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Real-Time Feasibility of Nonlinear Predictive Control for Semi-batch Reactors

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Abstract

In this work a nonlinear model predictive control scheme for on-line optimization of semi-batch reactors is presented. Since the true process optimum occasionally lies on a boundary of the feasible region defined by one or more active constraints, the process is forced into an infeasible region due to the uncertainty in the parameters and measurement errors. An alternative new approach is proposed to assure both robustness and feasibility with respect to input and output constraints. This approach is based on the backing off of the constrained output variable bound along the moving horizon. With this strategy, a trajectory of mathematical constraint limits will be formed. The trajectory of these bounds is dependent on the amount of measurement error and parameter variation including uncertainty. The performance of the proposed approach is assessed via an application to a semi-batch reactor under safety constraints, where a strongly exothermic series reaction conducted in a non-isothermal batch reactor is considered to show the analytical steps of the approach, and to demonstrate the efficiency of the proposed online framework.

Keywords: NMPC, Output-Constraints, Dynamic Real Time Optimization, Batch Processes, Safety.

1. Introduction

Batch processing provides greater flexibility in the production of specialty and pharmaceutical chemicals. The trend in the chemical industry towards high value products has increased interest in the optimal, model-based control of batch processes. These control problems are generally posed as tracking problems for time-varying reference trajectories defined over a finite time interval. However, during the course of a typical batch, process variables swing over wide ranges and process dynamics go through significant changes due to nonlinearity. Furthermore, batch processes are characterized by significant uncertainties, a certain number of noisy measurements and the fact that the controlled properties are usually not measured on-line. Therefore, the potential advantages of a model based control system are likely to lead to significant tracking errors. With the aim of dealing with model uncertainties and process disturbances, the optimal control problem can also be solved on-line. The on-line

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optimization problem is generally non-convex for NMPC. Thus, practical implementation of NMPC becomes difficult for any reasonably nontrivial nonlinear system (Mayne D. Q., 2000). However, critical issues are robustness and the feasibility of the optimization problem, i.e. the presence of an input profile that satisfies the constraints. In this contribution an alternative new approach is proposed to assure both robustness and feasibility with respect to input and output constraints.

2. Problem Formulation

A strongly exothermic series reaction conducted in a non-isothermal batch reactor is considered to demonstrate the efficiency of the proposed online framework. The reaction kinetics are second-order for the first reaction producing B from A, and an undesirable consecutive first-order reaction converting B to C. The intermediate product B is deemed to be the desired product. Since the heat removal is limited, the temperature is controlled by the feed rate of the reactant A and the flow rate of the cooling liquid in the nominal operation. The reactor is equipped with a jacket cooling system. At the start, the reactor partly contains the total available amount of A. The remainder is then fed and its feed flow rate is optimized to maximize the yield. However, the accumulation of A at the start of the batch time must be prevented, otherwise, as the batch proceeds; exhaustion of the cooling system capacity can not be avoided. Furthermore, whilst the reaction proceeds, the reactor's volume diminishes so that the computation of the corresponding cooling capacity is adapted according to the remaining cooling jacket area. The developed model takes in both the reactor and the cooling jacket energy balance. Thus, the dynamic performance between the cooling medium flow rate as manipulated variable and the controlled reactor temperature is also included in the model equations. Thereby, it can be guaranteed that later the computed temperature trajectory can be implemented by the controller. Moreover, by this means the limitations of the cooling system (pump capacity) can explicitly be taken into account for the optimization. The resulting model comprises 5 differential states, 2 algebraic state variables, and 3 time-varying operational degrees of freedom.
The objective is to maximize the production of C_B while minimizing the total batch time subject to diverse operational, quality as well as safety related constraints during the batch and at its final time. The objective function then reads:

$$\min_{\dot{V}_{cool},Feed,\Delta t} \left(-C_B\left(t_f\right)+\zeta\cdot t_f\right) \quad \text{with} \quad \zeta=\frac{1}{70} \tag{1}$$

There are path and end point constraints for the reaction process to be fulfilled by the open-loop optimal recipes. First, a limited available amount of A to be converted by the final time is fixed to $NA_{tot}(t_f)$=500mol. Furthermore, so as to consider the shut-down operation, the reactor temperature of at the final batch time must not exceed a limit.

