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Economic Multi-stage Output Feedback NMPC using the Unscented Kalman Filter

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Abstract: Nonlinear Model predictive control (NMPC) is a popular control strategy for highly nonlinear chemical processes. The ability to handle safety and environmental constraints along with the use of an economic objective makes NMPC highly appealing to industries. The performance of NMPC depends strongly on the accuracy of the model. In reality, there always are plant-model mismatch and state estimation errors. Hence the NMPC controller must be robust to uncertainties in the model as well as against estimation errors. Among the several approaches presented in the literature, the scenario-tree based multi-stage NMPC approach is a non-conservative and efficient formulation. In this approach, the evolutions of the plant for different realizations of the uncertainties are considered as different scenarios and the optimization problem is formulated as a multi-stage stochastic programming problem with recourse. In this work, we consider multi-stage output feedback NMPC using the Unscented Kalman Filter (UKF) where the nonlinearities are represented using deterministically chosen sigma points for state estimation. In the control problem, we explicitly consider the UKF estimation equations to predict the future evolution of the system. The proposed approach is illustrated by simulation results of fed-batch chemical reactor with an economic cost function.

Keywords: Model-based control, Output feedback Nonlinear model predictive control, Robust control, Unscented Kalman Filter, Economic control objective.

1. INTRODUCTION

Nonlinear Model predictive control (NMPC) is an advanced process control strategy for the control of nonlinear systems. The control problem is formulated as an optimization problem over a finite prediction horizon with an economic objective or a reference tracking objective. In addition to the possibility of optimizing an economic objective online, handling constraints with ease makes this approach highly attractive. The performance of the controller depends crucially on the accuracy in the prediction of the plant evolution. Plant-model mismatch and estimation errors cause the prediction to be less accurate and may lead to poor performance of the controller and in some cases it can even lead to instability. A practically relevant NMPC controller must be robust to the uncertainties and disturbances and satisfy the constraints at all times. The most prominent robust NMPC schemes in the literature are the min-max approach described in Scokaert and Mayne [1998], the tube-based approach in Mayne et al. [2011] and the multi-stage NMPC approach from Lucia et al. [2013]. Min-max approaches minimize the worst case cost of the predicted evolution enforcing the fulfillment of the constraints for all the cases of the uncertainty for one optimal input trajectory. The tube-based approach of nonlinear systems uses two controllers, a nominal controller and an ancillary controller. For the nominal controller more stringent constraints than the original constraints are imposed and the task of the ancillary controller is to make sure that the path of the plant remains close to the nominal path so that the original constraints are satisfied. In the multi-stage NMPC approach (see Lucia et al. [2013] and Lucia et al. [2012]), the possible future evolutions of the plant for different realizations of the uncertainties are considered as different scenarios of the problem. The important feature of this approach is that it takes future information about the realization of the uncertainty into account at every stage by admitting different control moves for different future scenarios that branch from different points. This makes the approach less conservative compared to open-loop min-max NMPC schemes. If the scenario tree is an exact representation of the future uncertainties, multi-stage NMPC provides the optimal solution under the given feedback information structure by solving an open-loop optimization problem. When the state vector is not measured at each sampling interval but only noisy measurements of some outputs are available, additional uncertainty about the current state as well as inexact information about the future states must be taken into account. Thus the controller needs to be robust to the estimation errors as well. Output based NMPC schemes have been researched extensively in the literature using the robust MPC schemes and accounting for the estimation errors as described e.g. in Rawlings and Amrit [2009], Findeisen et al. [2003], Lee and Ricker [1994]. Multi-stage Output feedback NMPC was presented for the first time in Subramanian et al. [2014] using an EKF for state estimation. The scheme was shown to be robust against parametric uncertainties and bounded estimation error. In this work, we formulate a multi-stage output feedback NMPC using the Unscented Kalman Filter (UKF) where the nonlinearities are better represented by using deterministically chosen sigma points. In this controller, we consider the UKF

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estimation equations for the prediction of the future evolution of the system. The innovations give the new information from the measurement at each sampling time and are used to update the predicted state using the system model. We model the samples of the innovations as new scenarios in the scenario tree in addition to the parametric uncertainties and we use the UKF estimation equations for the evolution of the future states along with the covariance information. The proposed approach is shown to be robust to plant-model mismatches and to estimation errors. The approach is illustrated by simulation results of a fed-batch chemical reactor with an economic cost function. In what follows, the UKF is discussed in Section 2 followed by standard multi-stage NMPC and multi-stage output feedback NMPC in Section 3. In Section 4, a case study of a highly nonlinear system is discussed followed by results which validate the method in Section 5. After discussing the results, we conclude this paper in Section 6.

