Robust NMPC for a Benchmark Fed-Batch Reactor with Runaway Conditions

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Summary. A nonlinear model predictive control (NMPC) formulation is used to prevent an exothermic fed-batch chemical reactor from thermal runaways even in the case of total cooling failure. Detailed modeling of the reaction kinetics and insight into the process dynamics led to the formulation of a suitable optimization problem with safety constraints which is then successively solved within the NMPC scheme. Although NMPC control-loops can exhibit a certain degree of inherent robustness, an explicit consideration of process uncertainties is preferable not only for safety reasons. This is approached by reformulating the open-loop optimization problem as a min-max problem. This corresponds to a worst-case approach and leads to even more cautious control moves of the NMPC in the presence of uncertain process parameters. All results are demonstrated in simulations for the esterification process of 2-butyl.

1 Introduction

Known from extreme accidents like in Seveso, Italy (1976), thermal runaways occur more frequently in smaller fine chemical reactors with high heat release potential. They lead to annoying production losses and equipment damages [2, 18]. To reduce difficulties, potentially dangerous processes are commonly run in fed-batch mode, yet with the most simple feeding strategy of constant dosing rates. The advent of detailed models of batch reactors including complicated reaction schemes can aid the development of more sophisticated feed strategies. A suitable framework for this goal is nonlinear model predictive control (NMPC). NMPC has the appealing attribute that constraints on states and controls are taken into account explicitly. In the fed-batch reactor case, a dosing rate profile delivered by NMPC will steer the process closer to the limits. At the same time, due to the predictive nature of NMPC, the system will be able to avoid runaway conditions.

Plant-model-mismatch in the form of uncertain parameters and initial values require NMPC schemes to be robust. Theoretical considerations have shown that NMPC controllers can inherently possess a certain degree of robustness [5]. For safety-critical processes, an explicit consideration of uncertainty is

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desirable. Some robust NMPC schemes have been proposed based on game-theoretic ideas [4], min-max formulations [11], H_∞-control [14], and chance constrained programming [13]. These methods tend to be computationally too complex for practical applications.

In this paper, the optimization problem is reformulated using a min-max approach similar to [15], extending the formulation to path constraints. The resulting semi-infinite control problem is then approximated to obtain a numerically tractable form ([8, 10]). To demonstrate this approach, it is applied to control the exothermic esterification of 2-butanol. While the main task of the state-feedback controller is to quickly finish the batch, safety constraints have to be met at any time of the process.

This paper is organized as follows: In Section 2, the fed-batch process and its mathematical model are described. The open-loop optimization problem needed for the NMPC scheme is developed in Section 3. Particular care is taken of the formulation of a safety constraint that prevents runaways even in the case of a total cooling failure. This section ends with simulation results for the process under nominal NMPC. To take parameter uncertainties directly into account, the approximated min-max formulation is stated in Section 4. It leads to a more robust version of the NMPC as is demonstrated via simulations at the end of the section. The paper concludes with further discussions and an outlook on future research directions.

2 Example: Exothermic Esterification of 2-Butanol

The esterification of 2-butanol (B) with propionic anhydride (A) to 2-butyl propionate (D) and propionic acid (C) is a mildly exothermic reaction that allows one to study runaway situations in a lab. The reaction is catalyzed by two forms of a catalyst, (K_1 and K_2), while the first degrades into the latter in a side reaction:

$$\begin{aligned} A + B &\xrightarrow{K_1,K_2} C + D \\ K_1 &\longrightarrow K_2 \end{aligned}$$