$$T_r\left(t_f\right) \leq 303\ K \tag{2}$$

There are path constraints for the reactor temperature and the adiabatic end temperature

$$T_r\left(t\right) \leq 356\ K \tag{3}$$

$$T_{ad}\left(t\right) \leq 500\ K \tag{4}$$

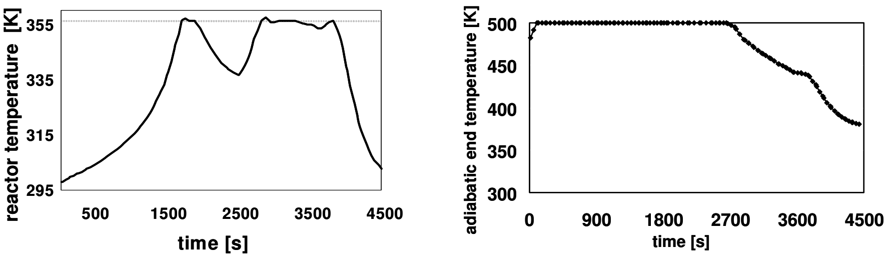

Figure 1. Path constraints: Reactor temperature (left) and adiabatic end temperature (right).

T_{ad} is used to determine the temperature after failure (Abel and Marquardt, 2000). Additionally, the cooling flow rate changes from interval to interval are restricted to an upper bound

$$abs\left[\dot{V}_{cool}\left(k+1\right)-\dot{V}_{cool}\left(k\right)\right] \leq 0,05 \tag{5}$$

The decision variables *u(t)* are the feed flow rate into the reactor, the cooling flow rate V_{cool}, and the different time intervals. A multiple time-scale strategy based on the orthogonal collocation method in finite elements is applied for both discretization and implementation of the optimal policies according to the controller's discrete time intervals (6-12s; 600-700 intervals). The resulting trajectories of the reactor temperature and the adiabatic end temperature for which constraints have been formulated are depicted in Fig. 1. It can be observed that during a large part of the batch time both states variables evolve along the upper limit. The adiabatic end temperature, in particular, is an active constraint over a large time period. Although operation at this optimum is desired, it typically cannot be achieved with simultaneous satisfaction of all constraints, because of the influence of external disturbances (Loeblein and Perkins, 1999). Thus, an NMPC based approach is proposed to implement such an optimal strategy despite disturbances.

3. Nonlinear Model Predictive Control

NMPC provides a systematic methodology to handle constraints on manipulated and controlled variables not being limited to a certain model structure. However, for the online optimization of the semi-batch process, the momentary criteria on the restricted controller horizon with regard to the entire batch operation are insufficient. Therefore, the original objective (eq. 1) must be substituted by an appropriate alternative which can be evaluated on the local MPC prediction horizon.

$$\min_{V_{cool}} \; J \; \left(\mathrm{N}_1, N_2, N_U\right) = \sum_{j=N_1}^{N_2} \delta(j) \cdot \left[\hat{y}(t+j \mid t) - w(t+j)\right]^2 + \sum_{j=1}^{N_U} \lambda(j) \cdot \left[\Delta u(t+j\text{-}1)\right]^2 \tag{6}$$

The optimization objective is reduced to a tracking problem. The first term stands for the task of keeping as close as possible to the calculated open loop optimal trajectory of the reactor temperature, whereas the second term corresponds to control activity under the consideration of the systems restriction's described above. Both reactor temperature and adiabatic end temperature are defined as hard-constraints. However, it is well known that hard output constraints can cause problems for two reasons: the optimization can become infeasible, and some of the constraints must then be relaxed or

