Preprints of the 8th IFAC Symposium on Advanced Control of Chemical Processes
The International Federation of Automatic Control
Furama Riverfront, Singapore, July 10-13, 2012

A new Robust NMPC Scheme and its Application to a Semi-batch Reactor Example

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Abstract: In this paper, a non-conservative robust nonlinear model predictive control scheme that can guarantee satisfaction of the constraints and optimal expected performance under uncertainty is introduced. The proposed control scheme is evaluated by simulations using a well known benchmark problem where the operation of a semi-batch polymerization reactors is optimized under very tight temperature tolerance limits. The simulation results show that the proposed scheme is capable of optimizing the process operation and, at the same time, it ensures robust operation within the whole range of uncertainties.

Keywords: Robust control; Model predictive control; Multistage optimization; Semi-batch reactors

1. INTRODUCTION

Model predictive control (MPC) is a control strategy that is widely used in process engineering mainly because of its ability to treat multi-input multi-output plants and to deal with constraints. In addition, it offers the possibility to optimize the plant performance by using an economic criterion in the cost function instead of using a classical set-point tracking formulation. MPC solves an open-loop optimization problem over a finite horizon at each sampling time, and feedback information enters only by the re-initialization of the calculation based on the available information. Therefore, one of the main problems is the fact that the performance and stability of the control loop relies strongly on the accuracy of the model that is used in the optimization.

The importance of this problem has attracted the attention of both the industrial and the research community to the field of robust model predictive control. However, there is still no approach that simultaneously handles nonlinear systems, is real-time implementable, guarantees robust constraint satisfaction and shows a low degree of conservatism.

Most robust approaches are based on a min-max formulation, firstly introduced in [Campo and Morari, 1987] where the cost of the worst-case realization over all possible values of the uncertainty is minimized. Min-max controllers can be classified into open-loop and closed-loop approaches, see [Lee and Yu, 1997]. The first ones are known to provide conservative solutions and they lead easily to infeasibilities during the optimization, as illustrated in [Scokaert and Mayne, 1998]. In contrast, closed-loop approaches take the presence of feedback directly into account by optimizing over different control policies, however in general this is a very difficult problem to solve. It can be simplified by formulating it as an optimization over a restricted type of control policies (e.g. affine policies), but this results in suboptimality, which can be bounded for linear time-varying systems [Hadjiyiannis et al., 2011].

In our approach we consider the two-stage robust MPC formulation proposed in [Dadhe and Engell, 2008] and [Engell, 2009]. The uncertainty is modeled as a scenario tree, as in [Scokaert and Mayne, 1998], and feedback information is taken explicitly into account by assuming that new information about the true state of the plant will become available at each sampling instant and that the future control inputs (also called recourse variables) can be adapted to the evolution of the uncertainties and hence, the conservativeness of the approach is largely reduced. Similar approaches have been used in [Muñoz de la Peña et al., 2005], and [Bernardini and Bemporad, 2009] for linear systems. Assuming that the scenario tree describes the uncertainty perfectly, this approach represents exactly the real-time decision problem and therefore is the best possible solution. However, it results in a problem the size of which grows exponentially with the prediction horizon and with the number of uncertainties and uncertainty levels.

In this work we apply this approach to a well-known benchmark problem on temperature control of semi-batch reactors that was presented by [Chylla and Haase, 1993]. This control problem is also known as the CHBR (Chylla-Haase Benchmark Reactor). Although several advanced control

⋆ The research leading to these results has received funding from the European Union Seventh Framework Programme FP7/2007-2013 under grant agreement number FP7-ICT-2009-4 248940 and from the Deutsche Forschungsgemeinschaft (DFG, German Research Council) in the context of the research cluster: Optimization-based control of uncertain systems.

