ADVANCED PROCESS CONTROL FOR CHEMICAL BATCH REACTORS APPLIED TO A POLYMERIZATION PROCESS

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Introduction

Advanced Process Control ('APC') has become widespread and even a commodity tool for certain continuous processes. APC encompasses model based control solutions, where control and on-line optimization go hand in hand, and a Model Predictive Controller is often used for this purpose.

The advantage of this technology is straightforward: while delivering a significantly improved process control result, it enables to optimize your process on-line taking operational constraints into account.

However, until recently these tools could not be applied to chemical reaction batch processes. The reasons for this are twofold: on the one hand the general APC tools as applied in continuous processes cannot deal with the more complex nature of batch processes (changing dynamics, nonlinear responses). On the other hand the modeling effort and related cost would also be prohibitive to implement an APC project on batch processes with a reasonable return on investment. This would even be more true in a multi-product multi-reactor environment.

Therefore a new strategy has been developed for chemical batch processes. A hybrid modeling solution is proposed which needs a limited engineering input, and delivers a high precision representation of the process. The hybrid model contains both a rigorous mechanistic process description as well as a parametric part. The mechanistic part is used to model often encountered devices in a batch process, like half tube jackets, coils, external heat exchangers, condensers and an overall mass and heat balance. The parametric part is used to describe the reaction kinetics.

This non-linear model is then used within the Model Predictive Control solution. This solution contains an EKF based observer, as well as an interbatch control and observer solution.

Objective of the control solution is to deliver improved control performance, however in a lot of applications batch cycle time optimization is the prime objective. As such the reaction phase of the batch is minimized while keeping the process within the allowable constraints (available heat exchange duty, adiabatic temperature, quality aspects…).

The above mentioned APC methodology has now been applied to several industrial processes. An application case at CYTEC Industries Inc. is shown on a polyacrylate polymerization process.

Some observations on batch control challenges

Batch reactor processes are commonly praised for their flexibility. Indeed, with limited variety in hardware equipment, a wide range of products can be produced, ranging from performance polymers to specialty chemicals, from pharmaceutical intermediates to food ingredients. This flexibility however results in much more complex operation. Recipes must be defined and implemented, while production scheduling is a challenge in a multi-reactor multi-product environment. Also the control task can be more complex since the process can no longer be characterized having a single process gain, but the changing product characteristics throughout the batch cause the gains to vary dynamically. This nonlinear behavior has made traditional linear MPC technology inadequate for solving the problem. One can only conclude that a different type of model is required.

Different types of nonlinear models come to mind. On the one hand, one could choose very descriptive mechanistic models based on phase descriptions and heat and mass balances of all the components in the reactor. These models can give a very accurate description of all phenomena occurring within the reactor. To be able to be used within an APC application these models should have a guaranteed short calculation time, be stable at all times, be validated and tuned on the process, and have a limited numbers of states. Even more importantly, although not always trivial, they should contain a proper input-output description for control. One has to be sure that all relevant control degrees of freedom and interactions are well modeled. If all these criteria are met, a mechanistic model approach may be used.

The financial picture however looks a bit different if the rigorous model has to be developed from scratch for a specific APC application. This is especially true in a multi-product reactor, where a given recipe is only utilized a limited time per year. If the APC application is commissioned for that recipe, the payback should be generated on that recipe as well. To cut project costs, modeling efforts must be reduced as much as possible. A simple modeling technology requiring limited implementation time is needed.

APC for Batch applications

Standard techniques which are applied in continuous APC applications offer no solution for batch processes. In order to enable online optimization of batch processes, novel modeling and control techniques must be developed.

Dedicated Batch APC Models: Hybrid Modeling

Optimization is implicitly embedded in a Model Predictive Control solution. A process model is required that features a short design time and sufficient accuracy to be used within a control and on-line optimization application. For reasons explained above, a purely mechanistic model does not address these requirements. A black box approach, which represents the opposite extreme, is not straightforward either. Linear black box models do not work in a highly nonlinear application as a batch process. General nonlinear black box functions (e.g. neural nets) possess insufficient extrapolation capability. It is the assertion of the authors that a hybrid combination of mechanistic and black box modeling delivers the best of both worlds.