2. THE UNSCENTED KALMAN FILTER

The most commonly used technique in the field of nonlinear estimation is the Extended Kalman filter (EKF) mainly because it is easy to implement. However because of the approximation of the nonlinearities present in the system using the Jacobian for the propagation of covariance information, higher order information gets lost and this leads to a less precise estimate of the states and the error covariance. The Unscented Kalman Filter offers an alternate and an efficient way to estimate states without the linearization of the model as presented in Julier and Uhlmann [1997]. In this method, $2\,n_x+1$ deterministically chosen sigma points are sampled from the initial confidence interval and are propagated in time using the system model. Here n_x is the number of states in the system. From the propagated sigma points, the mean of the state and the new covariance information is obtained. A nonlinear system is assumed to be given by

$$x_k = f(x_{k-1}, u_{k-1}) + q_{k-1}, \tag{1}$$
$$y_k = h(x_k) + r_k, \tag{2}$$

where x_k is the state vector, u_k is the input vector, q_k is the process noise at a given time step k and $f : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_x}$ is the model of the system with n_x being the dimension of the state and n_u being the dimension of the input. In the equation (2), y_k represents the output vector with the dimension n_y, $h : \mathbb{R}^{n_x} \to \mathbb{R}^{n_y}$ is the measurement model and r_k represents the measurement noise. The covariances of q_k and r_k are represented as Q_k and R_k respectively. The covariance of the state x_k is given as P_k. With the current state estimate $\hat{x}_k$ and the covariance matrix P_k, the $2\,n_x+1$ sigma points $\hat{x}_{\sigma_k}$ are calculated first as follows:

$$\lambda = \alpha^2(n_x+\kappa) - n_x, \tag{3a}$$
$$S_k = \sqrt{((n_x+\lambda)P_k)}, \tag{3b}$$
$$\hat{x}^0_{\sigma_k} = \hat{x}_k, \tag{3c}$$
$$\hat{x}^i_{\sigma_k} = \hat{x}_k + S^i_k, \forall i = 1, ..., n_x, \tag{3d}$$
$$\hat{x}^i_{\sigma_k} = \hat{x}_k - S^i_k, \forall i = n_x+1, ..., 2\,n_x, \tag{3e}$$

where λ here is a scaling parameter obtained by the tuning parameters α and κ. S_k is the square root of the scaled covariance matrix P_k which can be obtained using Cholesky factorization. S^i_k represents the i^{th} row of the square root matrix S_k. The sigma points are then assigned different weights for the calculation of the mean and covariance of the resulting state estimate (mean) and probability distribution. The associated weights are given below.

$$w^0_m = \frac{\lambda}{(n_x+\lambda)}, \tag{4a}$$
$$w^i_m = \frac{1}{2(n_x+\lambda)}, \forall i = 1, ..., 2\,n_x, \tag{4b}$$
$$w^0_c = \frac{\lambda}{(n_x+\lambda)} + (1-\alpha^2+\beta), \tag{4c}$$
$$w^i_c = \frac{1}{2(n_x+\lambda)}, \forall i = 1, ..., 2\,n_x, \tag{4d}$$

where $w^i_m, \forall i = 0, ..., 2\,n_x$ are the weights associated with the sigma points $\hat{x}^i_{\sigma_k}, \forall i = 0, ..., 2\,n_x$ for the calculation of the mean and $w^i_c, \forall i = 0, ..., 2\,n_x$ are the weights associated with the corresponding sigma points for the calculation of the covariance matrix and β is another tuning parameter to approximate the probability density function. With these details, the algorithm for the Unscented Kalman Filter is given as follows (Wan and Merwe [2000]). In the Algorithm 1, the weighted sum

