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Robust Nonlinear Model Predictive Control with Reduction of Uncertainty via Robust Optimal Experiment Design

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Abstract: This paper studies the reduction of the conservativeness of robust nonlinear model predictive control (NMPC) via the reduction of the uncertainty range using guaranteed parameter estimation. Optimal dynamic experiment design is formulated in the framework of robust NMPC in order to obtain probing inputs that maximize the information content of the feedback and simultaneously to guarantee the satisfaction of the process constraints. We propose a criterion for optimal experiment design which provides a minimization of parameter uncertainty in the direction of improved performance of the process under robust economic NMPC. A case study from the chemical engineering domain is studied to show the benefits of the proposed approach.

Keywords: Nonlinear model predictive control, Robust control, Optimal experiment design, Guaranteed parameter estimation

1. INTRODUCTION

Many studies have been devoted to the problem of real-time optimal process control. The most challenging problems involve handling of nonlinearities and uncertainties of the processes. This paper is focused on the reduction of the parametric uncertainties of the processes for performance improvement of nonlinear model-based control approaches.

We consider a model of the process described by a set of nonlinear ordinary differential equations (ODEs) and output equations in sampled form as

$$\boldsymbol{x}_{k+1} = \boldsymbol{f}(\boldsymbol{x}_k, \boldsymbol{u}_k, \boldsymbol{d}_k), \quad (1a)$$

$$\boldsymbol{y}_k = \boldsymbol{g}(\boldsymbol{x}_k), \quad (1b)$$

where k stands for the sampling instant, $\boldsymbol{x}$ denotes the n_x-dimensional vector of process states, $\boldsymbol{u}$ represents the n_u-dimensional vector of process control variables (inputs), $\boldsymbol{d}$ is the n_d-dimensional vector of uncertain parameters of the process model with a priori known bounds $\boldsymbol{D}_k := [\boldsymbol{d}_k^L, \boldsymbol{d}_k^U]$, and $\boldsymbol{y}$ denotes the n_y-dimensional vector of model outputs (predictions of measurable state combinations). The superscripts ^{L} and ^{U} representing the lower and upper bounds of an interval box are understood component-wise throughout the paper. We want to control the process, i.e. determine the control inputs for (1), such that

$$\mathcal{J}(\boldsymbol{y}_{k+1}, \boldsymbol{u}_k) := \sum_{k=0}^{N_p-1} \mathcal{L}(\boldsymbol{y}_{k+1}, \boldsymbol{u}_k), \quad (2)$$

representing the chosen economic performance criterion, is minimized on a finite prediction horizon of a length N_p subject to the set of constraints of the form

$$\boldsymbol{h}(\boldsymbol{y}_{k+1}, \boldsymbol{x}_{k+1}, \boldsymbol{u}_k, \boldsymbol{d}_k) \leq 0, \quad \forall k \in \{0, \ldots, N_p - 1\}, \quad (3)$$

being satisfied. Optimal trajectories of control inputs can be found by means of mathematical optimization.

Given the efficiency of modern optimization tools that provide fast and reliable resolutions to many of the arising problems of nonlinear constrained optimization (Houska et al., 2011), the handling of uncertainties, here present by parametric uncertainties $\boldsymbol{d}_k$, remains the most challenging problem of real-life applications of the optimizing control schemes. One of the possible approaches to optimizing control, in the presence of uncertain parameters in (1), is the utilization of robust control. Various schemes have been presented in this framework (Nagy and Braatz, 2004) while different levels of conservativeness of the resulting robust optimizing control scheme were observed.

The use of multi-stage robust nonlinear model predictive control (NMPC), suggested in Lucia et al. (2013), represents a recent approach that was shown to achieve a low degree of conservativeness compared to other state-of-the-art robust approaches. The strength of this approach lies in exploiting the future information that becomes available via feedback (measured outputs) at each sampling time of the process run. A scenario tree of possible realizations of uncertainties is considered to represent possible deviations of the process from nominal predictions. The robustly optimizing control is then found by recursive resolution of the NMPC problem over the set of generated scenarios with (2) as an objective evaluated on the prediction horizon subject to (3) where each scenario is assigned with the different probability of occurrence. The key here is

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the use of recourse, i.e. future control inputs along the scenario tree are adapted to the observations, reducing the conservativeness of the approach.

It is an obvious fact that by reducing the range of parametric uncertainty $\boldsymbol{D}_k$, i.e. narrowing the employed scenario tree, a dramatical improvement can be achieved in terms of the conservativeness of the resulting robustly optimal control input. Dual control, originally proposed in Feldbaum (1960) and also studied in Åström and Wittenmark (1971), tackles this problem. The aim of dual control is to strike the balance between finding the optimizing inputs for the criterion (2) and inputs that excite the process sufficiently to reduce the (a posteriori estimated) bounds on the parameter values $\boldsymbol{D}_k$ thanks to information incorporated in feedback. The dynamic programming formulation of the problem (Bertsekas, 2000) is often found computationally intractable for nonlinear systems, but the minimization of the uncertainty (the range of possible $\boldsymbol{d}_k$) can also be achieved via means of optimal design of dynamic experiments.