The envisaged model should give a good representation of the heat balance of the process. This will automatically include information on conversion, build up of unreacted feed material, and adiabatic run-away temperature and pressure.

In fact, most batch reactors share common principles. All of them use heat exchange devices, like jacketed reactors (half pipes or other design), coils or external heat exchangers. In some cases vapor builds up and a condenser is used. In a fed-batch or semi-batch reactor, mass is accumulated in the reactor while the reactor is being filled. All these principles can be modeled in a general mechanistic way that requires only a few parameters to be tuned to the actual process. This general mechanistic model can be applied to most batch reactors and drastically decreases the engineering time since one can take the advantage of general pre-built modules.

On the other hand the reaction scheme and kinetics, the phase behavior, etc. differ from process to process. Mechanistic modeling of these phenomena is the most time consuming part. Therefore a specific black box approach is chosen which uses a surface map to relate overall conversion and temperature to reaction energy or conversion speed (Figure 1). Some a priori knowledge is built into the map as well.

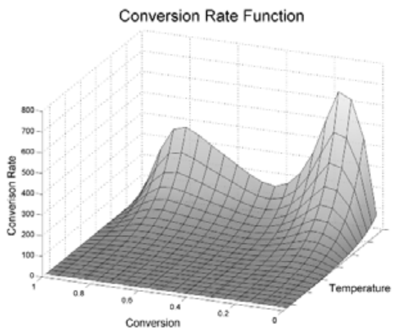

Figure 1. Reaction Surface Map

Experience with this method has revealed that combining the rigorous model part with the black box reaction part, results in a very accurate process model demonstrating nice extrapolation capability. All heat balance related issues such as reaction energy, conversion, reactant excess, and adiabatic temperature are taken into account. Design times are short as most of the information can be extracted from historical data and a limited number of tests on the process. Once a model has been validated on the process, generating extra models for new products on the same reactor is only a small effort.

Nonlinear MPC (NL-MPC)

Given the fact that the proposed model format is not standard and certainly nonlinear, traditional linear MPC principles, calculations, and procedures do not hold. A nonlinear MPC (INCA® for BATCH) solution is required.

The proposed strategy splits the NL-MPC problem into two stages: a prediction step and an optimization step. First a nonlinear prediction is made with the aid of the hybrid model. Based on the previous process inputs and the previous optimization result, a prediction emerges of the process behavior over a horizon into the future. Along this predicted batch trajectory a set of linear dynamic models is automatically provided. These models are combined into a linear time variant model (LTV model).

In the second stage this linear model is used to optimize the process. Based on the nonlinear prediction, the optimization observes the gap between where the process is heading and where the process is desired to be. The optimizer minimizes this gap by taking into account operating constraints on process inputs and process variables such as adiabatic temperature, and reactant excess. The model used during the optimization is the LTV model, enabling fast calculation speed since a QP algorithm can be applied. An Extended Kalman

Filter technology based observer modifies model states such that the hybrid model stays on track with the actual running batch.

In addition to the aforementioned optimization and observer, additional modules are optionally executed in between subsequent batches. Two of these modules are an inter-batch observer and an inter-batch controller. Both deal with phenomena which are only visible over longer time periods than one batch. The interbatch observer adapts the hybrid model in case of fouling or catalyst deactivation which only become tangible after several batch runs. The interbatch controller modifies the optimization targets and constraints from batch to batch to maintain the product at or within quality specifications. These specifications may be affected due to slowly varying feedstock quality and become visible only after a lab sample is analyzed after the batch has ended.

Application Example

INCA® for BATCH was applied on a water based polyacrylate process at CYTEC Drogenbos, Belgium. The site contains multiple workshops, amongst others a water based and solvent based polyacrylate process. It is a typical multi-product multi-reactor environment. The solvent based polyacrylate workshop counts 5 reactors covering 60 product grades, while the water based polyacrylate workshop produces 70 different product grades using 5 reactors.

The water based polyacrylate process is an exothermal fed batch process taking place under atmospheric conditions. A process lay-out is shown in Figure 2. Heat is exchanged by the means of a half-tubed jacket. The jacket temperature is controlled making use of a frequently applied configuration: a circulation loop with a fresh cooling water inlet to decrease the circulation water temperature and a heat exchanger to increase the circulation water temperature. Raw materials are dosed making use of premix vessels. An agitator is used to achieve proper mixing.

