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Handling uncertainty in economic nonlinear model predictive control: A comparative case study

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ABSTRACT

In the last years, the use of an economic cost function for model predictive control (MPC) has been widely discussed in the literature. The main motivation for this choice is that often the real goal of control is to maximize the profit or the efficiency of a certain system, rather than tracking a predefined set-point as done in the typical MPC approaches, which can be even counter-productive. Since the economic optimal operation of a system resulting from the application of an economic model predictive control approach drives the system to the constraints, the explicit consideration of the uncertainties becomes crucial in order to avoid constraint violations. Although robust MPC has been studied during the past years, little attention has yet been devoted to this topic in the context of economic nonlinear model predictive control, especially when analyzing the performance of the different MPC approaches. In this work, we present the use of multi-stage scenario-based nonlinear model predictive control as a promising strategy to deal with uncertainties in the context of economic NMPC. We make a comparison based on simulations of the advantages of the proposed approach with an open-loop NMPC controller in which no feedback is introduced in the prediction and with an NMPC controller which optimizes over affine control policies. The approach is efficiently implemented using CasADi, which makes it possible to achieve real-time computations for an industrial batch polymerization reactor model provided by BASF SE. Finally, a novel algorithm inspired by tube-based MPC is proposed in order to achieve a trade-off between the variability of the controlled system and the economic performance under uncertainty. Simulations results show that a closed-loop approach for robust NMPC increases the performance and that enforcing low variability under uncertainty of the controlled system might result in a big performance loss.
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1. Introduction

Model predictive control (MPC) and its nonlinear counterpart (NMPC) have become popular control strategies both for the process industry and for control researchers. The main reason for their success is the ability of NMPC to deal with multivariable nonlinear systems with constraints. Usually, a model of the system is used to predict the behavior of the system and to compute a sequence of optimal control inputs by minimizing a certain tracking objective which is mapped to a cost function. However, the ultimate goal of process control is not to track as well as possible a certain set-point that has been previously generated, but to maximize the profit (or minimize the costs) of a process as it is discussed in [1]. For this reason, in the last years the traditional tracking cost function of the MPC scheme has frequently been replaced by a more general cost function that can represent the plant economics and different results have been reported in e.g. [2–4], and in [5].

One of the problems of this modification is that it is not possible to extend directly the existing tools and theory for the stability analysis of standard tracking MPC (see [6] for a review) and new approaches are required, as stated in [7]. The main reason for this is that the central argument on which most of the stability analysis relies, that is, the optimal cost of the MPC problem is a Lyapunov function of the closed-loop system, does not hold for economic MPC under the usual assumptions. Recently, several modifications of the classical approaches have been proposed to guarantee the stability of economic MPC schemes. A Lyapunov function to prove stability

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of economic NMPC based on a strong duality assumption has been proposed in [8]. This assumption is relaxed in [9] using dissipativity assumptions. These methods need the use of a terminal constraint or of a terminal set as in standard NMPC, which can be dropped by introducing further assumptions as shown in [10].

Interestingly, very little attention has been paid to another important implication of economic MPC: the economic operation of a system typically drives the system to its constraints. This, together with the fact that models of real systems are never perfect, makes the handling of the uncertainty in economic NMPC a crucial issue in order to guarantee constraint satisfaction in the presence of the uncertainty and the disturbances that act on the system.

The consideration of uncertainties in tracking model predictive control has been extensively studied in the literature under the heading of robust MPC, but very little has been reported for the case of economic MPC. One of the few works in this direction is [11], where input-to-state stability of economic NMPC for uncertain cyclic processes is studied. In [12], robustness with respect to changes in the constraint set is analyzed based on dissipativity assumptions and [13] discusses the case of probabilistic constraints for linear economic MPC under uncertainty. For the case of traditional tracking MPC approaches, there is a large amount of literature which often considers a min–max formulation of the problem as originally proposed in [14] and later in the context of MPC in [15]. The traditional min–max MPC approaches are usually called open-loop min–max because they do not consider the fact that at the next sampling time the optimization problem resulting from the MPC scheme will be solved again. Closed-loop approaches as described in [16] optimize over a sequence of control policies instead of over a sequence of control inputs, taking feedback into account and reducing strongly the conservativeness of the controller as illustrated in [17]. However, the optimization over control policies results in an infinite-dimensional optimization problem that is very difficult to solve in general. In order to solve this problem, different approximations have been proposed such as optimizing over state feedback policies [18] or affine policies parametrized on the uncertainty [19,20]. In both cases, a certain degree of suboptimality is introduced.

Another possibility for robust NMPC that has become popular in the last years is the use of tube-based methods, that were first proposed in the context of linear MPC in [21]. The main idea of tube-based MPC is to decouple the robust control problem into the nominal solution and a second controller (called ancillary controller) that tries to steer the real system that is affected by the uncertainty to a set near the nominal trajectory. The approach was extended to nonlinear systems in [22] and different modifications have been proposed in the last years leading to different computational complexities and degrees of conservativeness (see e.g. [23–25]).

The stability properties of the mentioned strategies are always discussed in the literature for the case of tracking MPC. However, with the exception of [26], which proposes a method to estimate the suboptimality introduced by the choice of affine policies in the case of tracking MPC of linear systems, very little attention has been devoted to the analysis of the performance or conservativeness introduced by the different robust approaches, especially in the case of economic nonlinear model predictive control. For this reason, this paper focuses on analyzing the performance of different methods using robust economic NMPC for an industrially relevant batch polymerization reactor example provided by BASF SE. The theoretical stability analysis of the controllers is out of the scope of this paper and is not discussed.

In particular, we use the framework of multi-stage NMPC and we perform a comparison based on simulations with other typical robust MPC approaches by solving a challenging benchmark problem of an industrial polymerization reactor under large model uncertainty. Multi-stage NMPC uses ideas of closed-loop robust MPC [17] and is based on the representation of the uncertainty by a scenario tree. The multi-stage formulation represents the real-time decision problem that arises from the receding horizon strategy of MPC correctly because the future control inputs can depend on the realization of the uncertainty that will have been observed at the respective decision point, thus reducing the conservativeness of the approach considerably. Multi-stage NMPC has demonstrated a good potential for solving robust NMPC problems, as was demonstrated in [27,28]. The main drawback of the approach is that the size of the resulting optimization problem grows rapidly with the prediction horizon and with the number of uncertainties considered. This paper extends the results presented in [29] in several ways. The benchmark problem has been extended to consider an important safety constraint that modifies the optimal solution of the problem and we consider larger uncertainties. We compare the multi-stage approach with an open-loop robust NMPC approach and with robust NMPC using affine policies. We also present another novel contribution: a modification of the multi-stage NMPC approach inspired by tube-based MPC ideas in order to specify a trade-off between the variability of the trajectories for the different scenarios and the average economic performance. All optimization problems are solved in a very efficient way using CasADi, which makes it possible to solve the resulting Nonlinear Programming (NLP) problems with exact first and second order derivative information with a low implementation effort, significantly reducing the computation times reported in [28].

The remainder of the paper is structured as follows. Multi-stage NMPC is explained in Section 2 together with the implementations of open-loop robust NMPC and robust NMPC based on affine control policies that are applied in this work. Section 3 presents the case study considered in this paper: an industrial batch polymerization reactor provided by BASF SE. The numerical approach for the solutions of the resulting optimization problems using CasADi is presented in Section 3. A comparison which shows the benefits of multi-stage NMPC over traditional methods to achieve robustness (i.e. tracking a conservative-set point with a conservative choice of the uncertain parameters) is presented in Section 4. A comparison of multi-stage NMPC with other robust NMPC approaches is made in Section 5 and the modification of the multi-stage approach to reduce the variability of the system for the different values of the uncertainty is presented in Section 6. The main conclusions of the paper and future directions of work are stated in Section 7.

2. Robust economic nonlinear model predictive control

In this section, we describe several approaches to deal with uncertainty in model predictive control and we formulate all of them within the framework of multi-stage NMPC to enable a fair comparison for the proposed case study. First, we revisit the multi-stage NMPC approach and then the framework is extended to incorporate an open-loop approach in which a sequence of control inputs is calculated to satisfy the constraints for all the scenarios in the tree. Finally, the use of affine feedback control policies as a way to introduce feedback in the predictions of the NMPC scheme as described e.g. in [20] is shortly presented in the context of multi-stage NMPC.