The reaction is assumed to take place in a fed-batch reactor under isoperibolic conditions (constant jacket temperature). A similar, strongly simplified reaction has also been considered in [17]. The reaction system is modeled by a set of differential equations based on mass and energy balances. Note that the model is only valid for a total amount of A added which is smaller or equal to B. The full model reads as follows:

$$\begin{aligned} \dot{n}_A &= u - r\,V, & \dot{n}_B &= -r\,V, \\ \dot{n}_C &= r\,V, & \dot{n}_{K_1} &= -r_k\,V, \\ (C_{p,I} + C_p)\,\dot{T}_R &= r\,H\,V - q_{\mathrm{dil}} - U\,\Omega\,(T_R - T_J) \\ &\quad -\alpha(T_R - T_a) - u\,c_{p,A}\,(T_R - T_d), \end{aligned} \tag{1}$$

with n_i being the molar amount of component i, V the volume, T_R, T_J, T_a and T_d the reactor, jacket, ambient and dosing temperatures, respectively. r and r_k are reaction rates, H is the reaction enthalpy, q_{dil} the dilution heat, U is a heat transfer coefficient, Ω the heat exchange surface. $C_{p,I}$ denotes the approximated heat capacity of solid inserts (stirrer, baffles), C_p the approximated heat capacity of the entire mixture and $c_{p,A}$ is the specific molar heat capacity of component A. Equations for D and K_2 have been omitted: The number of moles of D equals the number of moles of C (i.e. $n_D(t) = n_C(t)\ \forall\ t$). The amount of ($K_2$) can be calculated as $n_{K_2}(t) = n_{K_1}(0) - n_{K_1}(t)$. The molarities c_i are calculated as $c_i = n_i/V$.

The dosing rate $u(t)$ of A to the batch reactor serves as the control input and can be assigned between upper and lower bounds.

The defining algebraic equations are:

$$V = 1000\left(\frac{n_A M_A}{\rho_A} + \frac{n_B M_B}{\rho_B} + \frac{n_C M_C}{\rho_C} + \frac{n_C M_D}{\rho_D}\right) \tag{2a}$$

$$\Omega = \Omega_{\min} + \frac{V - V_{\min}}{1000d} \tag{2b}$$

$$U = \left(U_1 + \frac{U_2 - U_1}{V_2 - V_1}\right)(V - V_1) \tag{2c}$$

$$x_A = \frac{n_A(t)}{n_A(t) + n_B(t) + 2n_C(t) + n_{K_1}(0)} \tag{2d}$$

$$q_{\text{dil}} = \frac{2232.74201}{0.13963}\, e^{\frac{-x_A}{0.13963}}\, \dot{n}_A \tag{2e}$$

$$r = (k_0 + k_2\, c_{K_1})c_A c_B + k_3 c_A\, c_{K_2} \tag{2f}$$

$$r_k = k_4 10^{-H_R} c_B c_{K_1}. \tag{2g}$$

In these equations, M_i, ρ_i, c_i denote the molar weight, density and molar concentration of component i respectively. V_1, V_2, U_1, U_2 are geometry-dependent parameters and d is the scaled reactor diameter. The rate of heat loss to the environment is modeled by a constant α of appropriate dimension derived from a constant heat transfer coefficient and an average heat transfer surface area. The constants in equation (2e) have been adjusted properly for the needed dimension (Watt). The reaction rate constants k_i are calculated following the Arrhenius approach as $k_i(t) = A_i e^{\frac{-E_i}{RT_R(t)}}$, and the acidity term H_R is computed as $H_R(t) = -\left(p_1 c_{K1}(t) + p_2 c_C(t)\right)\left(p_3 + \frac{p_4}{T_R(t)}\right)$.

The reactor is initially charged with B and K_1. Then, A is dosed to the reactor until the accumulated number of moles of A is equal to the initial number of moles of B. The batch is complete when nearly all of B is consumed.