The aim of this paper is to study possible improvements of the on-line robust NMPC scheme via a combination of inputs optimizing the chosen criterion of optimal experiment design and the inputs optimizing the economic criterion in the framework of multi-stage NMPC.

2. MULTI-STAGE NONLINEAR MODEL PREDICTIVE CONTROL

Multi-stage NMPC (Lucia et al., 2013) represents a robust NMPC approach that is based on modeling the uncertainty by a tree of discrete scenarios (see Fig. 1). The tree structure makes it possible to take into account future control inputs and disturbances explicitly. In this way, future control inputs depend on the value of the previous realization of the uncertainty, acting as recourse variables that counteract the effect of the uncertainty. Therefore, multi-stage NMPC is a closed-loop NMPC approach (Lee and Yu, 1997) in contrast to typical open-loop min-max approaches that optimize over a sequence of control inputs checking the constraints for all the cases of the uncertainty. This reduces the conservativeness of the approach considerably (Scokaert and Mayne, 1998).

The main assumption of the approach is that the uncertainty can be described by a set of discrete scenarios. In the case of discrete-valued uncertainties, multi-stage NMPC computes the exact optimal feedback policy and it is therefore the best solution possible of the robust NMPC problem within a finite horizon guaranteeing the constraint satisfaction as well. For the real-valued realizations of the uncertainty, the multi-stage NMPC computes approximate robust feedback when a suitable scenario tree is chosen as shown in different simulation studies (Lucia et al., 2012, 2013; Lucia and Engell, 2013). While for a general nonlinear system, constraint satisfaction is not guaranteed for the values of uncertainty that are not explicitly considered in the scenario tree, the values of parameters that produce the worst-case scenario are found on the boundaries of the parameter interval box very often (Srinivasan et al., 2003a). Therefore, a suitable scenario tree should include scenarios with extreme values of all the parameters. It is then clear that the main challenge of the approach is that the size of the resulting optimization problem grows exponentially with the number of uncertainties and with the length of the prediction horizon. Given a certain choice of N_p, a simple strategy to avoid the exponential growth of problem size is to consider the uncertainty to remain constant after a certain point in time (called robust horizon) as illustrated in Fig. 1. See Lucia et al. (2013) for a more detailed explanation of this concept.

The scenario tree setting assumes a discrete-time formulation of an uncertain nonlinear system that can be written as:

$$\boldsymbol{x}_{k+1}^j = \boldsymbol{f}(\boldsymbol{x}_k^{p(j)}, \boldsymbol{u}_k^j, \boldsymbol{d}_k^{r(j)}), \tag{4a}$$

$$\boldsymbol{y}_k^j = \boldsymbol{g}(\boldsymbol{x}_k^j), \tag{4b}$$

where each state vector $\boldsymbol{x}_{k+1}^j$ at stage $k+1$ and position j in the scenario tree depends on the parent state $\boldsymbol{x}_k^{p(j)}$ at stage k, the control inputs $\boldsymbol{u}_k^j$ and the corresponding realization r of the uncertainty $\boldsymbol{d}_k^{r(j)}$ (for example in Fig. 1, $\boldsymbol{x}_2^6 = \boldsymbol{f}(\boldsymbol{x}_1^2, \boldsymbol{u}_1^6, \boldsymbol{d}_1^3)$). The uncertainty at the stage k is defined by $\boldsymbol{d}_k^{r(j)} \in \{\boldsymbol{d}_k^1, \boldsymbol{d}_k^2, \ldots, \boldsymbol{d}_k^s\} \subset \boldsymbol{D}_k$ for s different possible combinations of values of the uncertainty. We define the set of occurring indices (j,k) in the scenario tree as $\boldsymbol{I}$.