2.1. Multi-stage nonlinear model predictive control

Multi-stage NMPC is a robust NMPC approach that is based on describing the evolution of the uncertainty by a scenario tree as depicted in Fig. 1. The tree structure visualizes that future control inputs can depend on the previous values of the uncertainty if full state measurement or perfect estimation is assumed, and thus can

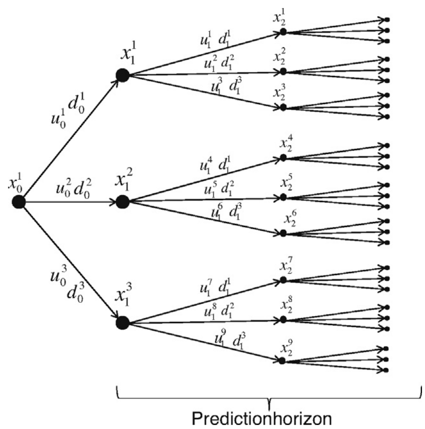

Fig. 1. Scenario tree representation of the uncertainty evolution for multi-stage NMPC.

act as recourse variables that counteract – to the extent possible – the effect of the future uncertainties. Thus, multi-stage NMPC is a closed-loop robust NMPC approach that exhibits a lower degree of conservativeness compared to other approaches, such as open-loop min–max NMPC, multi-model or multi-scenario approaches without recourse, as the one presented in [30] where in contrast to our formulation, no feedback is introduced in the predictions. The basic idea of the use of a scenario tree for MPC was suggested in [17] and some results for linear MPC have been reported in [31]. The same approach has been applied in planning and scheduling, see e.g. [32,33].

Note that the tree structure does not necessarily represent time-varying uncertainties or disturbances, but it reflects the fact that if the uncertainty is not known at one sampling time, it will remain unknown at the next sampling time when a new tree (shifted in time) will have to be considered. By using disturbance estimation (unknown input observers) or parameter estimation, some of this uncertainty can be reduced and this leads to a better performance, see e.g. [28].

It is clear that meeting the constraints is guaranteed for all the values of the uncertainty that are considered in the scenario tree, but for general nonlinear systems, robust constraint satisfaction cannot be guaranteed for values that are not represented explicitly in the tree. However, the values of the parameters that produce the worst-case scenario are often on the boundaries of the considered parameter interval as discussed in [34] and therefore a suitable scenario tree should include the combinations of the extreme values of the parameters, which produces good results in practice as shown in [28,35]. For this reason, in the remainder of the paper we say that an NMPC scheme is robust if it satisfies the constraints for a given (properly chosen) scenario tree. Since a suitable scenario is often generated by the combination of the different possible extreme values of the uncertainties, the main drawback of the approach is the exponential growth of the scenario tree with the prediction horizon and also with the number of uncertainties taken into account. A simple strategy to deal with the growth of the tree with the prediction horizon is to consider that the uncertainty remains constant after a certain point in time (called the robust horizon). The main idea of this simplification is that due to the receding horizon nature of NMPC, modeling the far future very accurately is not critical because all the control inputs will be recomputed at the next sampling time anyway. An example scenario tree illustrating this simplification can be seen in Fig. 2.

The control inputs cannot anticipate the values of the uncertainty that are realized after the corresponding decision point, and this is enforced by the non-anticipativity constraints that require all the control inputs that branch at the same node to be equal

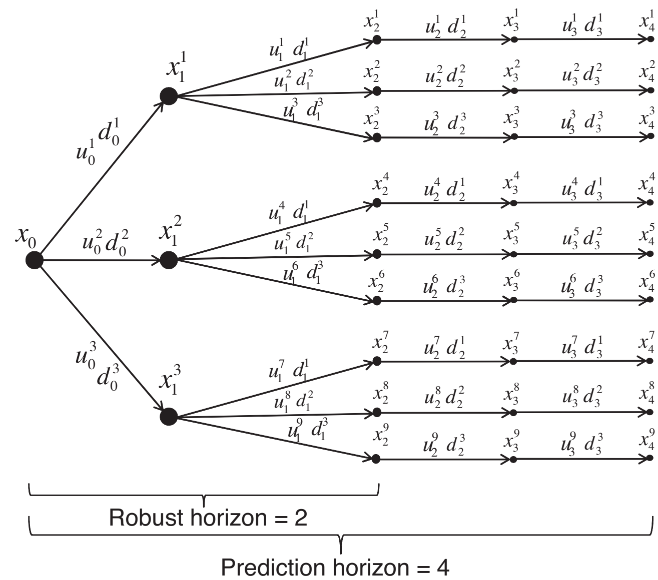

Fig. 2. Scenario tree representation of the uncertainty evolution for multi-stage NMPC with robust horizon.

(for example in Fig. 1, $u_0^1 = u_0^2 = u_0^3, u_1^1 = u_1^2 = u_1^3, \ldots$). The scenario tree setting assumes a discrete-time formulation of an uncertain nonlinear system that can be written as:

$$x_{k+1}^j = f(x_k^{p(j)}, u_k^j, d_k^{r(j)}), \tag{1}$$

where each state x_{k+1}^j is a function of the previous state $x_k^{p(j)}$, the control input u_k^j and the realization r of the uncertainty at stage k, $d_k^{r(j)}$ (for example in Fig. 1, $x_2^7 = f(x_1^3, u_1^7, d_1^1)$). For simplicity, in the presentation we consider that the tree has the same number of branches at all nodes, given by $d_k^{r(j)} \in \{d_k^1, d_k^2, \ldots, d_k^s\}$ at stage k for s different possible values of the uncertainty. Also, in order to clarify the notation, the index set of all occurring indices (j, k) is denoted by I. Each path from the root node x_0 to a leaf node x_K^i is called a scenario S_i such that

$$S_i = \{x_K^i, x_{K-1}^{p(i)}, x_{K-2}^{p(p(i))}, \ldots, x_0\}, \quad \forall i = 1, \ldots, N,$$

where N is the number of scenarios (or leaf nodes) and K is the prediction horizon. The optimization problem resulting from the multi-stage formulation in a scenario-based setting can be written as:

$$\min_{x_k^j, u_k^j \forall (j,k) \in I} \left(\sum_{i=1}^{N} (\omega_i J_i(x_{k+1}^j, u_k^j))^{\alpha} \right)^{1/\alpha} \tag{2a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, u_k^j, d_k^{r(j)}), \quad \forall (j, k+1) \in I, \tag{2b}$$

$$g(x_k^j, u_k^j) \le 0, \quad \forall (j, k) \in I, \tag{2c}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)} \quad \forall (j, k), (l, k) \in I, \tag{2d}$$

where $g(x_k^j, u_k^j)$ represents general and possibly nonlinear constraints on the states and the inputs at each node of the tree. The cost of each scenario S_i with weight ω_i is denoted by $J_i(x_{k+1}^j, u_k^j)$ defined as:

$$J_i(x_{k+1}^j, u_k^j) = \sum_{k=0}^{K-1} L(x_{k+1}^j, u_k^j), \ \forall x_{k+1}^j, u_k^j \in S_i, \tag{3}$$

where $L(x_{k+1}^j, u_k^j)$ is the stage cost, which represents a general – possibly economic – cost function. The non-anticipativity constraints in (2d) enforce that the decisions u_k^j with the same parent node $x_k^{p(j)}$ must be the same. Using the formulation parametrized on α, it is possible to represent the multi-stage NMPC approach if $\alpha = 1$ is chosen, whereas if $\alpha = \infty$ is chosen, a closed-loop min–max approach is obtained, in which feedback is taken explicitly into account. A comparison of both approaches was presented in [28]. If the number of scenarios is $N = 1$, the problem is reduced to standard NMPC. The weights ω_i can be adapted according to parameter estimation or stochastic information if it is available (see [28]) or chosen to be identical if no information is available. We do not consider terminal cost or terminal constraints in any of the schemes presented in this paper.

2.2. Open-loop robust nonlinear economic model predictive control

The formulation of multi-stage NMPC presented in (2) can be modified to represent the open-loop case in which no feedback is incorporated in the prediction of the NMPC controller. For this purpose the non-anticipativity constraints are modified such that they force all the control inputs to be equal at each stage. Thus a sequence of control inputs that satisfy the constraints for all the cases of the uncertainty in the scenario tree has to be computed. The optimization problem that has to be solved at each sampling time in this case is:

$$\min_{x_k^j, u_k^j \forall (j,k) \in I} \left(\sum_{i=1}^{N} (\omega_i J_i(x_{k+1}^j, u_k^j))^{\alpha} \right)^{1/\alpha} \tag{4a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, u_k^j, d_k^{r(j)}), \quad \forall (j, k+1) \in I, \tag{4b}$$

$$g(x_k^j, u_k^j) \leq 0, \quad \forall (j,k) \in I, \tag{4c}$$

$$u_k^j = u_k^l, \quad \forall (j,k), (l,k) \in I, \tag{4d}$$

where the only difference with respect to the multi-stage formulation is the modification of the non-anticipativity constraints in (4d).