Algorithm 1 The Unscented Kalman Filter (UKF)

Require: $\hat{x}_{k-1}$, u_{k-1}, y_k, P_{k-1}, Q_k, R_k, α, β, κ
1: **Calculate** $x^i_{\sigma_{k-1}}, \forall i = 0, ..., 2\,n_x$ as in equation (3)
2: **Calculate** $w^i_m, \forall i = 0, ..., 2\,n_x$ as in equation (4)
3: **Calculate** $w^i_c, \forall i = 0, ..., 2\,n_x$ as in equation (4)
4: **for** i=0 to $2\,n_x$ **do**
5: $\quad x^{i-}_{\sigma_k} = f(x^i_{\sigma_{k-1}}, u_{k-1})$
6: $\quad y^{i-}_{\sigma_k} = h(x^i_{\sigma_k})$
7: **end for**
8: $\hat{x}^-_k = \sum_{i=0}^{2\,n_x} w^i_m\, x^{i-}_{\sigma_k}$
9: $y^-_k = \sum_{i=0}^{2\,n_x} w^i_m\, y^{i-}_{\sigma_k}$
10: $P^-_k = \sum_{i=0}^{2\,n_x} w^i_c\, [x^{i-}_{\sigma_k} - \hat{x}^-_k][x^{i-}_{\sigma_k} - \hat{x}^-_k]^T + Q_k$
11: $P_{yy} = \sum_{i=0}^{2\,n_x} w^i_c\, [y^{i-}_{\sigma_k} - y^-_k][y^{i-}_{\sigma_k} - y^-_k]^T + R_k$
12: $P_{xy} = \sum_{i=0}^{2\,n_x} w^i_c\, [x^{i-}_{\sigma_k} - \hat{x}^-_k][y^{i-}_{\sigma_k} - y^-_k]^T$
13: $K_k = P_{xy} \cdot P^{-1}_{yy}$
14: $\hat{x}_k = \hat{x}^-_k + K_k(y_k - y^-_k)$
15: $P_k = P^-_k - K_k P_{yy} K^T_k$

of all the propagated (time updated) sigma points gives the a priori estimate $\hat{x}^-_k$ and the a priori covariance P^-_k is calculated as given in step 10 of the algorithm. Then the Kalman gain K_k is calculated from the cross covariance matrix P_{xy} and the measurement covariance matrix P_{yy}. The measurement information is added to the a priori estimate with the Kalman gain K_k via the innovations $\nu_k = y_k - y^-_k$. This gives the current state estimate $\hat{x}_k$ and with the update of the a priori state covariance matrix to the a posteriori covariance matrix P_k in step 15 of the Algorithm 1, the state estimation is complete.

3. MULTI-STAGE OUTPUT FEEDBACK NMPC

3.1 Multi-stage NMPC

We first shortly review the main concepts of the multi-stage NMPC approach presented in Lucia et al. [2013, 2014a] and then we discuss the main contribution of this paper: the integration of the Unscented Kalman Filter in the output based multi-stage NMPC setting. In multi-stage NMPC, the evolution of the uncertainty is represented by a tree of discrete scenarios that branches at each sampling instance until the end of the

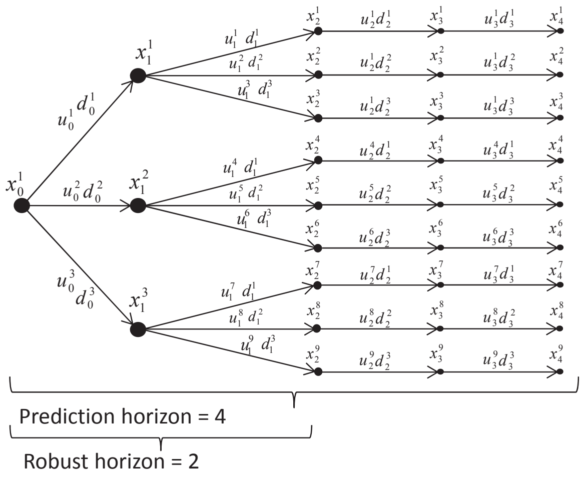

Fig. 1. Scenario tree representation of the evolution of the uncertainty for multi-stage NMPC.