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

$$\min_{\boldsymbol{y}_{k+1}^j, \boldsymbol{x}_{k+1}^j, \boldsymbol{u}_k^j, \forall (j,k) \in \boldsymbol{I}} \quad \tilde{\mathcal{J}}(\boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j) \tag{5a}$$

subject to:

$$\boldsymbol{x}_{k+1}^j = \boldsymbol{f}(\boldsymbol{x}_k^{p(j)}, \boldsymbol{u}_k^j, \boldsymbol{d}_k^{r(j)}), \qquad \forall (j, k+1) \in \boldsymbol{I}, \tag{5b}$$

$$\boldsymbol{y}_k^j = \boldsymbol{g}(\boldsymbol{x}_k^j), \qquad \forall (j,k) \in \boldsymbol{I}, \tag{5c}$$

$$0 \geq \boldsymbol{h}(\boldsymbol{y}_{k+1}^j, \boldsymbol{x}_{k+1}^j, \boldsymbol{u}_k^j, \boldsymbol{d}_k^{r(j)}), \qquad \forall (j,k) \in \boldsymbol{I}, \tag{5d}$$

$$\boldsymbol{u}_k^j = \boldsymbol{u}_k^l \text{ if } \boldsymbol{x}_k^{p(j)} = \boldsymbol{x}_k^{p(l)}, \qquad \forall (j,k), (l,k) \in \boldsymbol{I}, \tag{5e}$$

where $\tilde{\mathcal{J}}(\boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j) := \sum_{i=1}^{N} \omega_i \mathcal{J}_i(\boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j)$. Here we assign the probability ω_i for the scenario S_i, $i \in \{1, \ldots, N\}$ to occur. A scenario is defined as the path in the scenario tree from the root node $\boldsymbol{x}_0$ until each one of the leaf nodes. The cost of each scenario reads as:

$$\mathcal{J}_i(\boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j) := \sum_{k=0}^{N_p-1} \mathcal{L}(\boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j), \ \forall\, \boldsymbol{y}_{k+1}^j, \boldsymbol{u}_k^j \in S_i. \tag{6}$$

In order to represent the real-time decision problem correctly, the control inputs cannot anticipate the realization of the uncertainty at the instant k. This is modeled by the *non-anticipativity constraints* (5e) that force all the control inputs $\boldsymbol{u}_k^j$ that branch at the same parent node $\boldsymbol{x}_k^{p(j)}$ to be equal. The definition of problem (5) allows the uncertainty to vary over the time. In this study we will assume that the uncertain parameters are constant for simplicity, hence the notation $\boldsymbol{d}_0 \in \boldsymbol{D}_0 := [\boldsymbol{d}_0^L, \boldsymbol{d}_0^U]$.

3. ROBUST OPTIMAL DYNAMIC EXPERIMENT DESIGN

Optimal dynamic experiment design has been widely used since the seventies of the last century, especially in the field of system identification (see Gevers et al. (2011) for a review). In general, it can be formulated as the problem

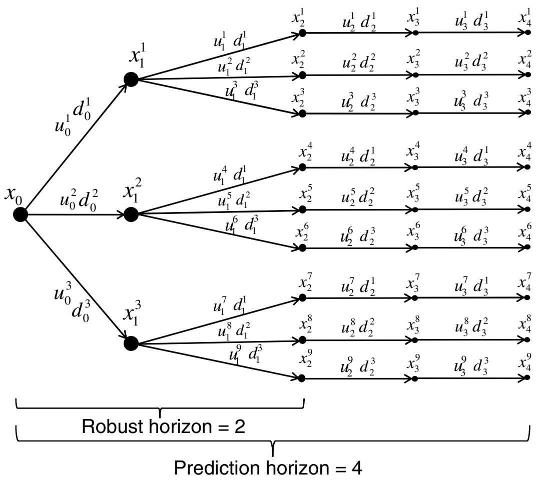

Fig. 1. Scenario tree representation of the uncertainty evolution for multi-stage NMPC.

of designing the input trajectories to the system (1) that generate measurements outputs from which parameters can be identified with maximal possible certainty.

Such a problem can be defined via minimization of an appropriate measure, $\phi(\mathbf{F})$, of the Fisher information matrix defined as:

$$\mathbf{F} := \sum_{k=0}^{N_e-1} \boldsymbol{s}_{\boldsymbol{y},k+1}^T \mathbf{Q} \boldsymbol{s}_{\boldsymbol{y},k+1}, \tag{7}$$

where N_e stands for the horizon where the optimal experiment is realized, $\mathbf{Q}$ is the inverse of the covariance matrix of the measurement noise, and $\boldsymbol{s}_{\boldsymbol{y},k+1}$ represents the matrix of parametric output sensitivities, here defined in the fully relative form suggested by Munack (1991):

$$\boldsymbol{s}_{x,k+1} = \boldsymbol{f}^s(\boldsymbol{s}_{x,k}, \boldsymbol{x}_k, \boldsymbol{u}_k, \boldsymbol{d}), \tag{8a}$$

$$\boldsymbol{s}_{y,k} = \boldsymbol{g}^s(\boldsymbol{s}_{x,k}, \boldsymbol{x}_k), \tag{8b}$$

where the sensitivity of the ith state w.r.t. the jth parameter obeys the dynamics

$$f_{i,j}^s = \frac{d_j}{x_{j,k}} \left(\frac{\partial f_i}{\partial \boldsymbol{x}^T} \{\boldsymbol{s}_{x,k}\}_j + \frac{\partial f_i}{\partial d_j} \right), \tag{9}$$

where $\{\cdot\}_j$ represents the jth column of a matrix. The function $\boldsymbol{g}_s$ is derived analogously respecting (1b).