2.3. Robust economic model predictive control with affine policies

It is well known that the computation of open-loop control policies can lead to very conservative solutions or even to infeasible optimization problems as has been illustrated by a simple example in [17]. A traditional way to introduce feedback in the predictions to achieve a closed-loop approach is to include a feedback matrix which depends on the future predicted state as an additional degree of freedom in the optimization problem. This was introduced in the context of MPC in [18]. In this case, the control input that is calculated at each sampling time in the prediction is $u_k^j = v_k^j + K x_k^{p(j)}$ where K is the new optimization variable. Other parametrizations, including time varying affine (state feedback) policies or affine policies parametrized on the uncertainty instead of on the states, have also been proposed in the literature (see e.g. [19] or [20]).

The constraints have to be satisfied for all the values of the uncertainty and in order to have a direct comparison with the other presented approaches we enforce this by applying the constraints for all the nodes of the tree. Following [20], we consider in the cost function only the nominal scenario (but this could easily be extended to the average value). The optimization problem that is solved at each sampling time in the case of constant affine policies is:

$$\min_{x_k^j, v_k^j, K \forall (j,k) \in I} \left(\sum_{i=1}^{1} (\omega_i J_i(x_{k+1}^j, v_k^j + K x_k^{p(j)}))^{\alpha} \right)^{1/\alpha} \tag{5a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, v_k^j + K x_k^{p(j)}, d_k^{r(j)}), \quad \forall (j, k+1) \in I, \tag{5b}$$

$$g(x_k^j, v_k^j + K x_k^{p(j)}) \leq 0, \quad \forall (j,k) \in I, \tag{5c}$$

$$v_k^j + K x_k^{p(j)} = v_k^l + K x_k^{p(l)}, \quad \forall (j,k), (l,k) \in I. \tag{5d}$$

For the case with time varying state feedback policies (K_k) the optimization problem is formulated as:

$$\min_{x_k^j, v_k^j, K_k \forall (j,k) \in I} \left(\sum_{i=1}^{1} (\omega_i J_i(x_{k+1}^j, v_k^j + K_k x_k^{p(j)}))^{\alpha} \right)^{1/\alpha} \tag{6a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, v_k^j + K_k x_k^{p(j)}, d_k^{r(j)}), \quad \forall (j, k+1) \in I, \tag{6b}$$

$$g(x_k^j, v_k^j + K_k x_k^{p(j)}) \leq 0, \quad \forall (j,k) \in I, \tag{6c}$$

$$v_k^j + K_k x_k^{p(j)} = v_k^l + K_k x_k^{p(l)}, \quad \forall (j,k), (l,k) \in I, \tag{6d}$$

Several possible parametrizations have been presented in the literature and we do not attempt to compare all the different approaches. The main goal of this work is to provide some insight into the possible conservativeness introduced by these approaches when solving an industrially relevant economic NMPC problem.

We briefly summarize here the four different designs for robust NMPC that have been presented in this section and which will be used in the remainder of the paper. Multi-stage NMPC is described in (2), which also includes standard NMPC if the number of scenarios is $N = 1$. An open-loop robust NMPC implementation in which a sequence of control inputs has to satisfy the constraints for all the cases of the uncertainty can be found in (4). Robust NMPC with affine constant policies is defined in (5) and robust NMPC with affine time-varying policies is described in (6). We will use these names for referring to the different approaches in the following sections of the paper.

3. Case study: an industrial batch polymerization reactor

3.1. Description of the model

The results of this paper are obtained for a realistic industrial batch polymerization reactor model provided by BASF SE as case study in the context of the EU-funded project EMBOCON [36]. A scheme of the system under consideration can be seen in Fig. 3. The system consists of a reactor into which monomer is fed. The monomer turns into a polymer via a very exothermic chemical reaction. The reactor is equipped with a jacket and with an External Heat Exchanger (EHE) that can both be used to control the temperature inside the reactor.

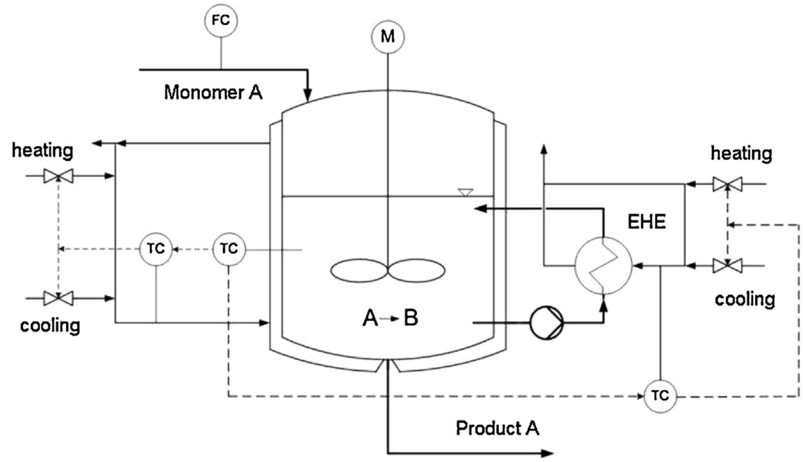

Fig. 3. Industrial batch polymerization reactor with an external heat exchanger.

The process is modeled by a set of 8 ordinary differential equations:

$$\begin{aligned}
\dot{m}_{\rm W} &= \dot{m}_{\rm F}\omega_{\rm W,F}\\
\dot{m}_{\rm A} &= \dot{m}_{\rm F}\omega_{\rm A,F} - k_{\rm R1}m_{\rm A,R} - k_{\rm R2}m_{\rm AWT}m_{\rm A}/m_{\rm ges},\\
\dot{m}_{\rm P} &= k_{\rm R1}m_{\rm A,R} + p_1k_{\rm R2}m_{\rm AWT}m_{\rm A}/m_{\rm ges},\\
\dot{T}_{\rm R} &= \frac{1}{c_{\rm p,R}m_{\rm ges}}[\dot{m}_{\rm F}c_{\rm p,F}(T_{\rm F}-T_{\rm R}) + \Delta H_{\rm R}k_{\rm R1}m_{\rm A,R} - k_{\rm K}A(T_{\rm R}-T_{\rm S})\\
&\quad - \dot{m}_{\rm AWT}c_{\rm p,R}(T_{\rm R}-T_{\rm EK})],\\
\dot{T}_{\rm S} &= \frac{1}{c_{\rm p,S}m_{\rm S}}[k_{\rm K}A(T_{\rm R}-T_{\rm S}) - k_{\rm K}A(T_{\rm S}-T_{\rm M})],\\
\dot{T}_{\rm M} &= \frac{1}{c_{\rm p,W}m_{\rm M,KW}}[\dot{m}_{\rm M,KW}c_{\rm p,W}\left(T_{\rm M}^{\rm IN}-T_{\rm M}\right) + k_{\rm K}A(T_{\rm S}-T_{\rm M})],\\
\dot{T}_{\rm EK} &= \frac{1}{c_{\rm p,R}m_{\rm AWT}}[\dot{m}_{\rm AWT}c_{\rm p,W}(T_{\rm R}-T_{\rm EK}) - \alpha(T_{\rm EK}-T_{\rm AWT})\\
&\quad + k_{\rm R2}m_{\rm A}m_{\rm AWT}\Delta H_{\rm R}/m_{\rm ges}],\\
\dot{T}_{\rm AWT} &= [\dot{m}_{\rm AWT,KW}c_{\rm p,W}(T_{\rm AWT}^{\rm IN}-T_{\rm AWT})\\
&\quad - \alpha(T_{\rm AWT}-T_{\rm EK})]/(c_{\rm p,W}m_{\rm AWT,KW}),
\end{aligned} \tag{7}$$

where

$$\begin{aligned}
U &= \frac{m_{\rm P}}{m_{\rm A}+m_{\rm P}},\\
m_{\rm ges} &= m_{\rm W} + m_{\rm A} + m_{\rm P},\\
k_{\rm R1} &= k_0 e^{\frac{-E_a}{R(T_{\rm R}+273.15)}}(k_{\rm U1}(1-U) + k_{\rm U2}U),\\
k_{\rm R2} &= k_0 e^{\frac{-E_a}{R(T_{\rm EK}+273.15)}}(k_{\rm U1}(1-U) + k_{\rm U2}U),\\
k_{\rm K} &= (m_{\rm W}k_{\rm WS} + m_{\rm A}k_{\rm AS} + m_{\rm P}k_{\rm PS})/m_{\rm ges},\\
m_{\rm A,R} &= m_{\rm A} - m_{\rm A}m_{\rm AWT}/m_{\rm ges}.
\end{aligned}$$

The model includes mass balances for the water, monomer and product hold-ups ($m_{\rm W}$, $m_{\rm A}$, $m_{\rm P}$) and energy balances for the reactor ($T_{\rm R}$), the vessel ($T_{\rm S}$), the jacket ($T_{\rm M}$), the mixture in the external heat exchanger ($T_{\rm EK}$) and the coolant leaving the external heat exchanger ($T_{\rm AWT}$). The variable U denotes the polymer-monomer ratio in the reactor, $m_{\rm ges}$ represents the total mass, $k_{\rm R1}$ is the reaction rate inside the reactor and $k_{\rm R2}$ is the reaction rate in the external heat exchanger. The total heat transfer coefficient of the mixture inside the reactor is denoted as $k_{\rm K}$ and $m_{\rm A,R}$ represents the current amount of monomer inside the reactor.