prediction horizon, as it can be seen in Fig. 1. The use of the scenario tree for the formulation of the real-time decision problem makes it possible to take into account that in future sampling times new measurements will be available and therefore it will be possible to adapt the future control inputs to the measurements that become available. In other words, it is not necessary to compute at the current sampling time a sequence of control inputs that satisfies the constraints for all the possible realizations of the uncertainty because the future decisions can be adapted to the new available information as time progresses. This reduces significantly the conservativeness of the controller. If the uncertainty present in the system takes only the discrete values which are included in the scenario tree (e.g. in the case of discrete faults), multi-stage NMPC provides the best solution possible for a given prediction horizon. Generally this is not the case, and multi-stage NMPC is an approximation of the best solution.

A possible strategy to generate a scenario tree is to consider as branches the combinations of the maximum, minimum and optionally also nominal values of all the uncertainties and disturbances. Although for the nonlinear case this strategy does not guarantee constraint satisfaction for the realizations that are not included in the tree, it is very common that the worst-case realization is located at one of the extrema of the uncertainty set. In that case, the multi-tage approach leads to robust constraint satisfaction for all the realizations of the tree (see e.g. Lucia et al. [2013]). If a rigorous guarantee for robust constraint satisfaction of all the possible values of the uncertainty (including those that are not in the tree) is required, the multi-stage approach can be combined with reachability analysis as shown in Lucia et al. [2014b].

It can be seen that the main challenge of the approach is that the size of the scenario tree and hence of the resulting optimization problem grows rapidly with the prediction horizon and also with the number of uncertainties considered. A possible strategy to avoid the exponential growth of the scenario tree with the prediction horizon is to consider that the uncertainty remains constant after a certain stage (called the robust horizon N_r) until the end of prediction horizon (Fig. 1).

In the multi-stage NMPC approach, we consider a discrete-time nonlinear system:

$$x_{k+1}^j = f\left(x_k^{p(j)}, u_k^j, d_k^{r(j)}\right), \tag{5a}$$

where each state vector $x_{k+1}^j \in \mathbb{R}^{n_x}$ at stage $k+1$ and position j depends on the parent state $x_k^{p(j)}$ at stage k, the vector of control inputs $u_k^j \in \mathbb{R}^{n_u}$ and the corresponding realization r of the uncertainty $d_k^{r(j)} \in \mathbb{R}^{n_d}$ (e.g. in Fig. 1, $x_2^6 = f(x_1^2, u_1^6, d_1^3)$). The uncertainty at stage k is defined by $d_k^{r(j)} \in \{d_k^1, d_k^2, \ldots, d_k^s\}$ for s different possible combinations of values of the uncertainty. We define the set of indices (j,k) in the scenario tree as I. S_i denotes ith scenario defined as the path from the root node x_0 to one of the leaf nodes and it contains all the states x_k^j and control inputs u_k^j that belong to the ith scenario.

The optimization problem that has to be solved at each sampling instant can be written as:

$$\min_{x_{k+1}^j, u_k^j, \forall (j,k) \in I} \quad \sum_{i=1}^{N} \omega_i J_i(X_i, U_i) \tag{6a}$$

subject to:

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

$$0 \geq g\left(x_{k+1}^j, u_k^j, d_k^{r(j)}\right), \quad \forall (j,k) \in I, \tag{6c}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)}, \quad \forall (j,k), (l,k) \in I. \tag{6d}$$

where X_i, U_i are the set of states and control inputs that belong to the scenario S_i with the probability of occurrence ω_i. The cost of each scenario is denoted by $J_i(\cdot)$ and can be written as:

$$J_i(X_i, U_i) := \sum_{k=0}^{N_p - 1} L\left(x_{k+1}^j, u_k^j\right), \ \forall x_{k+1}^j, u_k^j \in S_i. \tag{7}$$

$g : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \to \mathbb{R}^{n_g}$ represents general and possibly nonlinear constraints on the states and on the inputs of the control problem evaluated at each node of the tree. n_g denotes the number of constraints. The constraints (6d) are called non-anticipativity constraints which implies that the control inputs cannot anticipate the realization of the uncertainty, i.e. the control inputs u_k^j that branch at the same parent node $x_k^{p(j)}$ must be the same.