3 NMPC Formulation

The solution of an open-loop optimal control problem is a prerequisite for NMPC. For batch processes, the formulation of a suitable optimal control problem tends

Table 1. List of process parameters and initial values

$\Omega_{\min}$	0.011 m^2	p_1	0.200 l/mol	d	0.155 m
$V_{\min}$	0.124 l	p_2	0.032 l/mol	$T_{R,0}$	293.15 K
M_A	0.130 kg/mol	p_3	-21.375	α	0.1 W/K
M_B	0.074 kg/mol	p_4	12706.0 K	C_p	1523.3 J/K
M_C	0.074 kg/mol	E_0	80.479 kJ/mol	V_1	0.8 l
M_D	0.130 kg/mol	E_2	79.160 kJ/mol	V_2	1.6 l
M_{K1}	0.098 kg/mol	E_3	69.975 kJ/mol	$m_{A,0}$	0.00 g
ρ_A	979.381 kg/m^3	E_4	76.617 kJ/mol	$m_{B,0}$	510.98 g
ρ_B	772.288 kg/m^3	R	8.314 J/(mol K)	$m_{K_1,0}$	5.01 g
ρ_C	955.869 kg/m^3	$c_{p,A}$	238.519 J/(mol K)	U_1	195 W/(m^2K)
ρ_D	830.422 kg/m^3	$C_{p,I}$	89.859 J/K	U_2	155 W/(m^2K)
A_0	5.362e7 l/(mol s)	H	59458 J/mol	m_A	890.00 g
A_2	2.807e10 l^2/(mol^2 s)	H_{dil}	5070 J/mol	t_f	0.662 l
A_3	3.948e10 l/(mol s)	T_J	293.65 K	T_a	298.85 K
A_4	1.403e8 l/(mol s)	T_d	298.15 K		

to be difficult because of typically appearing end constraints. In this case, end constraints are avoided by observing that simply minimizing the amount of B over time leads to a meaningful solution. The batch is stopped when the amount of B is below a desired threshold. The optimal control problem is formulated as:

$$\begin{aligned} \min_u \quad & \int_0^{t_f} n_B(\tau)^2 \, d\tau \qquad (3) \\ \text{subject to} \quad & (1), (2) \\ & 0 \text{ mol/s} \le u(t) \le 0.004 \text{ mol/s} \\ & \int_{t_0=0}^{t_f} u(\tau) \, d\tau = 6.9 \text{ mol} \\ & T_R(t) \le 333.15 \text{ K} \\ & S(t) \le 363.15 \text{ K}. \end{aligned}$$

The safety constraint S (defined in the next section) has to ensure that even in the extreme case of a total cooling failure no runaway will occur. The prediction and control horizon of the NMPC controller are specified as 56 times the sample time of $t_s = 50$ s. With this choice, the horizon is slightly larger than the minimum batch time for this process. All states are assumed perfectly measured.

3.1 A Suitable Safety Constraint to Avoid Runaways

In the case of a cooling failure, the heat released during the reaction can no longer be removed from the reactor. This leads to a temperature rise which further accelerates the reactions. If enough reactant had accumulated before,

this mechanism results in a thermal runaway with severe safety risks [1]. Once a runaway has started, the best strategy is to immediately stop dosing the reactant. Then, the maximum temperature rise is related to the amount of reactants present in the reactor and can be calculated assuming adiabatic conditions [9].

Such an approach has been formulated more precisely in [17], where for two reactants A, B the safety constraint is $S(t) = T_R(t) + \min(n_A, n_B)\frac{H_A}{\rho c_p V} \leq T_{\max}$. Since the consumption rate for both species A and B is equal and all B is initially present in the reactor, n_A is smaller than n_B and we can set $\min(n_A, n_B) = n_A$ in order to avoid the nondifferentiable min-operator.

Note, that the calculated adiabatic temperature in $S(t)$ is rather conservative and will likely be smaller in reality because of heat losses to the jacket and ambient. Also, the heat capacity of the mixture is assumed to be constant with a value chosen at the upper limit.

