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Realization of online optimizing control in an industrial semi-batch polymerization

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ABSTRACT

In this work, the realization of an online optimizing control scheme for an industrial semi-batch polymerization reactor is discussed in detail. The goal of the work is the automatic minimization of the duration of the batch without violating the tight constraints for the product specification which translate into stringent temperature control requirements for a highly exothermic reaction. Crucial factors for a successful industrial implementation of the control scheme are the development and the validation of a process model that is suitable for process optimization purposes and the estimation of unmeasured process states and the online compensation of model uncertainties. Two implementations are proposed, a direct online optimizing control scheme and a simplified scheme that combines a model-predictive temperature controller and a monomer feed controller that steers the cooling power to a predefined value in a cascaded fashion. We show by simulation results with a validated process model that both schemes achieve the goals of tight temperature control and reduction of the batch time. The performance of the NMPC controller is superior, on the other hand the cascaded scheme could be directly implemented into the DCS of the plant and is in daily operation while the online optimizing scheme requires an additional computer and is currently in the test phase.

1. Introduction

Linear MPC (Model Predictive Control) was first proposed and implemented in the 1970s by Cutler and Richalet. Since then, it has emerged as the standard solution for multivariate high performance control problems in the chemical industry, especially in the petro-chemical sector. This technique was successfully applied in real production units long before it was well understood from the theoretical point of view. By now linear MPC is quite mature and it is routinely applied in industry [1]. However, as in the chemical industry most of the process dynamics are inherently nonlinear, linear models are often only capable to describe the behavior of the processes accurately near a fixed operating point. Especially in time-varying processes as batch and semi-batch processes with tight operating windows, linear MPC may fail to deal provide sufficient control performance. In such cases, the use of nonlinear models may improve the operation of the process, because the safety margins due to model inaccuracies can be reduced. Therefore, the use of NMPC (Nonlinear Model Predictive Control) has been motivated by the growing demands on process economics under tighter product quality specifications and environmental regulations. While the structure of MPC enables a straightforward extension by employing nonlinear models in the optimization over a finite prediction horizon, in contrast to the linear case, the resulting problems are usually non-convex and numerically demanding. A solid theoretical background has also been developed for NMPC over the last decades [2,3] and several successful applications in real systems have been reported [4,5]. But, despite of the effort that has been made, there are still several obstacles to be overcome for the implementation of NMPC controllers in real production units, in particular the need for accurate models or online compensation of model inaccuracies and the robustness of the online optimization under significant uncertainties. Therefore the utilization of NMPC in industry is still quite limited.

During the last years, it has been realized that the potential of MPC can go far beyond tracking references and rejecting disturbances. Instead, economic cost functions that are usually only considered in an upper steady state real time optimization layer can be optimized within the MPC formulation. This enables the possibility of updating the operation point or the trajectories to external factors (like changes in the availability of utilities or in the cost of the raw materials) online during the process operation, resulting in what is called DRTO (Dynamic Real Time Optimization) or online optimizing control [6]. Dynamic online optimization can also be realized by using economics-motivated cost functions

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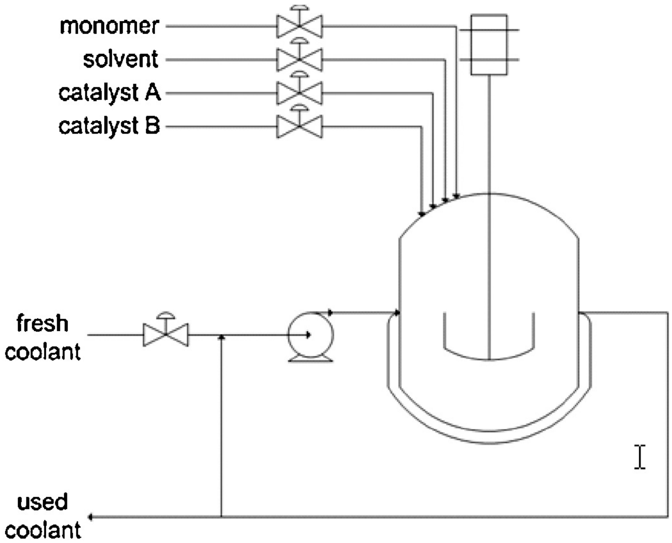

Fig. 1. Scheme of the industrial polymerization process.

or by tracking necessary conditions of optimality [7]. Our NMPC controller follows this approach by maximizing the monomer feed online over a finite prediction horizon.