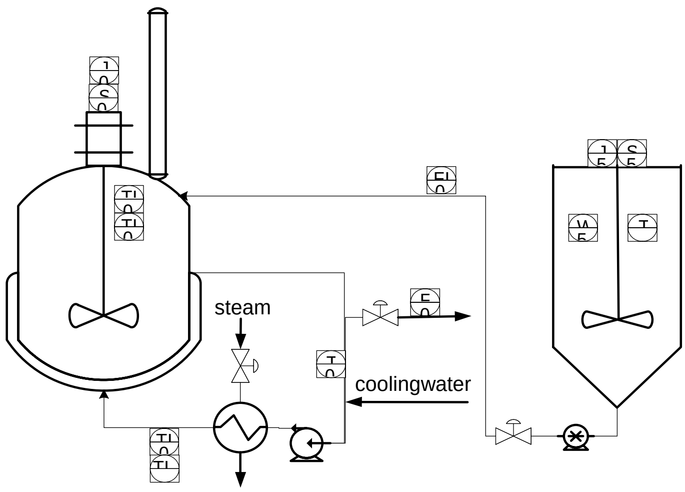

Figure 2. Batch reactor Layout

The project was implemented via a number of phases. In order to gather data for model development, a logging environment was set up to enable data logging at high sample rates without data compression. The logging software was installed on a PC and connected to the plant DCS via OPC. The next stage demonstrated significant benefits of the hybrid model approach. If using traditional model identification techniques, tests spanning many batches would have been required but the hybrid model approach only required tests to be executed during two batches. During a first batch a slightly elevated temperature profile was used. In a second batch a step disturbance was applied to the reactor feed flow (Figure 3). Both experiments were discussed thoroughly with key process engineers. The amplitudes of the applied changes were selected such that they would have minimal impact on the process operation and especially the batch-end quality, while the effect would still be observable in the measurements.

In a next step the hybrid model was identified. This was largely done based on historical data, enriched by the data delivered by the above described tests. The resulting reactor temperature profiles (hybrid model versus measurements) for two different product grades are shown in Figure 4. Hybrid model derivation for extra product grades becomes a smaller task, since large parts of the models can be reused.