3.2 NMPC Simulation Results

The open-loop control problem (3) is successively solved numerically with the direct multiple shooting approach by Bock and Plitt [3]. It is based on a parameterization of the controls and state trajectories. This leads to a large but favorably structured nonlinear program (NLP). The NLP is solved by a generalized Gauss-Newton sequential quadratic programming (SQP) method implemented in the software package MUSCOD-II [12]. Because SQP methods only find a local solution, the initial guess is of importance. For the nominal NMPC, an appropriate constant dosing rate served as an initial guess. For the robust NMPC introduced next, the nominal solution has been used as the initial guess. All integration and differentiation is performed with the DAE solver DAESOL [1], which applies a backward differentiation formula (BDF) method.

The batch is stopped once the remaining amount of 2-butanol falls below a threshold of $n_B \leq 0.01$ mol. Following the ideas of the real-time iteration scheme in [6], the optimization problem (3) is not solved to convergence at each sampling interval. Instead, the control is updated after each iteration step of the NLP solver. Due to a careful initialization from one problem to the next and the favorable contraction properties of the direct multiple shooting method, this procedure allows for close tracking of the optimal solution of the subsequent optimization problems. Note that nominal stability of this real-time iteration NMPC scheme can be shown [7]. Also, the scheme predicts active set changes and is therefore particularly suited for constrained control problems.

The CPU time for one control sample has been in the range of 0.9 to 1.2 seconds and hence is significantly smaller than the sampling time of 50 seconds.

The NMPC has been tested for the nominal set of parameters. Then, to test for robustness, the initial amount of catalyst K_1 has been increased. This

[1] Note, that such a runaway can also occur under normal cooling. However, this is not the focus of this study and, in the optimization results, is automatically suppressed by the upper bound on the process temperature.

process parameter has a rather strong impact on the process behavior. The simulation results for the nominal NMPC in the nominal case ($m_{\mathrm{K}_1}(0) = 5.01$ g) and two more cases with $m_{\mathrm{K}_1}(0) = 5.10$ g and $m_{\mathrm{K}_1}(0) = 5.50$ g are shown in Figure 1. In the nominal case, the dosing rate is at its maximum in the beginning, ensuring a fast ignition of the reaction and quick conversion. During this phase, A accumulates. This poses a potential threat and eventually the adiabatic temperature strongly rises. Once the bound on the adiabatic temperature becomes active, the dosing rate slides along a singular sub-arc until the reactor temperature will reach its upper operation limit. This is when the controller decides to stop the dosing to let the accumulated A be consumed. In the end, the remaining amount of A can safely be added at a maximum dosing rate.

The simulations show that the nominal NMPC scheme based on the open loop problem (3) keeps the batch process within safe operation conditions despite a moderate uncertainty in the initial amount of catalyst (remember that the model always assumes the nominal value of 5.01 g to be valid). Because of the higher temperatures in comparison to the model-based predictions and the feedback mechanism, the singular arcs become steeper and the dosing has to be stopped earlier. In the extreme case of 5.50 g of catalyst in the beginning of the batch, the upper limit of the reactor temperature is slightly violated. The NLP only remained feasible due to a relaxation procedure implemented in the optimization code.

In the following section, the NMPC scheme is modified to take the uncertainty explicitly into account.

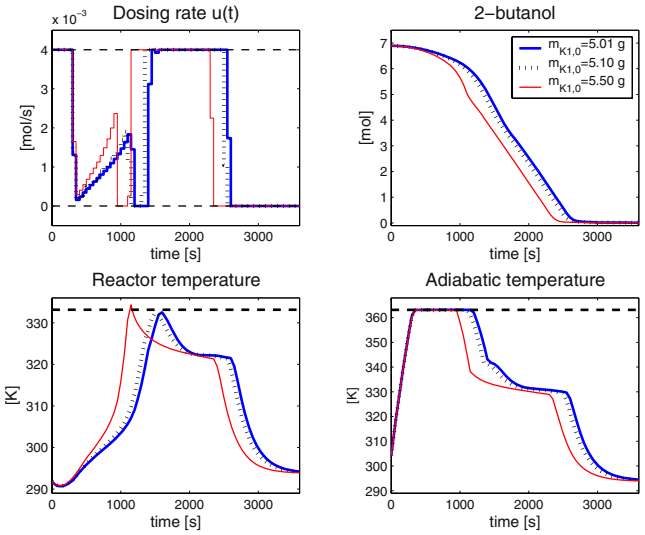

Fig. 1. Simulation results with nominal NMPC controller for the nominal value and two perturbed values of the initial amount of catalyst K_1. Dashed lines denote constraints.