The available control inputs are the feed flow $\dot{m}_{\rm F}$, the coolant temperature at the inlet of the jacket $T_{\rm M}^{\rm IN}$ and the coolant temperature at the inlet of the external heat exchanger $T_{\rm AWT}^{\rm IN}$.

The complete set of parameters of the model used in this work as provided by BASF SE, together with a short description of each parameter, are presented in Table 1.

3.2. Description of the control problem

The control task under consideration is the production of one batch of polymer in the minimum possible time while satisfying safety constraints and constraints on the quality of the resulting product by manipulating the control inputs $\dot{m}_{\rm F}$, $T_{\rm M}^{\rm IN}$ and $T_{\rm AWT}^{\rm IN}$.

The temperature at which the polymerization reaction takes place strongly influences the properties of the resulting polymer. For this reason, the temperature of the reactor should be maintained in a range of $\pm 2.0\,^\circ$C around the desired reaction temperature $T_{\rm set} = 90\,^\circ$C in order to ensure that the produced polymer has the required properties.

Real processes are also subject to important safety constraints that are incorporated to account for possible failures of the equipment. In this case, the maximum temperature that the reactor would reach in the case of a cooling failure is constrained to be below 109 °C. The temperature that the reactor would achieve in the case of a complete cooling failure can be calculated as:

$$T_{\rm adiab} = \frac{\Delta H_{\rm R}}{c_{\rm p,R}}\frac{m_{\rm A}}{m_{\rm ges}} + T_{\rm R}. \tag{8}$$

To model the safety constraint, we extend the model in (7) by an additional differential state ($T_{\rm adiab}$), the differential equation of which is obtained by differentiating (8) with respect to time:

$$\dot{T}_{\rm adiab} = \frac{\Delta H_{\rm R}}{m_{\rm ges}c_{\rm p,R}}\dot{m}_{\rm A} - (\dot{m}_{\rm W} + \dot{m}_{\rm A} + \dot{m}_{\rm P})\left(\frac{m_{\rm A}\Delta H_{\rm R}}{m_{\rm ges}^2 c_{\rm p,R}}\right) + \dot{T}_{\rm R}. \tag{9}$$

The new state is constrained to be below the safe temperature ($T_{\rm adiab} \leq 109\,^\circ$C).

The maximum amount of material that can be fed into the reactor is $\int \dot{m}_{\rm F}{\rm d}t = 30,000$ kg. After all the material has been fed into the reactor (feeding phase) the reaction continues with the

Table 1
Parameters of the industrial polymerization reactor model.

Parameter	Description	Value	Units
R	Gas constant	8.314	kJ kmol^{-1} K^{-1}
$c_{p,W}$	Specific heat capacity of the coolant	4.2	kJ kg^{-1} K^{-1}
$c_{p,S}$	Specific heat capacity of the steel	0.47	kJ kg^{-1} K^{-1}
$c_{p,F}$	Specific heat capacity of the feed	3	kJ kg^{-1} K^{-1}
$c_{p,R}$	Specific heat capacity of the reactor contents	5.0	kJ kg^{-1} K^{-1}
k_{WS}	Heat transfer coeff. water-steel	4800	W m−2 K^{-1}
T_F	Feed temperature	25	°C
A	Heat exchange surface of the jacket	65	m^2
$m_{M,KW}$	Mass of coolant in the jacket	5000	kg
m_S	Mass of reactor steel	39,000	kg
m_{AWT}	Mass of the product in the EHE	200	kg
$m_{AWT,KW}$	Mass of the coolant in the EHE	1000	kg
$\dot{m}_{M,KW}$	Coolant flow of the jacket	300,000	kg h^{-1}
$\dot{m}_{AWT,KW}$	Coolant flow of the EHE	100,000	kg h^{-1}
$\dot{m}_{AWT}$	Product flow to the EHE	20,000	kg h^{-1}
E_a	Activation energy	8500	kJ kmol^{-1}
ΔH_R	Specific reaction enthalpy	950	kJ kg^{-1}
k_0	Specific reaction rate	7	–
k_{U2}	Reaction parameter 1	32	–
k_{U1}	Reaction parameter 2	4	–
$w_{W,F}$	Mass fraction of water in the feed	0.333	–
$w_{A,F}$	Mass fraction of A in the feed	0.667	–
k_{AS}	Heat transfer coeff. monomer-steel	1000	W m^{-2} K^{-1}
k_{PS}	Heat transfer coeff. product-steel	100	W m^{-2} K^{-1}
α	Experimental coefficient	3,600,000	1 s^{-1}

remaining monomer (holding phase) and the batch is considered to be finished when the desired amount of polymer is produced ($m_P^{end} = 20,680$ kg). In order to avoid the switching between different optimization problems as in [28] for the feeding and the holding phase, we add an additional state that accounts for the accumulated material that has been fed, that is, $\dot{m}_A^{acc} = \dot{m}_F$ and another constraint is included such that $0 < m_F^{acc} < m_F^{max} =$ 30 000 kg. The constraints on the states and control inputs, as well as the initial conditions can be seen in Tables 2 and 3.

In a real system, usually the model parameters cannot be determined exactly, what represents an important source of uncertainty. In this work, we consider that two of the most critical parameters of the model are not precisely known and vary with respect to their nominal value. In particular, we assume that the specific reaction enthalpy ΔH_R and the specific reaction rate k_0 are constant but uncertain, having values that can vary ±30% with respect to their nominal values reported in Table 1.

Table 2
Initial conditions and state constraints.

State	Init. cond.	Min.	Max.	Unit
m_W	10,000	0	inf.	kg
m_A	853	0	inf.	kg
m_P	26.5	0	inf.	kg
T_R	90.0	$T_{set} - 2.0$	$T_{set} + 2.0$	°C
T_S	90.0	0	100	°C
T_M	90.0	0	100	°C
T_{EK}	35.0	0	100	°C
T_{AWT}	35.0	0	100	°C
T_{adiab}	104.897	0	109	°C
m_F^{acc}	0	0	30,000	kg

Table 3
Bounds on the manipulated variables.

Control	Min.	Max.	Unit
$\dot{m}_F$	0	30,000	kg h$^{=-1}$
T_M^{IN}	60	100	°C
T_{AWT}^{IN}	60	100	°C

3.3. Mathematical formulation

We formulate the control task as the following optimization problem:

$$\min_{x_k^j, u_k^j \forall (j,k) \in I} \quad J_{batch}(x_{k+1}^j, u_k^j) \tag{10a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, u_k^j, d_k^{r(j)}), \tag{10b}$$

$$T_{set} - 2.0 \le T_{R,k}^j \le T_{set} + 2.0, \tag{10c}$$

$$0 \le T_{S,k}^j \le 100, \tag{10d}$$

$$0 \le T_{M,k}^j \le 100, \tag{10e}$$

$$0 \le T_{EK,k}^j \le 100, \tag{10f}$$

$$0 \le T_{AWT,k}^j \le 100, \tag{10g}$$

$$0 \le T_{adiab,k}^j \le 109, \tag{10h}$$

$$0 \le m_{A,k}^{acc,j} \le m_A^{max}, \tag{10i}$$

$$0 \le \dot{m}_{F,k}^j \le 30000, \tag{10j}$$

$$60 \le T_{M,k}^{IN,j} \le 100, \tag{10k}$$

$$60 \le T_{AWT,k}^{IN,j} \le 100, \tag{10l}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)} \quad \forall (j,k), (l,k) \in I, \tag{10m}$$

where the constraints are applied to all the states and all control inputs along each scenario with

$$x_k^j = [m_{W,k}^j, m_{A,k}^j, m_{P,k}^j, T_{R,k}^j, T_{S,k}^j, T_{M,k}^j, T_{EK,k}^j, T_{AWT,k}^j, \times T_{adiab,k}^j, m_{A,k}^{acc,j}]^T,$$

$$u_k^j = [\dot{m}_{F,k}^j, T_{M,k}^{IN,j}, T_{AWT,k}^{IN,j}]^T.$$

The discretized dynamics of the system are included as constraints in (10b), (10c)–(10i) denote the constraints on the states, (10j)–(10l) represent the constraints on the input variables, and the non-ancitipativity constraints are included in (10m).