3.2 Multi-stage output feedback NMPC based on the UKF

As discussed in Section 2, the estimated states are not accurate but are assumed to lie in a certain confidence interval given by the covariance matrix P_k. We propose here a method to propagate the current state estimate and the covariance matrix given by the UKF algorithm in order to predict the future evolution of the system in a more robust way by accounting for the initial uncertainty and the future measurement noise. The UKF combines initial state covariance information along with the system model and the measurement information and estimates the state of the plant. This can be used as a part of NMPC to predict the future evolution of the system. However the future measurements are not known. The innovations $\nu_k = y_k - h(\hat{x}_k^-)$ are the new information used to update the predicted state using the system model to get the optimal estimate. The innovations information is in general bounded for a properly tuned filter, and we exploit this fact by sampling them and adding those samples as additional scenarios in the scenario tree in addition to the parametric uncertainties. The UKF estimation equations are used for the prediction of the future state estimates for the sampled innovations. The prediction and the measurement update are carried out simultaneously as a part of the NMPC algorithm as given by the UKF equations in Algorithm 1. With the assumption that the worst-case innovations always lie on the boundary given by $N_k := [\nu_k^L, \nu_k^U]$, the scenarios on the boundary can be included in the scenario tree leading to robust controller performance against the worst-case estimation errors. The Kalman gain K_k is updated taking into account that new information on the innovations will be available at the next sampling times and the future control inputs can act as recourse variables to counteract the effect of the uncertainties including the estimation error. The feedback information that is present in the scenario tree not only makes the approach less conservative but also helps in the propagation of the covariance matrices along the possible future realizations of the states for all the considered scenarios. Based on the covariance of the state estimates along the prediction horizon for all scenarios, the prediction of the Kalman gain K_k at all time-stages is possible leading to a good predicted state estimate for all the scenarios. In order to simplify the notations used in the problem formulation, the details given in the Algorithm 1 are simplified as follows. The covariance propagation (given in step 15 of Algorithm 1) is represented using $P_k = \Phi(\hat{x}_{k-1}, u_{k-1}, d_{k-1}, P_{k-1})$ and the Kalman gain equation shown in step 13 of the Algorithm 1 is represented as $K_k = \Psi(\hat{x}_{k-1}, d_{k-1}, u_{k-1}, P_{k-1})$. With this simplification, the multi-stage output feedback NMPC problem formulation is given as follows,

$$\min_{x_{k+1}^j, u_k^j, \forall (j,k) \in I} \quad \sum_{i=1}^{N} \omega_i J_i(X_i, U_i) \tag{8a}$$

subject to:

$$x_{k+1}^j = f\left(x_k^{p(j)}, u_k^j, d_k^{r(j)}\right) + K_k^j \nu_k^{r(j)}, \quad \forall (j, k+1) \in I, \tag{8b}$$

$$P_{k+1}^j = \Phi\left(x_k^{p(j)}, u_k^j, d_k^{r(j)}, P_k^{p(j)}\right), \quad \forall (j, k+1) \in I, \tag{8c}$$

$$K_{k+1}^j = \Psi\left(x_k^{p(j)}, u_k^j, d_k^{r(j)}, P_k^{p(j)}\right), \quad \forall (j, k+1) \in I, \tag{8d}$$

$$0 \geq g\left(x_{k+1}^j, u_k^j, d_k^{r(j)}\right), \quad \forall (j, k) \in I, \tag{8e}$$

$$u_k^j = u_k^l \text{ if } x_k^{p(j)} = x_k^{p(l)}, \quad \forall (j, k), (l, k) \in I. \tag{8f}$$

The innovations part of the uncertain parameters is assumed to be bounded and given by $\nu_k \in N_k := [\nu_k^L, \nu_k^U]$. The UKF equations (8c) and (8d) are used in the prediction of the state as shown in the problem formulation and the method is thus robust to plant-model mismatch and estimation error.