4 A Min-Max NMPC Formulation

This paper has presented an open-loop optimization problem for NMPC with safety constraints for a given process model with exact parameters. In reality, at least some of the parameters will not be known exactly and methods for optimization under uncertainty become important (see [16] for an overview).

It is clear that a changed parameter can deteriorate the performance of a supposedly optimal (open-loop) solution. It seems natural to see parameters as adverse players that try to disturb any control efforts as strongly as possible. One remedy is to minimize the success of parameters to maximally worse the optimization results. In the context of robust batch optimization, such a min-max formulation has been used by Nagy and Braatz [15] who also point out the possibility to extend these ideas to NMPC. Such min-max formulations lead to a semi-infinite programming problem, which is numerically intractable in the real-time context. To overcome this obstacle, Körkel et al. [10] propose an approximated min-max formulation which is also applied in this paper.

The min-max formulation considered here reads as the semi-infinite programming problem

$$\begin{aligned} \min_{u\in\mathcal{U}} \quad & \max_{\|p-\bar{p}\|_{2,\Sigma^{-1}}\leq\gamma} \; J(x(u,p)) \\ \text{s.t.} \quad & \max_{\|p-\bar{p}\|_{2,\Sigma^{-1}}\leq\gamma} \; r_i(x(u,p)) \leq\ 0, \quad i=1,\ldots,n_r. \end{aligned} \tag{4}$$

The parameters p are assumed to lie within a given confidence region with the symmetric covariance matrix Σ and an arbitrary confidence level γ. The state x implicitly depends on the discretized control u and parameters p as a solution to the system equations (1,2). The cost function J is the same as in the nominal problem (3), while $r_i(x(u,p))$ summarizes those constraints in (3) that are considered critical with respect to uncertainty and shall be robustified. All other constraints are treated as in the nominal problem.

First order Taylor expansion of the inner maximization part yields a convex optimization problem that has an analytical solution (cf. [10] for this problem and [8] for a more general problem class). Using this closed form, we finally obtain a minimization problem that can efficiently be solved numerically:

$$\begin{aligned} \min_{u\in\mathcal{U}} \quad & J(x(u,\bar{p})) + \gamma \left\| \frac{\mathrm{d}}{\mathrm{d}p} J(x(u,\bar{p})) \right\|_{2,\Sigma} \\ \text{s.t.} \quad & r_i(x(u,\bar{p})) + \gamma \left\| \frac{\mathrm{d}}{\mathrm{d}p} r_i(x(u,\bar{p})) \right\|_{2,\Sigma} \leq\ 0, \quad i=1,\ldots,n_r, \end{aligned} \tag{5}$$

where the bar denotes the nominal value of the parameters as assumed for the nominal optimization problem.

In an NMPC scheme, the robust version (5) can replace the nominal control problem (3). In the next section, numerical results for such a robust NMPC are presented and compared to the nominal NMPC.