We propose two possible cost functions $J_{\text{batch}}(x^j_{k+1}, u^j_k)$. The first one, (11), represents the maximization of the mass of polymer together with a set-point tracking term for the reactor temperature. In addition, small regularization terms are added in order to penalize the control movements so that a smooth control input is achieved as a result of the optimization problem. The mixed tracking cost function results as:

$$
\begin{aligned}
J_{\text{track}}(x^j_{k+1}, u^j_k) = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{K-1} - m^j_{\text{P},k+1} + q(T^j_{\text{R},k+1} - T_{\text{set}})^2 \\
+ r_1(\Delta \dot{m}^j_{\text{F},k})^2 + r_2(\Delta T^{\text{IN},j}_{\text{M},k})^2 + r_3(\Delta T^{\text{IN},j}_{\text{AWT},k})^2, \\
\forall m^j_{\text{P},k+1}, T^j_{\text{R},k+1}, \dot{m}^j_{\text{F},k}, T^{\text{IN},j}_{\text{M},k}, T^{\text{IN},j}_{\text{AWT},k} \in S_i, \qquad (11)
\end{aligned}
$$

where q, r_1, r_2 and r_3 are tuning parameters. A different possibility is to avoid the use of a tracking term and to use only an economically motivated cost function:

$$
\begin{aligned}
J_{\text{eco}}(x^j_{k+1}, u^j_k) = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{K-1} - m^j_{\text{P},k+1} + r_1(\Delta \dot{m}^j_{\text{F},k})^2 \\
+ r_2(\Delta T^{\text{IN},j}_{\text{M},k})^2 + r_3(\Delta T^{\text{IN},j}_{\text{AWT},k})^2, \\
\forall m^j_{\text{P},k+1}, \dot{m}^j_{\text{F},k}, T^{\text{IN},j}_{\text{M},k}, T^{\text{IN},j}_{\text{AWT},k} \in S_i. \qquad (12)
\end{aligned}
$$

For both cases the cost is calculated as the sum over all the N scenarios S_i along the prediction horizon K. Here we implicitly assume that the batch time is minimized by maximizing the amount of polymer produced within the prediction horizon. For the multi-stage NMPC implementation we consider a scenario tree with 9 scenarios that result from the combination of the maximum, the minimum and the nominal values of the uncertain parameters. The tree is branched only in the first stage (robust horizon = 1) because a higher robust horizon results in a very similar performance as it was also illustrated in [28] but with a higher computation cost. For all the results shown in the remainder of the paper the sampling time of the NMPC controller is $T_s = 50$ s with a prediction horizon of $K = 20$ steps. The tuning parameters chosen for the cost functions presented in (11) and (12) are $r_1 = 0.1$, $r_2 = 0.02$, $r_3 = 0.01$ and $q = 10,000$.

All the algorithms presented in this paper have been implemented using the optimization tool CasADi [37], which makes it possible to greatly improve the computational speed reported in [28] with very little implementation effort. CasADi is an open-source framework for C++and Python for numerical optimization and optimal control. The main feature of CasADi is that it provides the users with a flexible framework to implement a wide range of optimal control algorithms in an easy and efficient way, rather than providing the user with a black-box Optimal Control Problem (OCP) solver. The generation of the Jacobian of the nonlinear constraints and of the Hessian of the Lagrangian function is done automatically via a state-of-the-art implementation of algorithmic differentiation as presented in [38]. If ODE or DAE integrators are part of the symbolic expressions, forward and adjoint sensitivity analysis is invoked automatically, see [39] for more details. The results presented in [37] suggest that CasADi is faster than other state-of-the-art software such as the AMPL Solver Library (ASL) when solving standard benchmark problems.

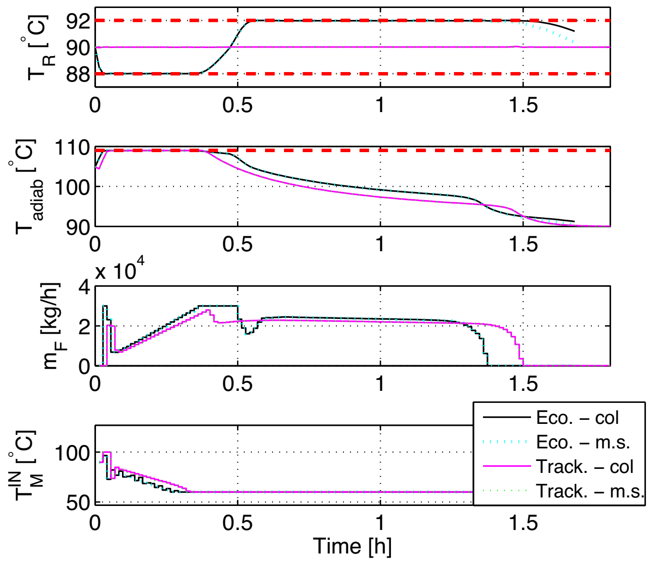

Fig. 4. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for mixed and for economic NMPC using collocation and multiple shooting for a perfect model (no uncertainty).

In this work all the resulting nonlinear programming optimization problems were solved using IPOPT [40] which uses first and second order exact derivative information provided automatically by CasADi. As described before, CasADi makes it possible to solve the optimal control problem using direct multiple-shooting or direct collocation for the discretization of the ODEs. For the collocation approach we used Radau collocation points, with interpolating polynomials of order 2. For the multiple shooting approach we used the integrators from the SUNDIALS toolbox [41]. The real plant is simulated with the calculated control input using also the integrators from the SUNDIALS toolbox with a high accuracy. All the optimization problems were solved on a standard laptop with an Intel i-5 processor at 2.30GHz running Ubuntu on a virtual machine with one core and 2 GB of RAM.

4. Tracking NMPC vs. multi-stage economic NMPC of a polymerization reactor under uncertainty

This section presents first a comparison of tracking and economic NMPC without uncertainty and afterwards a comparison of standard tracking NMPC (with typical modifications to account for uncertainty) and multi-stage NMPC under uncertainty.

First assume that the model is perfect, i.e. there is no plant-model mismatch. Then the described control problem can be solved by standard NMPC, using either the economic cost function $J_{\text{eco}}(x^j_{k+1}, u^j_k)$ or the mixed cost function $J_{\text{track}}(x^j_{k+1}, u^j_k)$ in which the center of the allowed temperature range is tracked. As expected, the use of economic NMPC improves the performance of the controller as can be seen in Fig. 4. The batch time is reduced by around 7.5%. We also show in Fig. 4 a comparison between the solution obtained using collocation and multiple shooting. Since both results are very similar, only the results with the collocation approach are shown in the remainder of the paper. The current multiple-shooting implementation has not been optimized for the performance and therefore the computation times are much higher than the ones obtained by the collocation approach (73.23 s vs. 0.072 s per optimization problem for standard NMPC with a mixed tracking objective).

