successful lab scale application it was possible to find a plant that fulfills all necessary criteria for a first industrial application: Economic potential for improvement by increasing the production rate, only moderate quality constraints resulting in the necessary degree of freedom for the nMPC to improve the process, already existing process model, and modern instrumentation with all necessary measurements.

As a consequence of aiming for a sustainable process improvement only commercial solution providers (IPCOS, Cybernetica, Honeywell) have been considered for implementing the nMPC. The final decision between the different approaches provided by these companies was not only based on the technology, but a life-cycle analysis was performed considering project costs, risks, maintenance concept, and also technology in an integral approach. Results of this first industrial semi-batch nMPC project are expected at the beginning of 2008. From this example it can be concluded that it takes several years to introduce a new technology in industry and that an elaborated approach should applied. Being ahead of times might lead to short term improvements but the risk is high to deliver no sustainable success.

Conclusion

Model based process operation methods have a high potential to increase the cost efficiency of polymer production plants. Although these methods are not applied in every plant yet, there is a clear trend from large scale continuous plants to large scale and even medium scale batch plants. Depending on the specific process characteristics and economic potentials, methods for model based operation are scalable from high-end nMPC to relatively simple models running in parallel to the plant on the DCS to estimate unmeasured process variable and/or to predict product properties. It is very important to recognize, that trying to implement the most complex solution (e.g. nonlinear closed-loop online optimization) for every plant is neither possible nor reasonable but that process specific tailor-made solutions are necessary.

Several challenges are associated with implementing model based operation concepts in an industrial environment. A suitable model must be available, the model must be implemented in a robust way on a reliable, commercially available and affordable software platform, and the lifelong maintenance must be ensured. Because of these difficulties many achievements of academic research do not yet reach the industrial end-user.

The economic break-even for model based applications using the currently available methods and tools is still relatively high. To provide solutions for smaller polymer plants, intelligent methods and convenient software tools facilitating the modeling step are urgently needed to promote the technology more widely. 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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