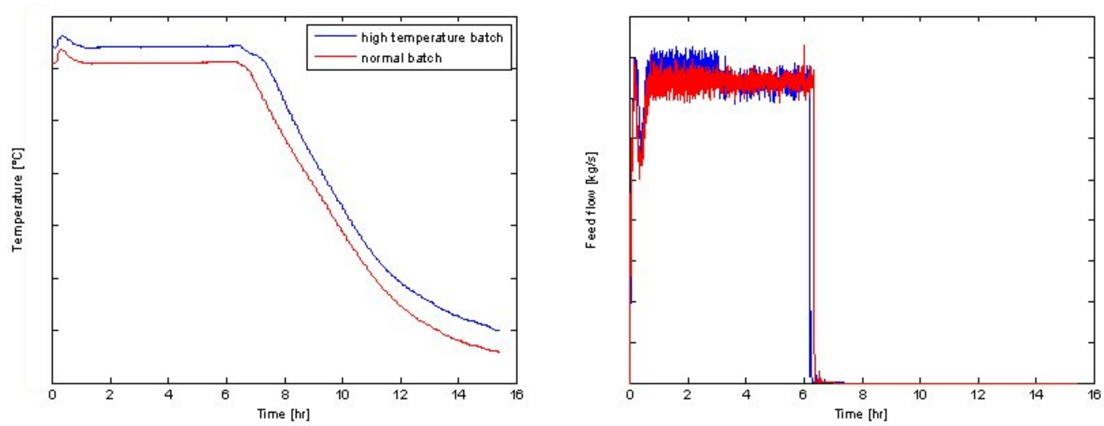

Figure 3. Applied tests to identify hybrid model

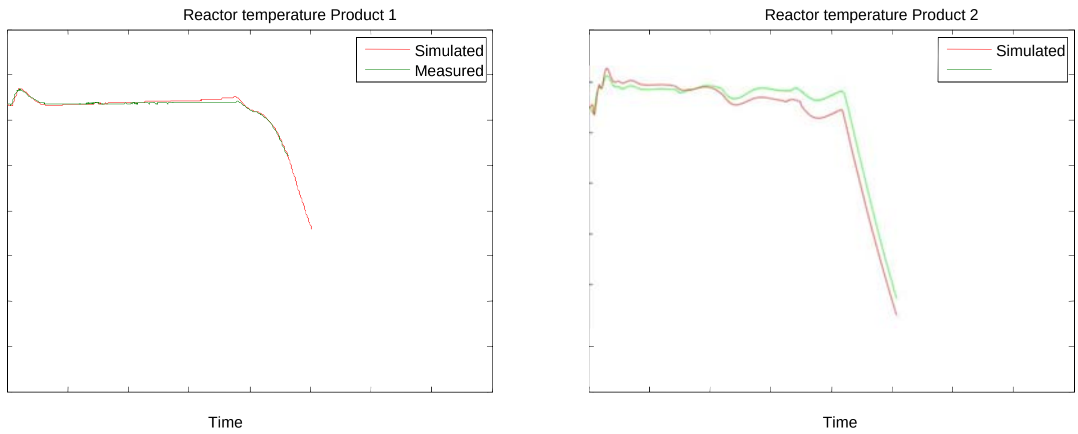

Figure 4. Modeling Results

Comparing to the measured signal, one can notice a slow drift on the model simulation for the second product shown in Figure 4. To improve model predictions, an Extended Kalman Filter based observer is tuned. The observer updates model states such that the model stays in track with the process despite unmodeled disturbances and model shortcomings. Next, a complete offline simulator was set up, consisting of a controller, an observer, and a modified hybrid model to represent the process-model mismatch. Based on this environment, controller tuning was performed and several process scenarios were analyzed. This simulator was then used for the Factory Acceptance Test where satisfactory performance for multiple case studies and sensitivity analyses was demonstrated. The control environment supports a broad set of different product grades, each represented by its dedicated hybrid model.

Due to the computationally intensive calculations required by the technology described in this paper, the controller is implemented in a separate, dedicated PC. This PC is typically connected to the process DCS or PLC via OPC. A separate interface is designed on the control system operator screen to permit the operator to interact with the application. Under normal operation, batch parameters are defined when the batch recipe is scheduled. It is especially worth noting that this is also when the choice to utilize MPC is defined. The recipe ensures that DCS/PLS controllers are switched into the proper input mode (local, remote, supervisory) and the MPC controller is then automatically started at the proper moment. At any given moment the operator can decide to switch off the MPC controller, and then a fallback is initiated towards a safe PID control solution. In rare cases of PC hardware, communication, or software malfunction the fallback is also triggered by means of a watchdog timer.

The results for two different product grades are discussed next. In Figure 5 the implementation results are shown for a first product grade. In this case limited operational freedom was available due to product quality related constraints. Therefore the focus was geared on batch reproducibility and product consistency. It is shown that a hybrid model predictive approach enables a tight process control, reducing the variance dramatically compared to conventional PID control. Mainly the overshoot at the start of the introduction phase was recognized as being critical to control the desired product end-quality parameters. Elimination of this overshoot was therefore essential to improve product consistency.