As can be seen in Fig. 4 and in general when using an economic cost function, the process is typically operated at one of its constraints, which might vary along the operation. Since

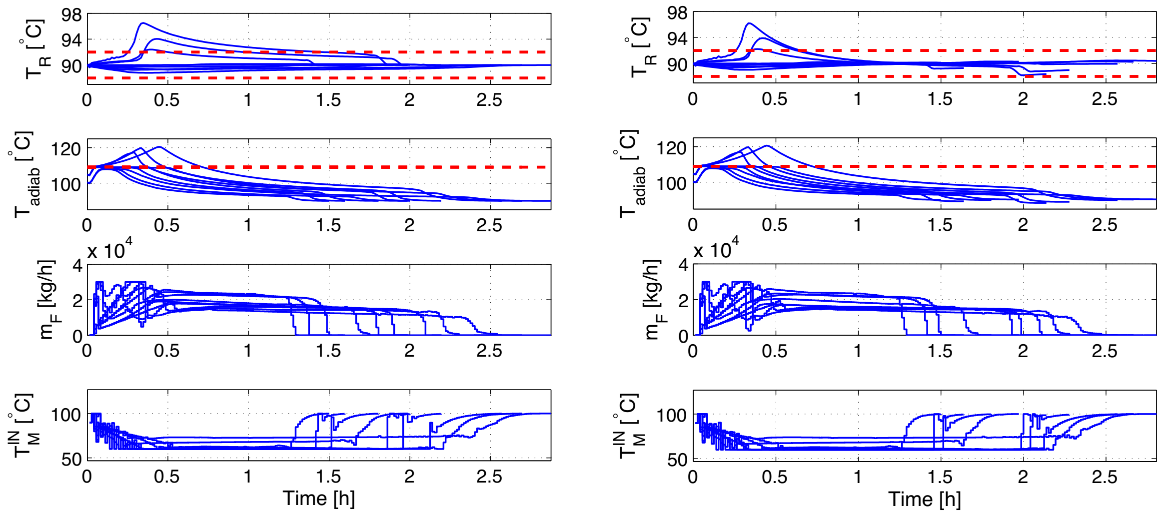

Fig. 5. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for standard NMPC (left) and for standard NMPC with bias term (right) with a mixed tracking cost function.

models for industrial applications are imperfect, constraints violations will be unavoidable, unless additional measures are taken. A typical approach used in practice is to track a conservative set-point and to expect that the tracking controller is able to maintain the system near the set-point despite the several uncertainties affecting it. This is however not enough to deal with significant uncertainties. Fig. 5 (left) shows the results of standard NMPC for different values of the uncertain parameters ΔH_R and k_0. Note that each line in the plot (and for the rest of the plots in this paper) represents the state and control trajectories with different values of the uncertain parameter for each batch (varying between ±30% with respect to their nominal values) using the same controller. The parameters are kept constant along each batch. It is clear that the standard NMPC controller with tracking of the mean value of the allowed temperature range fails to satisfy the constraints for several scenarios.

In order to increase the amount of feedback used in the standard NMPC scheme, a simple modification which introduces a bias-term for the set-point can be used. By doing this, the set-point that is used in the optimizer at each sampling time (T_{set}^{opt}) is updated using a proportional rule, i.e. $T_{set}^{opt} \leftarrow T_{set}^{opt} + K(T_{set} - T_R)$, with $K = 0.015$ where T_{set} is the real setpoint and T_R is the state of the real plant. The performance of the controller is improved (see Fig. 5 (right)) but there still are important violations of the safety constraints and for the reactor temperature that could lead to a deficient quality of the product and are not tolerable for safety reasons.

If the results are carefully analyzed, the violations occur only for certain values of the uncertain parameters, normally when the real ΔH_R and k_0 values are higher than expected, because then more heat than expected is generated, leading to constraint violations. A possible way to deal with this problem with the standard NMPC scheme with a tracking cost function is to consider the worst-case value of the uncertain parameters, i.e. $\Delta H_R = 1.30 \cdot \Delta H_R$ and $k_0 = 1.30 \cdot k_0$ in the prediction model. With this conservative choice of the uncertain parameters, standard NMPC with a mixed tracking cost function and a bias-term is able to satisfy the constraints for all cases of the uncertainty as can be seen in Fig. 6 (left). However, the obtained batch times are significantly higher than the ones obtained with the proposed multi-stage NMPC with economic cost function (Fig. 6 (right))

A summary of the results obtained with the different controllers for all the scenarios is shown in Table 4. It is clear that the use of multi-stage NMPC with a simple scenario tree can improve the performance of the controller significantly compared to a conservative choice of the uncertain parameters. Even in the case of the nominal value of the parameters, multi-stage NMPC achieves a very similar performance compared to the standard NMPC approach, while being robust for all the possible values of the uncertainty. This is due to the fact that an economic cost function is used in the multi-stage case and that the uncertainty is taken into account by using a scenario tree, whereas a tracking term of a conservative set-point is used in standard NMPC. Note that in this case, the improvement in the batch time averaged over all the scenarios is approximately 60%, which clearly shows the economic potential of the multi-stage approach compared to a conservative choice of parameters.

Table 4
Performance comparison between standard NMPC, standard NMPC with bias term, standard NMPC with bias term using the worst-case value of the parameters in the model used in the optimizer and multi-stage NMPC.

Unc. in ΔH_R	Unc. in k_0	Batch time in hours			
		Standard NMPC	Standard NMPC + bias	Std. worst-case NMPC + bias	Multi-stage NMPC
+30%	+30%	Infeasible	Infeasible	2.15	2.03
+30%	+0%	Infeasible	Infeasible	2.72	2.24
+30%	−30%	Infeasible	Infeasible	4.05	2.69
+0%	+30%	1.60	1.64	2.22	1.60
+0%	+0%	1.81	1.81	3.00	1.84
+0%	−30%	2.69	2.67	4.57	2.50
−30%	+30%	1.50	1.50	2.72	1.43
−30%	+0%	1.99	1.97	3.57	1.86
−30%	−30%	2.88	2.80	5.11	2.68
Av. batch time (h)		Infeasible	Infeasible	3.35	2.10

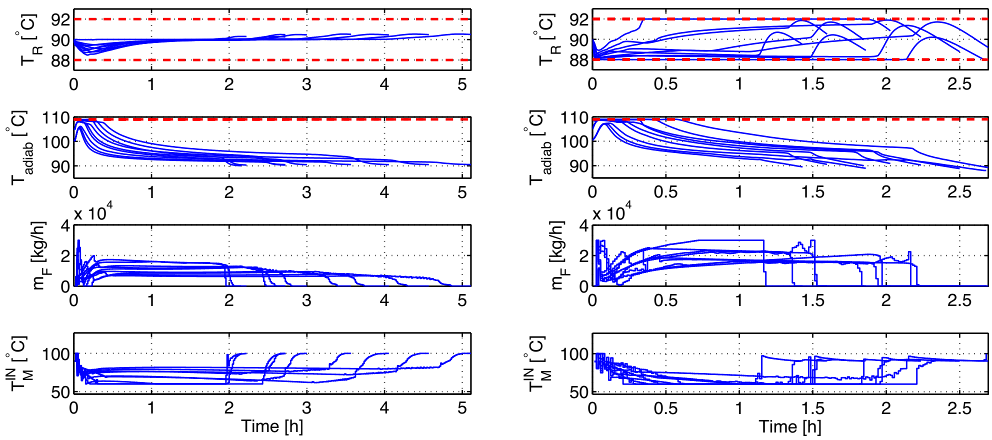

Fig. 6. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for standard NMPC with bias term and the worst case value of the parameters in the model with mixed tracking cost function (left) and for multi-stage NMPC with an economic cost function (right).

This improvement is achieved by considering the uncertainty explicitly using a robust NMPC closed-loop approach by means of a scenario tree, which increases the computational complexity of the approach. However, if efficient tools are used – as the ones described in this paper – it is possible to solve the resulting optimization problems consistently faster than the sampling time of the system ($T_s = 50$ s) which enables an implementation of the proposed scheme for this industrial case study. The average and maximum computation times per optimization problem obtained for each controller are reported in Table 5.

5. Comparison of robust economic NMPC formulations for a polymerization reactor under uncertainty

In this section we present a comparison of different robust NMPC approaches that have been presented in the literature over the last years and that were described in Section 2, i.e. multi-stage NMPC, open-loop robust NMPC, robust NMPC with affine constant policies and robust NMPC with affine time-varying policies. Our goal is to perform a comparison of the performance of each controller and we do not discuss the theoretical stability properties of the different methods, which are out of the scope of this paper. No stability or recursive feasibility problems were encountered for any of the simulations presented here.

The robustness of the controllers is achieved in all cases by enforcing the constraints on each node of a scenario tree which is obtained by combining the maximum, minimum and nominal values of the uncertain parameters as in the previous section. The same tree and the same economic cost function (12) are used for all the controllers.

Fig. 7 shows the results obtained when solving the optimization problem (3.3) in the form of a robust open-loop NMPC approach as formulated in (4). Since the constraints are checked for all the nodes in the scenario tree, no constraint violations occur for any of the scenarios. However, in the open-loop robust approach, the fact that at the next sampling time a newly computed control input will be able to counteract the effect of the realized uncertainty is ignored. This leads to a higher degree of conservativeness and therefore to longer batch times.

This can be partially compensated if a certain amount of feedback is introduced in the prediction by including a feedback gain as an additional optimization variable. If a robust NMPC controller with affine constant feedback policies is used by formulating the optimization problem as in (5) with the nominal case in the cost function, shorter batch times are obtained, as can be seen in Fig. 8 (left). If the degrees of freedom are increased by optimizing over time-varying state feedback policies (as in (6)) the performance can be increased even more, while preserving the robustness of the solution for all the different scenarios at the cost of a higher computation cost. The results for robust NMPC with time-varying feedback policies can be seen in Fig. 8 (right).