4. CASE STUDY

We consider as a case-study a semi-batch reactor with a cooling jacket. A chemical reaction $A + B \to C$ takes place in the reactor. The problem has been adapted from Srinivasan et al. [2003] and Ubrich et al. [1999].

The reaction system can be described by the following set of ODEs:

$$\frac{dc_A}{dt} = -kc_A c_B - \frac{u}{V} c_A, \qquad c_A(0) = c_{A,0}, \tag{9}$$

$$\frac{dc_B}{dt} = -kc_A c_B + \frac{u}{V}(c_{B,in} - c_B), \qquad c_B(0) = c_{B,0}, \tag{10}$$

$$\frac{dc_C}{dt} = kc_A c_B - \frac{u}{V} c_C, \qquad c_C(0) = 0, \tag{11}$$

$$\frac{dV}{dt} = u, \qquad V(0) = V_0. \tag{12}$$

where c_i represents the concentration of the substance i, k stands for the reaction rate, V is the volume of the reactor, and the control input u represents the feed flow-rate of reactant B with concentration $c_{B,in}$=10 mol L^{-1}. We study the case where the reaction is run under isothermal conditions, i.e., the inlet cooling jacket temperature is adjusted to maintain the temperature in the reactor at $T = 70°$C. The evolution of the temperature of the cooling jacket is given by

$$T_j(t) = T - \frac{(-\Delta H) k c_A(t) c_B(t) V(t)}{\alpha_H A(t)}, \tag{13}$$

where ΔH is the reaction enthalpy, α_H is a heat transfer coefficient and A is the contact area between the jacket and the reactor content.

In order to prevent an uncontrollable behavior of the reaction in the case of a cooling failure, a safety-related constraint is considered in which the reactor temperature is restricted by

$$T_{cf} = T(t) + \min_{i \in \{A,B\}} c_i \frac{(-\Delta H)}{\rho c_p} \leq T_{\max}, \tag{14}$$

where ρ denotes the density and c_p the specific heat of the reaction mixture. Additionally, the volume of the reactor is bounded by its maximum value, $V \leq V_{\max}$ and the control input is bounded ($u_{\min} \leq u \leq u_{\max}$). The parameters of the problem and the initial conditions are given by Table 1. The control goal is to produce a certain amount of product C (n_C) in the minimum possible time respecting the constraints. This goal has to be achieved for all the possible values of the uncertain parameters k, ΔH and α_H which are assumed to vary by $\pm 10\%$ with respect to its nominal value. We approximate this goal by considering the maximization of n_C for a finite horizon, which according to different simulation studies provides almost identical results compared to the minimum time problem.

We consider that we know the reactor temperature T (assumed isothermal) and that noisy measurements of the jacket temperature T_j are available at each sampling time with a measurement noise that follows a normal distribution with $\sigma = 0.1$ K bounded by $\pm 3\sigma$.

Table 1. Parameter values, initial conditions and bounds.

Parameter	Value	Units
k	0.0482	L mol^{-1} h^{-1}
ΔH	-60000	J mol^{-1}
α_H	20	W m^{-2} K^{-1}
T	70	°C
ρ	900	g L^{-1}
c_p	4.2	J g^{-1} K^{-1}
$c_{B,in}$	10	mol L^{-1}
$c_{A,0}$	2	mol L^{-1}
$c_{B,0}$	0.54	mol L^{-1}
V_0	0.7	L
u_{min}	0	L h^{-1}
u_{max}	0.1	L h^{-1}
T_{max}	80	°C
V_{max}	1	L
$n_{C,des}$	0.45	mol

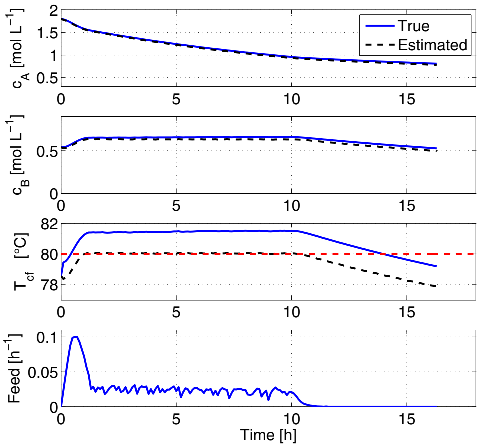

Fig. 2. Concentration c_A, Concentration c_B, temperature T_{cf} and the input feed u obtained from using nominal NMPC without accounting for parametric uncertainty and estimation error.