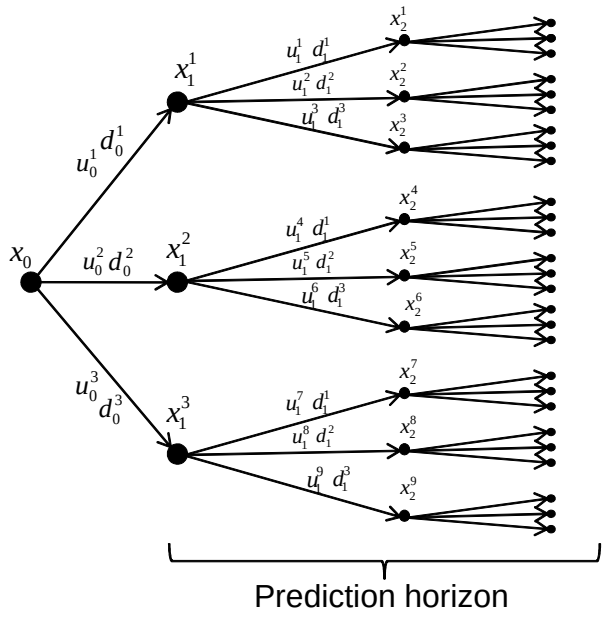

Fig. 1. Scenario tree representation of the uncertainty evolution

schemes that can considerably improve the performance of the temperature control of the CHBR have been already reported (see [Graichen et al., 2006] for a review), there is still no scheme that can guarantee robustness under the whole range of uncertainties.

After this introductory section, this paper is organized as follows. The proposed robust NMPC scheme is introduced in Section 2 and some additional information about its implementation are given in Section 3. In section 4, the CHBR is briefly revisited. In Section 5, simulation results are discussed. The paper is then concluded in Section 6.

2. MULTI-STAGE NMPC

In the multi-stage robust NMPC approach the uncertainty is modeled by a tree of discrete scenarios (see Fig. 1) where the uncertainty is resolved at each node and the control inputs are separated into stages. Each path from the root node x_0 until the leaf nodes is called a scenario. In this manner, at each node of the tree, a decision is computed based on the information up to that time, taking into account explicitly the uncertainty about the future evolutions from this node, as well as the future decisions on these branches. In order to model the real-time decision problem correctly, decisions based upon the same information must be equal. This is imposed by the so-called *non-anticipativity* constraints. They force all control inputs that branch at one node to be the same (i.e., in Fig. 1 $u_0^1 = u_0^2 = u_0^3$, $u_1^1 = u_1^2 = u_1^3$, ...). We consider a discrete-time formulation of an uncertain nonlinear system described by:

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

where $x_k^j \in \mathbb{X} \subseteq \mathbb{R}^n$, $u_k^j \in \mathbb{U} \subseteq \mathbb{R}^m$ are the j-th state and control vectors at stage k, and d_k^l describes the uncertainty at stage k. It can include parametric uncertainties or unknown disturbances within known bounds. It is assumed that the evolution of the uncertainty can be represented by a tree of discrete realizations. The state at stage k, x_k^j, depends on the values of the previous stage, denoted as (x_k, u_k, d_k), following the structure of the tree depicted in Fig. 1. For simplicity, the uncertainty and therefore the scenario tree are assumed to be uniform, i.e., it has the same number of branches at all nodes, given by $d_k^l \in \{d_k^1, d_k^2 ... d_k^s\}$ at stage k for s different possible values of the uncertainty. For ease of notation, the vector of nodes is defined as $\tilde{x} = [x_0, x_1^1, x_1^2, ..., x_{N_p}^N]$, and the vector of control inputs as $\tilde{u} = [u_1^1, u_1^2, ..., u_{N_p}^N]$, where N is the number of scenarios (or leaf nodes) and N_p is the prediction horizon. These vectors contain all states and controls in the scenario tree. Finally, we define the scenario vector S_i that contains all states and controls belonging to the scenario i.

Then, the optimization problem is formulated as:

$$\begin{aligned} \min_{\tilde{u}} \quad & \sum_{i=1}^{N} \omega_i J_i \\ s.t. \quad & x_{k+1}^j = f(x_k, u_k, d_k), \\ & x_k^j \in \mathbb{X}\,, \forall\, x_k^j \in \tilde{x}, \\ & u_k^j \in \mathbb{U}\,, \forall\, u_k^j \in \tilde{u}, \\ & \tilde{u} \in \mathbb{T}, \end{aligned} \tag{2}$$

where $\mathbb{T}$ is the set of all possible vectors of control inputs that satisfy the *non-anticipativity* constraints, ω_i is the probability of each scenario and J_i is the cost of each scenario, defined by:

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

where $L(x_{k+1}^j, u_k^j)$ is the stage cost. This formulation includes a closed-loop min-max approach if the summation in (2) is substituted by the *max* operator.