A summary of the performance of each controller for all the scenarios is given in Table 6. It can be seen that the use of any of the approaches presented in this section leads to a significant reduction of the batch times with respect to the ones obtained with standard NMPC and a conservative choice of the uncertain parameters. It is important to note that the open-loop approach leads to significantly higher batch times (25% with respect to multi-stage NMPC) because recourse is not introduced in the predictions of the NMPC

Table 5
Average and maximum computation times per optimization problem (in s) of standard NMPC, standard NMPC with bias term, standard NMPC with bias term using the worst-case value of the parameters in the model used in the optimizer and multi-stage NMPC.

	Standard NMPC	Standard NMPC + bias	Std. worst-case NMPC + bias	Multi-stage NMPC
Average (s)	0.072	0.071	0.059	1.134
Maximum (s)	0.230	0.190	0.179	1.550

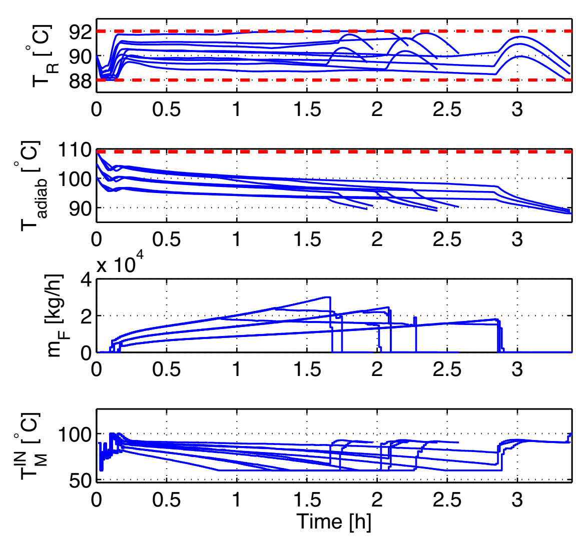

Fig. 7. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for open-loop robust NMPC with an economic cost function.

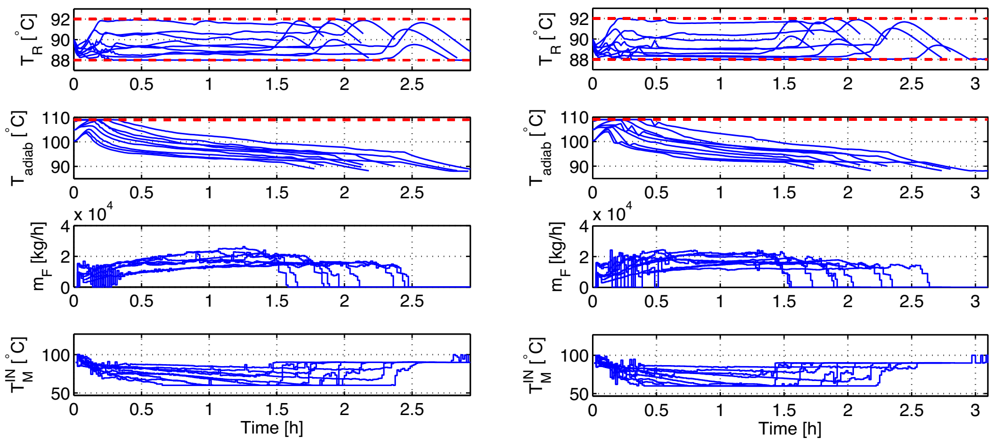

Fig. 8. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for robust NMPC with constant (left) and time varying (right) affine control policies with an economic cost function.

controller. The performance can be enhanced by using constant affine or time-varying affine feedback policies but the best performance is still achieved by multi-stage NMPC. Note that even for the nominal case of the uncertainty, which is the only one entering the cost function of the affine controllers, multi-stage NMPC achieves a better performance. This is due to the conservativeness introduced in the system by the fixed structure of the feedback. The computation times needed for the solution of each controller are reported in Table 7. The computation time needed by the open-loop approach is very similar to the one needed by the multi-stage even though it has less degrees of freedoms (free control inputs) but the same constraints are needed in order to enforce robustness. The introduction of the state feedback matrix K as optimization variable includes new degrees of freedom (see Table 8 for a comparison) and many non-zero entries in the Jacobian of the constraints and in the Hessian of the Lagrangian due to the feedback structure, which leads to computation times per iteration that are much higher than the ones obtained for multi-stage NMPC, especially in the case of time-varying feedback policies. Following [20], we use only the nominal case in the cost function for the cases of affine policies. If all the scenarios are included in the cost, the average performance for the robust NMPC with affine policies (both constant and time-varying) is slightly improved, but it is still worse than the multi-stage case for all the scenarios and it leads to larger computation times.

6. Multi-stage economic NMPC with reduced variability

From a practical point of view, operating a system that behaves consistently in the same manner despite the presence of changes in the plant dynamics or of disturbances that act on the plant can be beneficial. For this reason, some control approaches try to achieve a similar control performance of an uncertain system for all the possible cases of the uncertainty. In some of the formulations of tube based-MPC, as the one presented in [23], the variability of

Table 6
Performance comparison between open-loop robust NMPC, robust NMPC with affine constant policies, robust NMPC with affine time-varying policies and multi-stage NMPC.

Unc. in ΔH_R	Unc. in k_0	**Batch time in hours**			
		Open-loop robust NMPC	Constant affine policies	Time-varying affine policies	Multi-stage NMPC
+30%	+30%	2.22	2.14	2.09	2.03
+30%	+0%	2.58	2.38	2.31	2.24
+30%	−30%	3.38	2.93	2.81	2.69
+0%	+30%	1.97	1.85	1.74	1.60
+0%	+0%	2.42	2.13	2.01	1.84
+0%	−30%	3.38	2.83	2.74	2.50
−30%	+30%	1.93	1.78	1.74	1.43
−30%	+0%	2.43	2.18	2.18	1.86
−30%	−30%	3.39	2.92	3.00	2.68
Av. batch time (h)		2.63	2.34	2.29	2.10

Table 7
Average and maximum computation times per optimization problem (in s) of open-loop robust NMPC, robust NMPC with affine constant policies, robust NMPC with affine time-varying policies and multi-stage NMPC.

	Open-loop robust NMPC	Constant affine policies	Time-varying affine policies	Multi-stage NMPC
Average (s)	1.113	13.87	45.43	1.134
Maximum (s)	2.540	128.2	182.6	1.550

Table 8
Degrees of freedom (free control input variables) available for open-loop robust NMPC, robust NMPC with affine constant policies, robust NMPC with affine time-varying policies and multi-stage NMPC.

	Open-loop robust NMPC	Constant affine policies	Time-varying affine policies	Multi-stage NMPC
D.o.F.	60	90	660	540

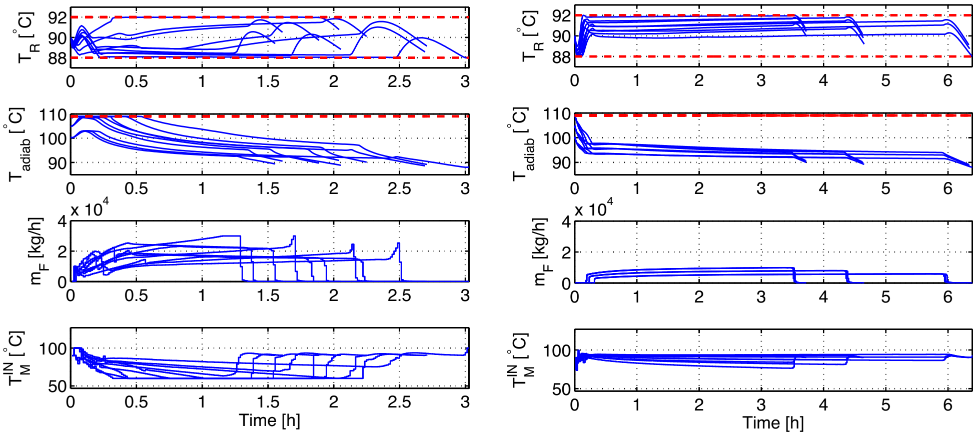

Fig. 9. Reactor temperature, safety temperature (with constraints indicated), monomer feed and jacket temperature for multi-stage NMPC with reduced variability with $k_{var} = 0.1$ (left) and $k_{var} = 1$ (right) in the economic cost function (13a).

the different trajectories can be influenced by tuning a parameter that controls how strong the influence of the ancillary controller is. Using a high value of this parameter leads to less variability, but also to a reduction of the average performance.