5. RESULTS

This section shows the results for standard NMPC, multi-stage NMPC and multi-stage output feedback NMPC for the case-study presented above. In all cases we estimate the necessary states for the initialization of the NMPC controller using an UKF based on the nominal model at each sampling time. For this case study, the tuning parameters are given as $\alpha = 0.9$, $\beta = 3.0$ and $\kappa = 4.0$. The initial state covariance is given as

$$P_0 = \begin{pmatrix} 1 \cdot 10^{-4} & 0 & 0 & 0 \\ 0 & 1 \cdot 10^{-4} & 0 & 0 \\ 0 & 0 & 1 \cdot 10^{-4} & 0 \\ 0 & 0 & 0 & 1 \cdot 10^{-2} \end{pmatrix}.$$

The process noise covariance matrix was chosen as

$$Q_k = \begin{pmatrix} 2 \cdot 10^{-4} & 0 & 0 & 0 \\ 0 & 2 \cdot 10^{-4} & 0 & 0 \\ 0 & 0 & 1 \cdot 10^{-4} & 0 \\ 0 & 0 & 0 & 1 \cdot 10^{-1} \end{pmatrix}.$$

The measurement noise covariance matric R_k is given by 0.01. For all the results presented in this paper we discretized the dynamics of the nonlinear system using orthogonal collocation on finite elements. The resulting nonlinear programming problem is solved using IPOPT (Wächter and Biegler [2006]) via CasADi (Andersson et al. [2012]), which calculates exact first- and second-order derivative information, leading to a very efficient implementation as illustrated in Lucia et al. [2014a]. We consider a prediction horizon of $N_p = 5$ steps with a sampling time of $t_{\text{step}} = 0.1$ h. The cost function minimized at each stage is the negative amount of product C ($n_{\text{C}} = C_{\text{C}}V$) with a penalty on the control moves:

$$L = -n_{\text{C}} + r\Delta u^2, \tag{15}$$

where the penalty term for the control movements is chosen as $r = 0.2$.

Fig. 2 shows that standard NMPC (for the case of $k = 0.0434$, $\Delta H = -66,000$ and $\alpha_H = 18$) is not able to satisfy the temperature constraint on T_{cf} resulting in significant constraint violations which can produce a dangerous operation of the reactor and should therefore be avoided. In order to account for the parametric uncertainty we build a scenario tree considering the maximum and minimum values of the uncertain parameters ($k = \{0.0434, 0.0530\}, \Delta H = \{-54000, -66000\}, \alpha_H = \{18, 22\}$) and we branch the scenario tree only in the first stage ($N_r = 1$), which gives a total of $s = 2^3 = 8$ scenarios. The results of this multi-stage NMPC approach can be seen in Fig. 3 for the case of $k = 0.0434$, $\Delta H = -66,000$ and $\alpha_H = 18$. It can be seen that the performance of the controller is improved but there are minor violations of the constraints because the estimation errors are ignored. Though the estimated values of T_{cf} satisfies the constraints, the true value of the plant violates the constraints marginally. In order to avoid violations of the constraints due to the estimation error, it must be taken into account in the design of the controller. We generate now a scenario tree considering the maximum and minimum values of the uncertain parameters ($k = \{0.0434, 0.0530\}, \Delta H = \{-54000, -66000\}, \alpha_H = \{18, 22\}$) and also its combinations with the maximum and minimum values of the innovations ($\nu_k = \{-0.6, 0.6\}$) which result from the UKF approach, as described in the Section 3. This gives a total of $s = 2^4 = 16$

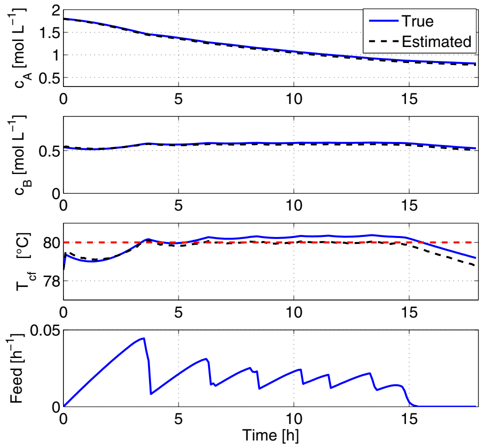

Fig. 3. Concentration c_A, Concentration c_B, temperature T_{cf} and the input feed u obtained from using standard multi-stage NMPC without accounting for the estimation error in the scenario tree.