2.1 Dealing with the problem size

The main drawback of this approach is the size of the resulting optimization problem. It grows exponentially with the number of uncertainties, with the number of uncertainty levels, and with the prediction horizon. However, there exist some techniques that allow to control the growth of the tree or approximate it by using only representative scenarios [Römisch, 2009].

A simple strategy to control the size of the tree is to consider the branching of the tree only up to a certain stage (called the *robust horizon*) and then to consider the uncertainty to be constant until the end of the prediction horizon. A similar idea has been applied in the contexts of scheduling [Cui and Engell, 2010] and linear min-max MPC in [Muñoz de la Peña et al., 2006].

Different strategies have been studied for the approximation of scenario trees based for example on machine learning techniques [Defouny et al., 2011], or others reviewed in [Römisch, 2009].

3. IMPLEMENTATION

The formulation presented in the previous section assumes a discrete nonlinear model. However, most chemical pro-

cesses are modeled using ordinary differential equations, that can be written as follows:

$$\dot{x} = \Phi(x, u, d). \tag{4}$$

It is possible to formulate the multi-stage NMPC problem with first principles models as a big but very structured Nonlinear Programming Problem (NLP) in the standard form. A very simple direct collocation method is applied here for the discretization of the differential equations. Using the implicit Euler's discretization, the discretized system can be written as:

$$x_{k+1} = x_k + \Delta T(\Phi(x_{k+1}, u_k, d_k)). \tag{5}$$

An implicit method is chosen because since a simultaneous method is used for the solution of the optimal control problem, both the states (x) and the control inputs (u) are optimization variables. Therefore, the discretized model equations are added as nonlinear constraints to the NLP and the computation complexity is similar to the one using explicit methods, but with the advantages of the implicit ones.

The formulation of the NLP is:

$$\min_{x^{opt}} \quad x^{opt'} Q x^{opt} \tag{6a}$$

$$s.t. \quad x_l \leq x^{opt} \leq x_u, \tag{6b}$$

$$b_l \leq A x^{opt} \leq b_u, \tag{6c}$$

$$c_l \leq c(x^{opt}) \leq c_u, \tag{6d}$$

where x^{opt} is the augmented optimization vector. It includes all the states (nodes) and control inputs as indicated in Fig. 1. That is, $x^{opt} = [x_0, x_1^1, x_1^2, ..., x_{N_p}^N, u_1^1, u_1^2, ..., u_{N_p}^N]$.

The matrix Q in the objective function (6a) is a big and sparse matrix that includes all the penalty weights in the correct order and structure to create an objective function in the form of (2). The constraints in (6b) express the bounds on the optimization variables, that is, the state and control constraints imposed on the real system. It is also necessary to include the *non-anticipativity* constraints in the linear constraints (6c). Finally, in (6d), the discrete model described in (5) is introduced for all the nodes in the tree. Therefore, the Jacobian of the nonlinear constraints is a sparse and highly structured matrix.

The fact that the problem is sparse and very structured, allows for an explicit exploitation of the structure that could lead to a fast solution despite of the size of the problem [Steinbach, 2000], but this issue is not addressed in this paper. The problem is solved here using the sparse nonlinear solver SNOPT (see [Gill et al., 2008]) via MATLAB/TOMLAB.

4. DESCRIPTION OF THE BENCHMARK PROBLEM

The Chylla-Haase Reactor, which is described in detail in [Chylla and Haase, 1993], consists of a stirred tank reactor where an emulsion polymerization reaction takes place and a heat exchanger system with a jacket and a recirculation loop. The heat exchanger can be used either to heat the reactor or to cool it. In the heating mode, a steam valve that manipulates the injection of medium-pressure steam into the recirculation water is activated, and in the cooling mode, a dumping valve that manipulates the amount of cold water that enters the recirculation loop is actuated. The reactor is used to produce different products which are obtained from different recipes. The different recipes consist of a sequence of charging, heating, feeding and holding steps that may or not be repeated. A detailed description of the individual steps can be found in [Graichen et al., 2006]. As the end-use properties of the product mainly depend on the temperature at which the polymerization takes place, a very precise temperature control is required. According to [Chylla and Haase, 1993] the reactor temperature must stay within a very tight range of 0.6 K around the specified reaction temperature in order to guarantee that the final product will have acceptable quality. [1]