In this work, we follow the same idea to introduce a novel formulation of the multi-stage NMPC approach described before. The cost function is modified by introducing an additional term which penalizes the deviations between the scenarios. The new optimization problem can be written as:

$$\min_{x_k^j, u_k^j \forall (j,k)\in I} \left(\sum_{i=1}^{N} (\omega_i J_i(x_{k+1}^j, u_k^j))^\alpha\right)^{1/\alpha} + k_{var}\left(\sum_{k=1}^{K}\sum_{j=1}^{T_k-1}(x_k^j - x_k^{j+1})^2\right) \tag{13a}$$

subject to:

$$x_{k+1}^j = f(x_k^{p(j)}, u_k^j, d_k^{r(j)}), \quad \forall (j, k+1) \in I, \tag{13b}$$

$$g(x_k^j, u_k^j) \le 0, \quad \forall (j,k) \in I, \tag{13c}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)} \quad \forall (j,k), (l,k) \in I, \tag{13d}$$

where k_{var} is a tuning parameter that controls the trade-off between robust economic performance and variability of the different scenarios. The number of nodes in the scenario tree at stage k is denoted by T_k. The new term introduced in (13a) penalizes (with a quadratic term) the deviations between two *neighboring* scenarios along the prediction horizon K for all the scenarios. Note that the presented approach is not a tube-based approach, although it was inspired by tube-based ideas. There are three main differences of the presented approach compared to the usual tube-based MPC approaches. Firstly, tube-based approaches guarantee that the real system remains in a robust positively invariant set around some trajectory, which is not guaranteed in the proposed method. Secondly, the use of the typical structure consisting of a nominal MPC and an ancillary controller is substituted by a single optimizing controller with a multi-objective cost function (13a). Thirdly, the trajectories of the system are not forced to track the nominal trajectory, but they are free to stay close around any trajectory which is optimal in average for the different scenarios in the tree. This formulation is comparable to minimizing an approximation of the sensitivities of the states with respect to the uncertain parameters. It is important to note that in the multi-stage approach the sensitivities are indirectly computed when predicting over all the scenarios and therefore it is not necessary to compute the sensitivities explicitly, which might be expensive. In this way it is possible to use the scenarios for a twofold purpose. First, to guarantee robust constraint satisfaction, and second to reduce the variability of the system in the presence of uncertainties.

The results obtained with the approach proposed in (13) are shown in Fig. 9 for different values of k_{var}. The results show that by increasing k_{var} the state trajectories are closer for the different values of the uncertainties, obtaining also smoother control inputs, but the batch times are much higher.

We define the variability obtained by the controller as the difference of each trajectory to the average trajectory summed up over the batch time

$$\text{Variability} = \sum_{i=1}^{N} \frac{1}{K_i^f} \sum_{k=1}^{K_i^f} \frac{|x_k(i) - x_k^{av}|}{x_k^{av}}, \tag{14}$$

where $x_k(i)$ represents the real state of the plant at sampling time k for the scenario (realization of the uncertainty) i and all the operators are applied element-wise. The number of sampling times that are necessary to end the batch for each scenario are denoted as K_i^f and x_k^{av} is the average state of the real system at sampling time k over all the scenarios, that is:

$$x_k^{av} = \frac{1}{N}\sum_{i=1}^{N} x_k(i). \tag{15}$$

Using this definition it is possible to perform an analysis of the system by comparing the variability obtained by the controller with the resulting batch times for different values of k_{var}. This analysis is shown in Fig. 10. As it can be seen, trying to reduce the

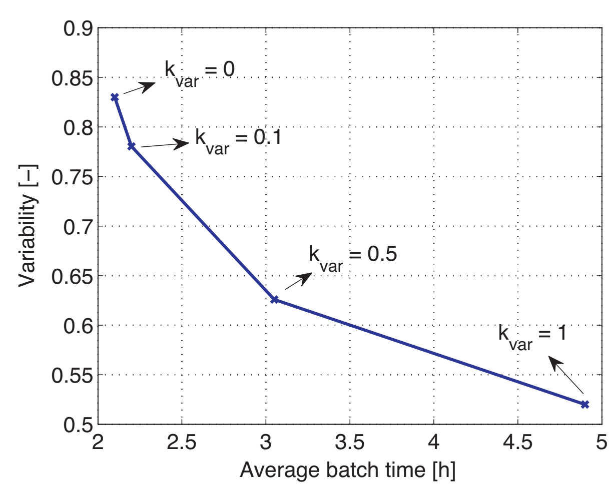

Fig. 10. Average batch time and variability over the different scenarios for different values of k_{var}.

variability (increasing k_{var}) of the system causes a significant loss of the economic performance of the process.

Reducing the variability of the system with respect to a certain trajectory might be a good idea if the cost function is a classical tracking term, since both goals go in the same direction, that is, if the nominal trajectory tracks the set-point well and if the uncertain trajectories are near the nominal one, then the average performance will be good. However, if an economic cost function is used, very often the objective of a reduced variability and of an optimal economic performance are contradictory. This can be clearly illustrated with a simple example used often in the MPC literature. If a driver wants to track the center of a road and the driver wants to minimize the variability of his trajectory despite the uncertain conditions of the road, the solution of this problem is to drive very slowly such that the center of the road can be tracked well for all the conditions of the road. This result will be good if the ultimate goal is just to track the center of the road. However, this solution will provide very poor results if the real goal is to drive a certain distance in the minimum time possible fulfilling the constraints for all the cases of the uncertainty. The same happens in the presented case-study, where the result with a big value of k_{var} (Fig. 9 (right)) leads to slow feeding of the monomer $\dot{m}_F$ in order to achieve low variability but leading to very long batch times.

Note that it is also possible to choose k_{var} such that only the variability of certain states (or other algebraic variables) is penalized. It is also possible to choose $k_{var} < 0$ in order to excite the system. This can be useful in the context of Optimal Experiment Design (OED) to increase the identifiability of certain parameters with respect to the available measurements. OED can be also used to reduce the uncertainty range of the uncertainty and to generate a new scenario tree accordingly that leads to improved performance as it has been shown in [42].

Our goal in this section is not to compare different tube-based approaches. We try to illustrate with simulation results the fact that, in the same way as the concepts and tools that are needed for stability guaranteeing formulations of economic MPC are different to those of classical tracking MPC [7], some typical approaches used in robust tracking MPC that try to minimize the variability of the system may not be suitable in the case of economic MPC because they might lead to significant losses of performance.

The powerful tools of set theory used in some tube-based methods for establishing stability and constraint guarantees could be combined with the multi-stage approach in order to make use of the advantages of both approaches by considering, for example, *slim* tubes centered along the different scenarios of the scenario tree.

7. Conclusions and future work

The stability properties of different economic MPC settings have been studied recently in the literature. However, the fact that uncertainty plays a crucial role in economic MPC because real models are imperfect and the economic operation of a plant typically operates the system at one of its constraints has received little attention yet. This paper presents a comprehensive comparison of the performance of different robust NMPC methods for the solution of an economic NMPC problem of an industrial batch polymerization reactor provided by BASF SE.

We use multi-stage NMPC in order to deal with uncertainties in the context of economic MPC. Multi-stage NMPC is based on the representation of the uncertainty evolution as a scenario tree, which makes it possible to introduce feedback explicitly in the prediction of the controller, thus improving its performance. Simulation results show that multi-stage NMPC with an economic cost is able to satisfy tight temperature constraints and safety-related constraints for all the scenarios under consideration that represent variations of ±30% in critical parameters, while standard NMPC and standard NMPC with bias term violate the constraints. Choosing a standard NMPC scheme with tracking term and with a conservative choice of the uncertain parameters results in no constraint violations but increases the obtained batch times significantly compared to multi-stage NMPC. We also compare multi-stage NMPC with other robust approaches proposed in the literature. Although the results have been obtained only for an industrial polymerization reactor, we believe that the main conclusions are useful for the design of robust economic NMPC controllers of many nonlinear systems with tight constraints. It has been shown that the use of a robust open-loop approach can lead to an important decrease of the performance compared to approaches with feedback or recourse. The introduction of feedback using state feedback policies (constant or time-varying) improves the performance, but for nonlinear systems it can be far from the performance obtained from multi-stage NMPC as in this case. Finally, we presented a novel extension of multi-stage NMPC that was inspired by tube-based MPC ideas that makes it possible to have a trade-off between system variability under uncertainty and robust economic performance. We show that trying to reduce the variability of the trajectories obtained for the different values of the uncertainty – as done for some robust NMPC schemes – might lead to a significant loss of performance, especially for economic robust NMPC.

Future work includes the extension of the approach to account for estimation and measurement noise and the implementation of the approach at a real reactor.

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