In this work, which is an extended version of [8], the challenge of implementing an optimizing NMPC controller in a real production unit is addressed using an industrial semi-batch polymerization process as a case study. An online optimizing NMPC scheme that simultaneously optimizes the cooling power and the monomer dosage is proposed and thoroughly tested in simulations. Because of a simpler implementation and good robustness properties that have been shown in [9,10], a simplified batch time minimization scheme that combines a scalar MPC temperature controller and a monomer feed rate controller is also investigated. The effectiveness of both control schemes is illustrated by simulations and by results taken from the application at the real plant. Crucial factors for a successful industrial implementation of the NMPC, as the development and validation of a process model that is suitable for online optimization purposes, the estimation of unmeasured states and the online compensation of uncertainties, are discussed in detail.

After this introductory section, the remainder of the paper is organized as follows. In Section 2, the industrial polymerization process is described, different control schemes that have been proposed in the literature are briefly discussed and the need for an advanced control solution is exposed by means of historical process data. In Sections 3 and 4 issues regarding the development, calibration and validation of a semi-rigorous process model are discussed. Aiming at using the model for online optimization of the batch operation, the issues of state estimation and online compensation of model errors are dealt with in Section 5 and a NMPC scheme for the online optimization of the process is proposed and investigated in the Section 6. In Section 7, the improvement of the currently used control solution is revisited on the basis of the developed process model and the alternative optimizing scheme that can be easily implemented in the DCS is introduced and real results from the plant are shown. Conclusions are drawn in Section 8.

2. Process description and motivation

The unit investigated in this work is an industrial semi-batch polymerization reactor that produces a liquid polymer with a relatively low molecular weight in a catalyzed solution polymerization. The reactor system, which is schematically shown in Fig. 1, is composed of the reactor vessel where a solution polymerization reaction takes place, a mechanical stirrer that keeps the reactant mixture homogeneous and a cooling circuit that removes the heat of reaction. The reactor is equipped with four inlet ports through which solvent, monomer, and two catalyst components can be independently dosed into the reactor.

As it is usual in the chemical industry, this reactor is used to produce different commercial polymer grades which, in this case, differ from each other by the polymer viscosity. Since this property is mainly determined by the temperature at which the polymerization takes place, a precise temperature control is required to ensure that the end-product will have an acceptable quality. Currently, the product quality is checked by off-line measurements of the viscosity of the product. The different products are obtained by different recipes that can be generally described by the three following steps. Firstly, during the pre-reaction step, the two catalyst compounds and a certain amount of solvent are inserted into the reactor. During the feeding or reaction step, monomer and solvent are continuously fed into the reactor, the polymerization starts and the reactor temperature is raised to the desired value. Finally, during the holding step, the monomer feed is stopped and the reactant mixture is kept inside the reactor for a pre-established period such that a high monomer conversion (low residual monomer content) is achieved.

The standard operation strategy for this process consists in running the batch with constant monomer feed during the whole reaction period while a cascade of PID controllers, which is illustrated in Fig. 2, takes care of controlling the reaction temperature to the desired value. Although this operation strategy has been successfully applied during the last years, several difficulties related to the control of the reaction temperature (especially at the beginning of the reaction period) have been reported by the operators. In Fig. 3, some real process trends are presented in order to illustrate potential for improving the operation and control of the process.[1]

These process trends show that, for both products, a relatively large temperature peak (which has a negative impact on the product quality) is observed at the beginning of the reaction period. For Product B, the system can be operated with the maximum monomer feed rate during the whole batch and the cooling constraint is not active (the opening of the cooling valve is below 50% during almost the whole reaction period). There is a relatively large temperature peak at the beginning of the reaction period, but the controller can then bring the reaction temperature back to the setpoint without intervention. For Product A, the cooling constraint becomes active at the beginning of the feeding period. When the temperature peak occurs, the maximum cooling power is reached and the operators are forced to reduce the monomer feed to bring the system under control. After the intervention by the operator, the system is operated close to the limit of the cooling capacity and during most of the reaction period the quality of the temperature control is not good. An alternative for eliminating the temperature peak is to feed the monomer more slowly into the reactor. This could improve the product quality but would also increase the batch duration, which is not desired. The problem of finding the right compromise between the quality of the temperature control and the batch duration, i.e. to choose the velocity at which the reactants are fed into the reactor, is a well-known problem in the operation of semi-batch reactors. Several possible control schemes to handle this challenge can be found in the literature. For example, [8,11,12] investigate the idea of maximizing the monomer conversion by tracking optimal trajectories that were computed offline by manipulating the reactant feed and the jacket temperature. In semi-batch emulsion polymerizations, usually a

[1] Note that, for confidentiality reasons, all the values are scaled.