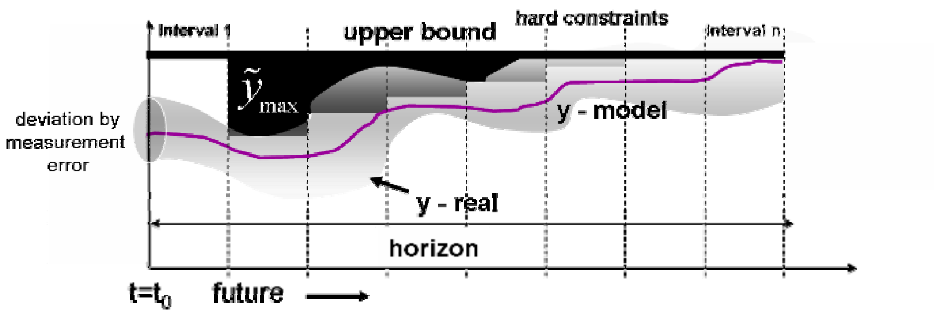

Figure 2. Back-off strategy within moving horizon.

eliminated. In the latter both approaches rely on relaxation which is, in fact, inapplicable for safety restrictions. In this work an alternative new approach is proposed to assure both robustness and feasibility with respect to input and output constraints. This approach is based on the backing-off of the bound of the hard-constrained output variable along the moving horizon (8intervals). Thus, a trajectory of mathematical constraint limits will be formed. For the near future time points within the horizon, these limits (bounds) are more severe than the real physical constraints and will gradually be eased (logarithmic) for further time points (see Figure 2). The trajectory of these bounds is dependent on the amount of measurement error and parameter variation including uncertainty.

The back-off strategy is introduced into the optimization to guarantee that the safety restrictions are not violated at all when the calculated trajectory is applied to the batch process. The basic idea is shown in Fig. 3. The true process optimum lies on the boundary of the feasible region defined by the active constraint. Due to the uncertainty in the parameters and the measurement errors, the process optimum and the set-point trajectory would be infeasible. By introducing a back-off from the active constraints in the optimization, the region of the set-point trajectory is moved inside the feasible region of the process to ensure, on the one hand, feasible operation, and to operate the process, on the other hand, still as closely to the true optimum as possible.

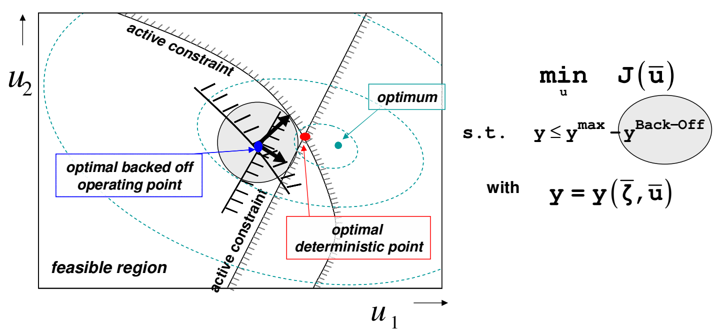

Figure 3. Back-off from active constraints

Table 1.Objective function parameter and hard-constraints back-off.

T_P	prediction horizon	8 intervals
T_C	control horizon	8 intervals
λ	MV variation weighting factor	3000
δ	offset weighting factor	$\alpha^{(\mathrm{Tp-j})}$ with $\alpha=0,7$
T_{max}	maximum allowable Reactor temperature $T_{max}=356K$	$T_{\max}\left(j=2...8\right)=T_{\max}^{offline}-\tilde{T}_{\max}.\alpha^{(j-2)}$ $with\quad \tilde{T}_{\max}=4K,\quad \alpha=0.5$
T_{ad}	maximum allowable adiabatic end temperature $T_{max}=508.5K$	$T_{\max}\left(j=2...8\right)=T_{\max}^{offline}-\tilde{T}_{\max}.\alpha^{(j-2)}$ $with\quad \tilde{T}_{\max}=3K,\quad \alpha=0.5$

For the formulation of the NMPC-based online optimization, the objective function parameters (eq. 6) and the hard-constraints back-off are presented in Table 1, respectively. The decision variable is again the cooling flow rate. In order to compare the performances of the open-loop nominal solution and the nominal NMPC with the proposed on-line framework under uncertainty, different disturbances have been considered, namely: catalyst activity mismatch and fluctuations of the reactor jacket cooling fluid temperature. Additionally, all measurements are corrupted with white noise e.g. component amount 8%, Temperature 2%.