In the original version of the Chylla-Haase problem the monomer is dosed into the reactor with a constant flow rate and there is almost no degree of freedom for process optimization. In [Finkler et al., 2012], a modified version of the CHBR in which variable monomer inlet flow rates can be employed has been proposed. This turns the CHBR into a much more challenging problem that involves simultaneous optimization of monomer dosage and cooling usage along the semi-batch run. As the goal of this work is to investigate robust optimizing NMPC, this modified version of the CHBR is considered here.

4.1 Modeling of the Process

In [Chylla and Haase, 1993], an experimentally validated model that describes the system behavior is given. This model has been extensively investigated by the process control community and several mistakes in its formulation have been identified and corrected. For brevity, these corrections issues are not covered here and the reader is directed to [Graichen et al., 2006] for more detailed discussion. The corrected model used in this investigation consists of a set of ODE's given by equations (7) to (11), which are written as:

$$\dot{m}_M = \dot{m}_M^{in} - r_P, \tag{7}$$

$$\dot{m}_P = r_P, \tag{8}$$

$$\begin{aligned} \dot{m}_T = &\frac{\dot{m}_M C_{p,M}(T_{amb} - T) + UA(\bar{T}_J - T)}{m_M C_{p,M} + m_P C_{p,P} + m_W C_{p,W}} \\ &+ \frac{UA_{loss}(T_{amb} - T) + r_P \Delta H_P}{m_M C_{p,M} + m_P C_{p,P} + m_W C_{p,W}}, \end{aligned} \tag{9}$$

$$\dot{T}_j^{out} = \frac{\dot{m}_C C_{p,W}(T_j^{in}(t - \theta_1) - T_j^{out}) + UA(T - \bar{T}_j)}{m_C C_{p,W}}, \tag{10}$$

$$\dot{T}_j^{in} = \dot{T}_j^{out}(t - \theta_2) + \frac{T_j^{out}(t - \theta_2)}{\tau_p} + \frac{K_p(c)}{\tau_p}, \tag{11}$$

where m_M, m_P, and m_W are the holdups of monomer, polymer, and water inside the reactor, T, T_J^{out}, T_J^{in}, T_{amb} are the inner reactor temperature, the water temperature

[1] Although such a tight tolerance may be questioned from a practical point of view, e.g. because of the limited accuracy of the temperature sensors, we stick to it here. This is important in order to compare the performance of the proposed scheme with other control solutions for this problem.

at the jacket outlet, the water temperature at the jacket inlet, and the ambient temperature, r_P is the polymerization rate, ΔH_P is the reaction heat, U is the overall heat transfer coefficient, A is the heat transfer area, $\dot{m}_M^{in}$ is the monomer inlet flow, $\dot{m}_C$ is the flow rate of water across the jacket, m_C is the mass of water inside the jacket, $C_{p,M}$, $C_{p,P}$, and $C_{p,W}$ are the thermal capacities of monomer, polymer, and water, respectively, θ_1 and θ_2 are time delays, τ_P is the jacket time constant; the heating/cooling usage c is a control command that can vary from 0 to 100%, and the heating/cooling function K_p is a function of c with the split-range characteristic given by (12), with T_{inlet} and T_{steam} being the cold water and the medium-pressure steam temperatures:

$$K_p(c) = \begin{cases} 0.8 \times 30^{-c/50}(T_{inlet} - T_j^{in}), & c < 50\% \\ 0, & c = 50\% \\ 0.15 \times 30^{c/50-2}(T_{steam} - T_j^{in}), & c > 50\%. \end{cases} \quad (12)$$

The empirical relations for the computation of r_P and U can be written as:

$$r_P = ikm_M \quad (13)$$

$$U = \frac{1}{h^{-1} + hf^{-1}} \quad (14)$$

where i is the purity factor, k is the first order kinetic constant, $1/h$ is the film heat transfer coefficient and $1/hf$ is the fouling factor which depends on the batch number. Other variables and parameters that appear in the model equations, can be easily found in the literature on the CHBR. The readers can consult [Graichen et al., 2006] for more information.