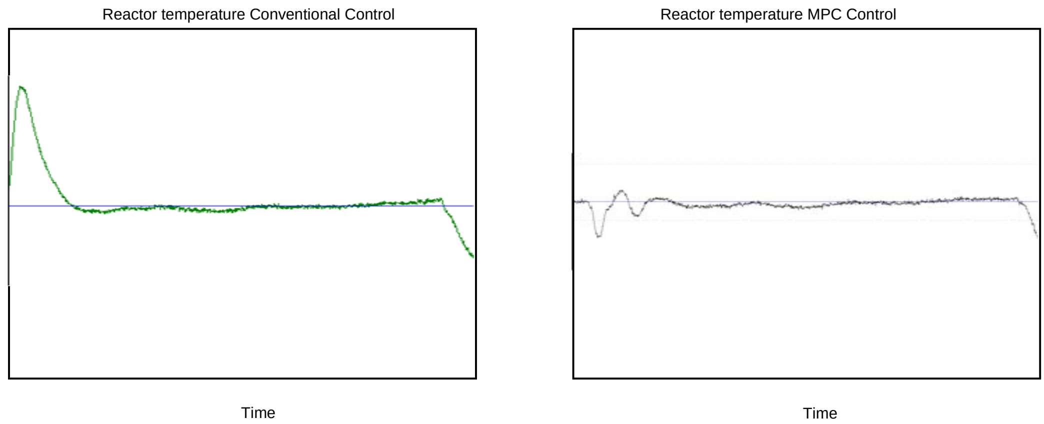

Figure 5. MPC results for polyacrylate product grade 1

In Figure 6 the results for another product grade are shown. In this case the focus was directed upon batch cycle time reduction. The MPC controller is configured such that the feed flow is maximized, while guaranteeing that at the current time instant and in the future the available cooling power will not be exceeded. The eventual control result shows an operation switching between the cooling constraint and the feed flow constraint, while keeping the process temperature on the setpoint. As a result 60 minutes batch cycle time is eliminated.

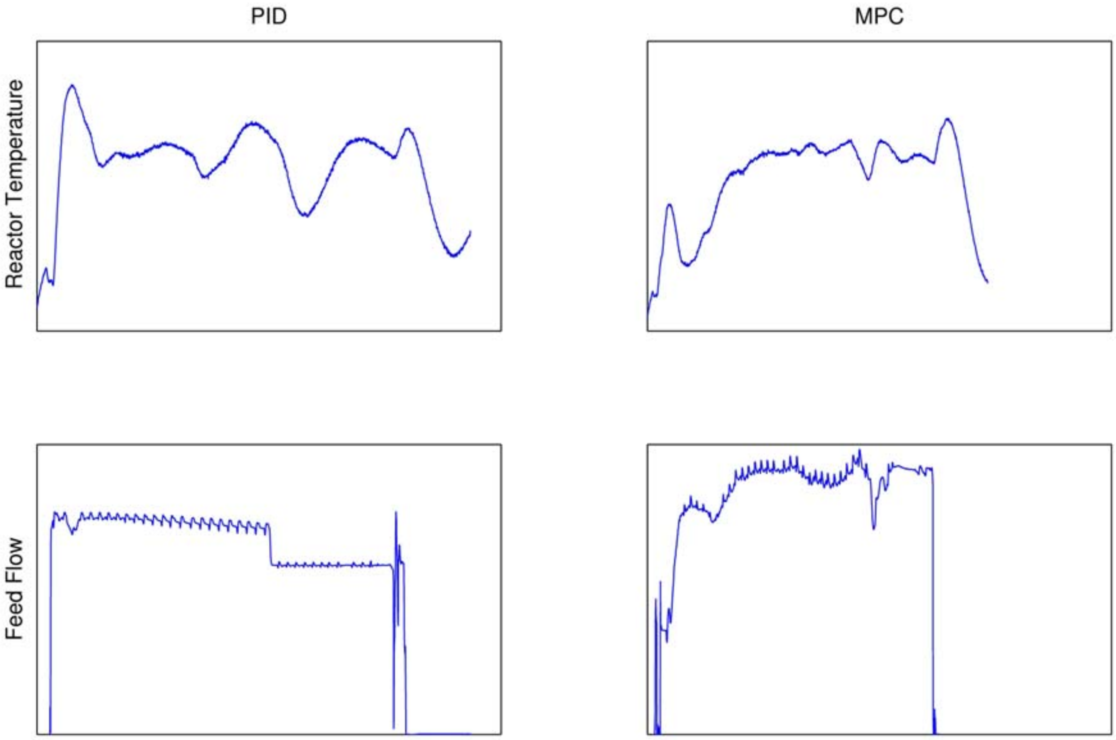

Figure 6. MPC results for polyacrylate product grade 2

Conclusion

In this paper an industrial application is shown of a hybrid non-linear model predictive control technology. The solution is specifically geared towards batch reactor systems, and aims at achieving two goals. At first a technical solution is provided to address the non-linear dynamical complexity of a batch reactor, encompassing a modeling and optimizing control solution. Secondly, the technology is set up to minimize modeling and configuration time, in order to achieve acceptable payback time in an industrial multi-reactor multi-product setting. Industrial results for different polyacrylate product grades show enhanced batch reproducibility and significant cycle time reduction.