4.1 Min-Max NMPC Simulation Results

For the numerical solution of (5) the direct multiple shooting approach was used. The NMPC settings are the same as described in Section 3.2. The confidence factor γ was slowly increased from zero to the desired level. For each optimization with a respective γ, the previous result has been used to initialize the states and control. In the case presented here, the initial amount of catalyst K_1 is assumed to be uncertain. The standard deviation of K_1 is 0.17 g. The confidence level has been chosen to be 99.7 %, i.e. we have $\gamma = 3$ to obtain the 3σ-interval. Figure 2 shows the simulation results for the robust version of the NMPC for the nominal amount of catalyst and an increased amount. The solution is compared to the solution of the nominal NMPC for the nominal catalyst amount charged to the reactor. One can see that the robust solution strongly resembles the nominal solution. Only, the dosing is stopped earlier. This ensures that less A is accumulating in the reactor and leaves a safety margin to the adiabatic temperature as can be seen in the lower right graph. When the robust NMPC controller is confronted with a plant-model mismatch it reacts by dosing A more carefully. The singular sub-arc becomes flatter than computed with the nominal NMPC. Eventually, less A is present in the reactor and the temperature peak gets lower. This also leads to a slower consumption of B which, however, is accounted for by a higher reactor temperature at the end of the batch so that the final productivity losses are very small.

The safety margins for the reactor temperature and the adiabatic temperature are the main feature of the robust NMPC scheme. The fact that they are also

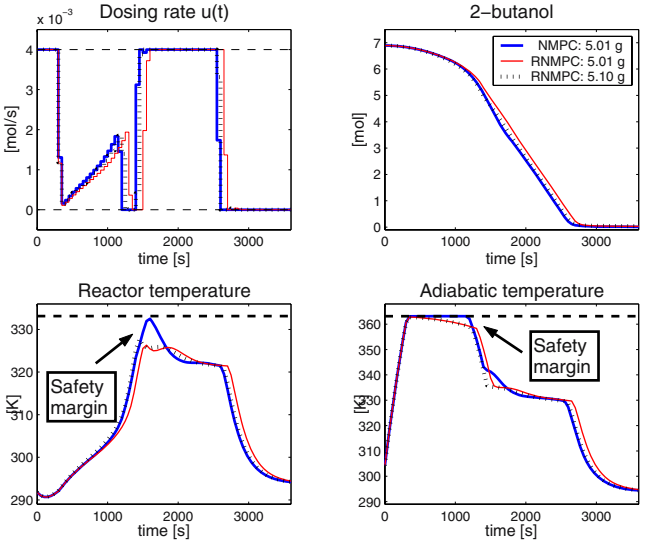

Fig. 2. Simulation results of robust (RNMPC) compared with nominal NMPC. The RNMPC is shown for the nominal and a perturbed initial amount of catalyst K_1. Dashed lines denote constraints. Note the RNMPC safety margins.

present in the nominal catalyst case reflects the conservatism inherent to the min-max approach. For the investigated cases, we have seen that already the nominal controller is robust against the uncertain parameter. So, any further robustification in the presence of uncertainty makes the controller more cautious. Also, the systematic robustness obtained via the min-max formulation is not fully exploited by the closed-loop dynamics. Instead of relying on the old, robustified solution, the optimization problem (5) is newly solved at every iteration with the new, unforeseen temperatures and concentrations. This is why the trajectories of the robust NMPC differ for the nominal and the perturbed realization of the initial amount of catalyst.

5 Conclusions

A detailed model of a fed-batch reactor has been used to demonstrate that a suitable NMPC scheme can avoid runaway situations. This nominal NMPC was robust against small perturbations of the initial amount of catalyst charged to the reactor. A robust formulation of the optimization problem based on an approximated min-max formulation led to additional safety margins with respect to the adiabatic temperature and the reactor temperature. The approximation does not guarantee full robustness for the nonlinear model, but it offers a systematic way to obtain safety margins that explicitly take into account uncertain parameters and their stochastic properties. The simulation also showed the conservatism of the proposed min-max formulation which is due to the open-loop formulation. The optimization method used to solve the nominal and the robust open-loop problems was able to deal with the complex state constraints and delivered control updates fast enough to be applicable to real batch processes. Future studies will treat larger numbers of uncertain parameters and focus on methods to efficiently solve the eventually enlarged optimization problems.

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