4.2 Modeling of the Uncertainties

In [Chylla and Haase, 1993], the main uncertainties and disturbances that affect the process are condensed in three variables, the purity factor i, the fouling factor $1/hf$ and the ambient temperature T_{amb}. The purity factor i, which varies from 0.8 to 1.2 and describes the fluctuations in the reaction rate caused by impurities in the row-materials. It is constant during one batch, but it changes randomly from batch to batch. The fouling factor $1/hf$ varies from 0 to 0.704 m^2KkW^{-1} in order to simulate the decrease in U due to the formation of a polymer film on the reactor wall during the successive batches. Finally, the ambient temperature, which affects the monomer inlet feed and the initial conditions, can vary from 280 to 350 K from winter to summer. In, [Chylla and Haase, 1993] it is also suggested that the time delays θ_1 and θ_2 may vary by 25% when compared to the nominal values. For simplicity, these time delays are neglected here. Finally, although data for two different products, A and B, is given in [Chylla and Haase, 1993], this work is restricted to product A only.

5. ECONOMIC ROBUST NMPC OF THE CHYLLA-HAASE REACTOR

The robust model predictive control approach presented above has been applied to the CHBR. The method was implemented as explained in Section 3. We use an economic cost function in which the monomer feed is maximized in order to minimize the batch time, that is, the objective function is:

$$J = \sum_{i=1}^{N} \omega_i \sum_{k=0}^{N_p-1} (\dot{m}_{M,k}^{in,j} - \dot{m}_M^{max})^2 \ , \forall \ \dot{m}_{M,k}^{in,j} \in S_i, \quad (15)$$

where $\dot{m}_M^{max}$ is the maximum allowed feeding rate, as explained in [Finkler et al., 2012]. Since the reactor is cleaned every 5 batches, the fouling factor can be easily guessed. Moreover, the ambient temperature can be measured and therefore only the impurity factor is considered as an uncertainty here. With this configuration, the scenario tree is quite simple and the problem can be solved faster than real time. A prediction horizon of $N_p = 4$ time steps with $T_{step} = 20$ s has been chosen. The probabilities of the different values of the uncertainty are chosen to be the same, that is, all scenarios have the same probability to occur. In this section, the proposed robust NMPC scheme is first compared with the standard NMPC solution assuming that full state feedback measurement is available. Furthermore, the robust NMPC scheme is evaluated in the situation where only noisy temperature measurements are available and a state estimator has to be used to reconstruct the state vector in order to initialize the controller.

5.1 Standard NMPC

The problem has been solved with the standard nominal NMPC formulation for the different values of the purity, i.e., 0.8, 1.0, and 1.2 respectively. To be fair in the comparison with the robust approach, the three different values have also been used in the model of the optimizer, so, nine different simulations were carried out. For most of the cases where the model of the optimizer is not exactly the same as the model of the real plant, the temperature constraints along the batch are not satisfied. A simulation where the purities used in both the optimizer model and the simulated plant are equal to 0.8 is presented in Fig. 2. An example of the violations of the constraints can be seen in Fig. 3 where the purity used in the optimizer is 1.2 and the purity of the real plant is 0.8.

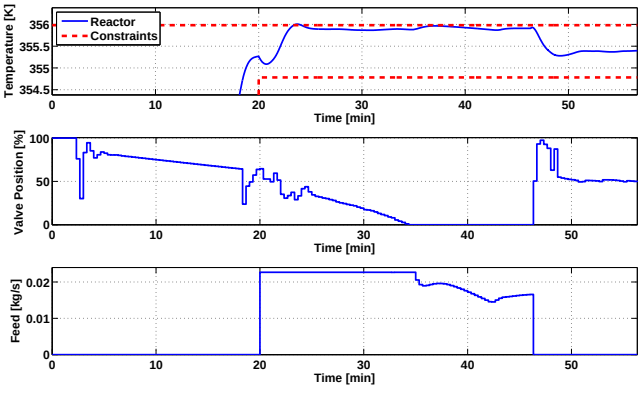

Fig. 2. Reactor temperature, valve position and monomer feed for standard NMPC, controller purity = plant purity = 0.8

5.2 Robust NMPC

The problem is formulated as a big NLP, including the *non-anticipative* constraints in the first stage. The results