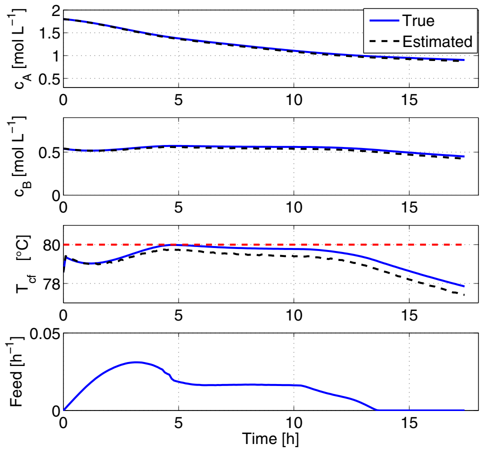

Fig. 4. Concentration c_A, Concentration c_B, temperature T_{cf} and the input feed u obtained from using multi-stage output feedback NMPC accounting for the estimation error in the scenario tree.

Table 2. Performance comparison between standard NMPC (ST), multi-stage NMPC (MS) and multi-stage output feedback NMPC (MSOF) for 100 random batches.

NMPC Controller	**ST**	**MS**	**MSOF**
Batch time [h]	15.08	16.57	16.71
Batches with violations [-]	60	11	0
Avg. constraint violations [K h]	3.22	0.12	0
Avg. comp. time per iter. [ms]	17	178	1620

scenarios. When the bounds on the innovations hold at all times, it is possible to satisfy the constraints on the temperature for all the values of the uncertain parameter and realizations of the error using such an approach, as it can be seen in Fig. 4. The robustness is achieved because the multi-stage output feedback NMPC calculates an additional backoff from the constraint to account for the estimation error. The additional backoff leads to a smooth operation of the system in contrast to the correction actions that happen because of the constraint violations when estimation errors are ignored (see Fig. 3 and Fig. 4). Thus the proposed method provides a robust, safer (avoids oscillatory inputs) method which results only in a slightly longer batch time. The UKF based scheme presented in this paper has the added advantage of possessing an inherent robustness compared to the EKF based scheme given in Subramanian et al. [2014] because the sigma points which are propagated along the scenario tree are also constrained in addition to the predicted evolution of the system with the innovations update. This already adds a certain degree of robustness to the state estimation error because even if the innovations sequence is 0 in the problem formulation, the initial error is propagated through sigma points and this gives the approach its inherent robustness to the estimation error.

We show in Table 2, a comparison of the performance for standard NMPC, multi-stage NMPC and multi-stage output feedback NMPC for 100 batches with random values of the uncertain parameters (following a uniform distribution) and different realizations of the initial conditions (following a normal distribution) in addition to the measurement noise (also following a normal distribution). It can be clearly seen that the multi-stage output feedback NMPC avoids violations of the constraints for all the cases (also for those not included in the scenario tree) at the cost of a higher average computation time per iteration and a slightly longer batch time. It can also be noted here that multi-stage NMPC can be applied in real time as the maximum average computation time is less than 2 seconds.

6. CONCLUSION

This paper shows that an Unscented Kalman Filter strategy can be combined with the multi-stage NMPC method to achieve a controller which is robust not only to model uncertainties and disturbances but also to estimation errors. The tree structure of the multi-stage NMPC approach fits perfectly with the design of the Unscented Kalman Filter, leading to a simple and non-conservative approach with a superior performance compared to standard NMPC or to a multi-stage NMPC which ignores estimation errors. We illustrate the performance of the proposed approach using simulation results of a fed batch reactor case study.

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