4. Dynamic Real-Time Optimization

The size of the dynamic operating region around the optimum (see Figure 3) is affected by fast disturbances. These are, however, efficiently rejected by the proposed regulatory NMPC-based approach. On the other hand, there are, in fact, slowly time-varying non-zero mean disturbances or drifting model parameters which change the plant optimum with time. Thus, a re-optimization i.e. dynamic real-time optimization (D-RTO) may be indispensable for an optimal operation. When on-line measurement gives access to the system state, on-line re-optimization promises considerably improvement. Moreover, additional constraints can be formulated. In this work, we assume that the state information is available.

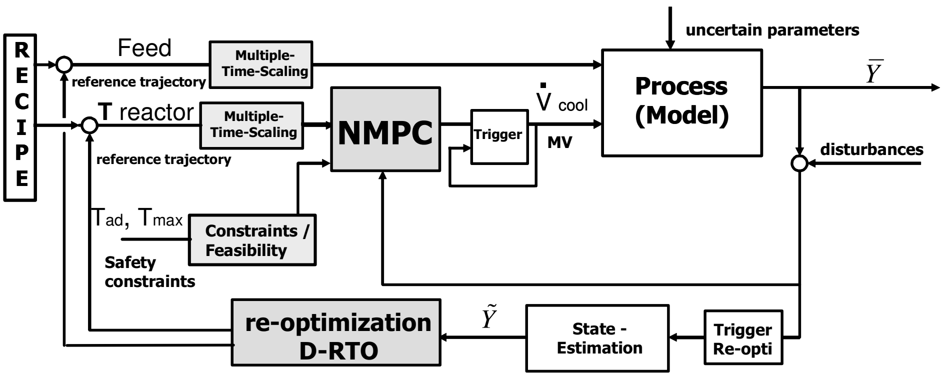

Figure 4. On-line Framework: Integration of NMPC and dynamic re-optimization

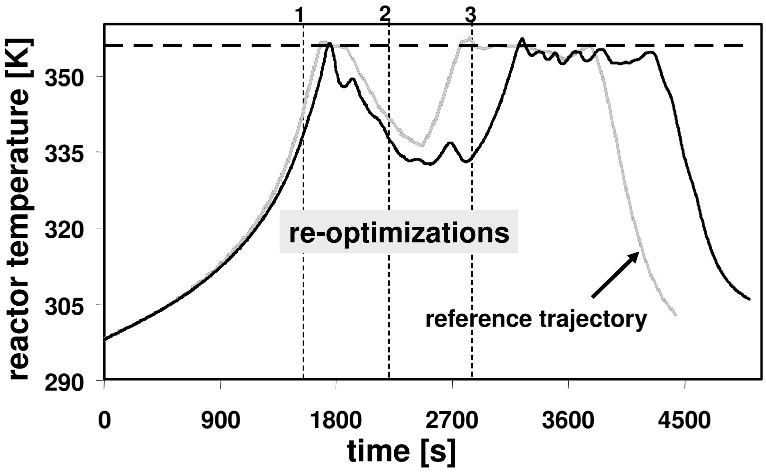

Figure 5. On-line re-optimization: reactor temperature

In order to compensate slow disturbances, the on-line re-optimization problem is automatically activated three times along the batch process time according to a trigger defined as the bounded above difference between the reactor temperature and the temperature reference trajectory (see Figure 5). New recipes resulting from this are then updated as input to the on-line framework. Due to the different trigger time-points the current D-RTO problem progressively possesses a reduced number of variables within a shrinking horizon (Nagy and Braatz, 2003). As a result of this, and a catalyst contamination the total batch time increases. But, despite the large plant mismatch and the absence of kinetic knowledge nearly perfect control is accomplished.

5. Conclusions

Feasibility and robustness with respect to input and output constraints have been achieved by the backing-off strategy. The resulting NMPC scheme embedded in the on-line re-optimization framework is viable for the optimization of the semi-batch reactor recipe while simultaneously guaranteeing the constraints compliance, both for nominal operation as well as for cases of large disturbances e.g. failure situation. The proposed scheme yields almost the same profit as the one of the off-line optimization operational profiles. Currently, the approach is extended to a probabilistically constrained nonlinear model predictive controller.

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