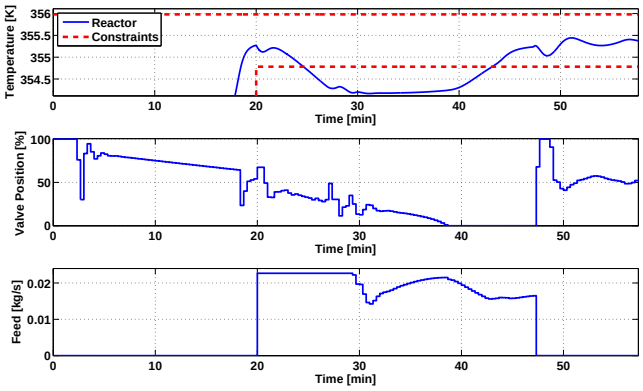

Fig. 3. Reactor temperature, valve position and monomer feed for standard NMPC, controller purity = 1.2, plant purity = 0.8

show that the controller is capable of maintaining the reactor temperature between the specified bounds for all values of the uncertainty. An example of the behavior can be seen in Fig. 4. The use of robust horizon $RH = 1$ and $RH = 2$ is compared and since in this case using $RH = 1$ gives a satisfactory performance with a lower computational cost, $RH = 1$ will be used in the remainder of the paper. A comparison of the performance of standard, multi-stage and min-max NMPC approaches is summarized in Table 1. The min-max approach is implemented by using the *max* operator instead of the summation in (2). When compared to the nominal NMPC cases, the performance losses of the robust multi-stage approach are minimal and it is never worse than the min-max case.

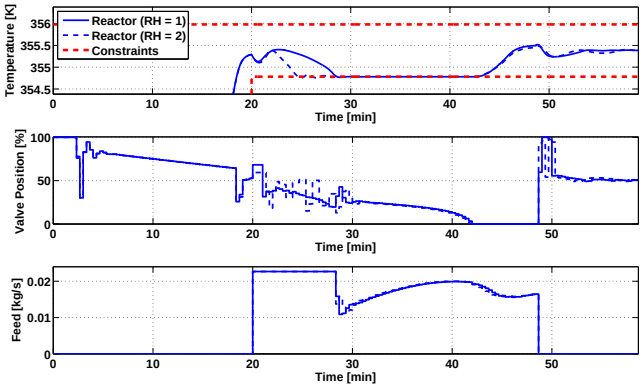

Fig. 4. Reactor temperature, valve position and monomer feed for multi-stage NMPC, plant purity = 0.8

With respect to computation speed, each iteration of the multi-stage NMPC controller takes around 0.59 s. ($RH = 1$) and 3.25 s. ($RH = 2$); the time is of 0.70 s. in the case of min-max NMPC with $RH = 1$ while the sampling time is 20 s. Therefore, this non-conservative approach can handle nonlinear systems with robust constraint satisfaction and is real-time implementable. It is important to note that the performance of the NMPC controller for intermediate values of the uncertainty, between the ones considered in scenario tree design is also satisfactory, as can be seen in Fig. 5. The different monomer feed trajectories, and the resulting batch durations are shown in Fig. 6.

		Feeding time in minutes		
Plant imp.	**Impurity controller**	**Standard NMPC**	**Multi-stage NMPC**	**Min-max NMPC**
0.8	0.8	26.33	28.67	29.33
	1.0	infeasible		
	1.2	infeasible		
1.0	0.8	infeasible	25.67	26.00
	1.0	25.67		
	1.2	infeasible		
1.2	0.8	infeasible	25.67	25.67
	1.0	25.67		
	1.2	25.67		

Table 1. Performance comparison between standard, multi-stage ($RH = 1$) , and min-max ($RH = 1$) NMPC.

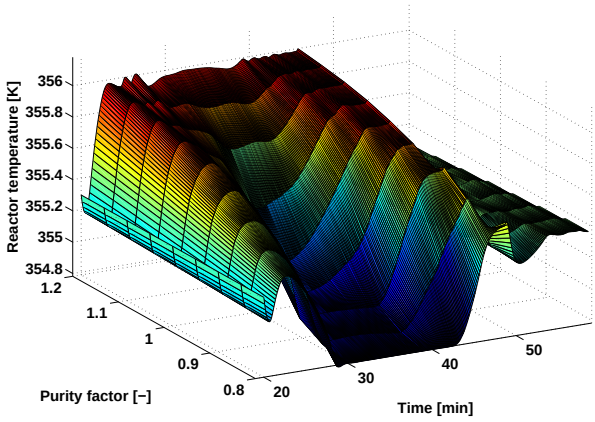

Fig. 5. Reactor temperature for different values of the purity factor in the plant for multi-stage NMPC

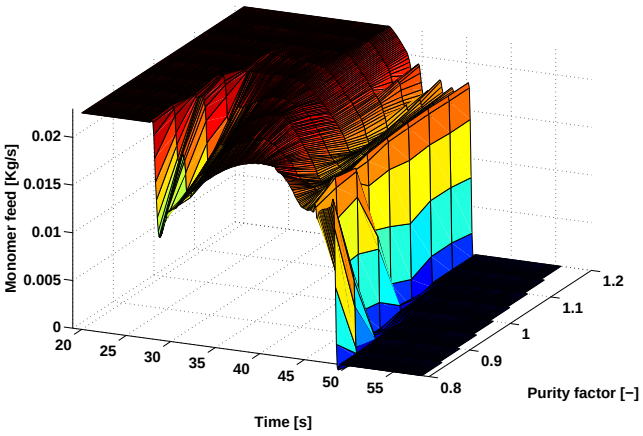

Fig. 6. Monomer feed trajectories for different values of the purity factor in the plant for multi-stage NMPC

5.3 Robust NMPC with Extended Kalman Filter

In this subsection it is assumed that only noisy temperature measurements with a standard deviation $\sigma = 0.05$ K are available, as it is the case in the real process. Therefore, the other states have to be estimated in order to initialize

the NMPC controller along the batch. In this work, an Extended Kalman Filter (EKF) which uses the nominal model of the plant is used for this task. The results of a simulation where the robust NMPC scheme is combined with the EKF are presented in Fig. 7. In this case a sampling time $T_{step} = 40$ s is used. Because of the estimation error, it is not possible to strictly guarantee robust constraint satisfaction and the temperature tolerance bounds are violated slightly during the reaction period. It can be observed that the noise of the measurements is propagated and it results in small oscillations in the control inputs. This issue, as well as the small constraint violations, could be avoided if the measurement and estimation errors are taken explicitly into account in the design of the scenario tree. Nevertheless, the results show that the performance of the robust NMPC is still good and that the small constraint violations are negligible from the practical point of view.

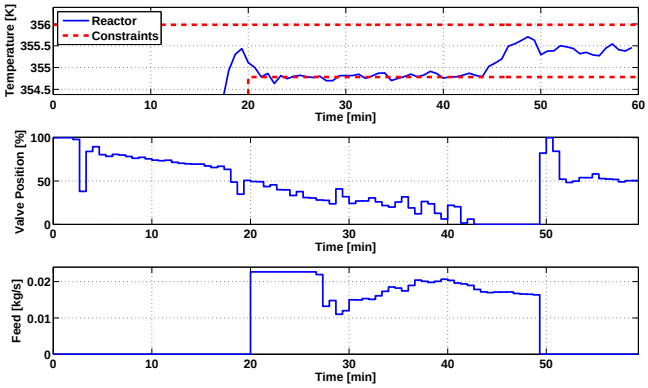

Fig. 7. Reactor temperature, valve position and monomer feed for multi-stage NMPC with EKF, plant purity = 0.8

6. CONCLUSION

In this paper, a robust nonlinear model predictive control approach has been presented. The uncertainty is taken into account explicitly by considering discrete disturbances that are represented as a scenario tree. The problem is formulated as a structured NLP that can be solved fast enough for real-time applications. The approach has been applied to the Chylla-Haase problem, which is a well-known case study for polymerization reactor control. Promising results are obtained with the combination of multi-stage NMPC and an economic cost function. The control scheme fulfills the temperature requirements for all values of the uncertain parameter and robustly minimizes the batch time.

Future work will include the stability analysis and problem formulations that guarantee closed-loop stability, as well as an analysis of the influence on the performance of the robust horizon and the different discretization methods that are used. Furthermore, scenario reduction techniques and decomposition approaches will be investigated for the consideration of more uncertainties and disturbances.

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