Among the several different possible experiment design criteria (Munack, 1991), we choose a modified E-design criterion:

$$\phi_{\mathrm{mE}}(\mathbf{F}) = \left(\max_i \lambda_i(\mathbf{F})\right) / \left(\min_i \lambda_i(\mathbf{F})\right), \tag{10}$$

where λ_i represents ith eigenvalue of $\mathbf{F}$. This choice is motivated by the minimization of the most uncertain parameter while achieving uncorrelated parameter estimates and it represents one of the generally recommended choices (Franceschini and Macchietto, 2008).

As we aim primarily at the minimization of the economical criterion (2) under uncertainty we propose a new optimal experiment design criterion. This uses the modified E-design with a scaled Fisher matrix such that:

$$\phi(\mathbf{F}) = \phi_{\mathrm{mE}} \left(\mathrm{diag}^{-1} \left[\frac{\partial \tilde{\mathcal{J}}^*}{\partial w(\boldsymbol{D})} \right] \mathbf{F} \, \mathrm{diag}^{-1} \left[\frac{\partial \tilde{\mathcal{J}}^*}{\partial w(\boldsymbol{D})} \right] \right), \tag{11}$$

where the scaling matrix contains the sensitivities of the optimal value of the robust economic objective w.r.t. the width of the range of parametric uncertainty.

A similar scaling was proposed in Recker et al. (2013) where the sensitivity of the economic cost is considered w.r.t. the parametric uncertainty. In contrast to that approach, we directly take into account the fact that if parametric uncertainty is present, a robust operation will be needed. As mentioned above, the conservativeness of the robust operation directly depends on the range of the uncertainty. Therefore we use as scaling factor the potential gain in the robust economic operation w.r.t. reduction in the parameter uncertainty range. Note that modern nonlinear programming solvers are capable of providing parametric sensitivity information w.r.t. the calculated optimum and thus, gathering of the scaling matrix can be automated when solving the problem (5) for some $\boldsymbol{D}$. In this work, the problem of optimal dynamic experiment design is formulated in the framework of multi-stage NMPC, hence Eq. (11) is reformulated as (6), in order to strike for the uncertainty in the objective and in the process constraints which are formulated accordingly.

4. GUARANTEED PARAMETER ESTIMATION

Given a set of output measurements $\boldsymbol{y}^{\mathrm{m}}$ at N_e time points $1, \dots, N_e$, *classical* parameter estimation seeks for *one* particular instance $\boldsymbol{d}_{\mathrm{e}}$ of the parameters for which the (possibly weighted) normed difference between measurements and the corresponding model outputs $\boldsymbol{y}$ is minimized. This optimization problem, for instance in the least-square sense, is given by:

$$\boldsymbol{d}_{\mathrm{e}} \in \arg\min_{\boldsymbol{d} \in \boldsymbol{D}_0} \sum_{i=1}^{N_e} \|\boldsymbol{y}_k^{\mathrm{m}} - \boldsymbol{y}_k\|_2^2, \tag{12a}$$

$$\text{s.t.} \quad \text{model (1)}, \tag{12b}$$

The confidence of the parameter estimates subject to measurement noise can then be approximated via ellipsoidal set whose shaping matrix (variance-covariance matrix of the estimates) can be approximated as an inverse of (7).

In contrast, *guaranteed* (bounded-error) parameter estimation accounts explicitly for the fact that the actual process outputs, $\boldsymbol{y}^{\mathrm{p}}$, are only known to be corrupted by some bounded measurement errors $\boldsymbol{e} \in \boldsymbol{E} := [\boldsymbol{e}^L, \boldsymbol{e}^U]$, so that

$$\boldsymbol{y}_k^{\mathrm{p}} \in \boldsymbol{y}_k^{\mathrm{m}} + [\boldsymbol{e}^L, \boldsymbol{e}^U] =: \boldsymbol{Y}_k. \tag{13}$$

Here, the main objective is to estimate the set $\boldsymbol{D}_{\mathrm{e}}$ of *all* possible parameter values $\boldsymbol{d}$ such that $\boldsymbol{y}_k \in \boldsymbol{Y}_k$ for every $k = 1, \dots, N_e$; that is,

$$\boldsymbol{D}_{\mathrm{e}} := \left\{ \boldsymbol{d} \in \boldsymbol{D}_0 \,\middle|\, \begin{array}{l} \exists \boldsymbol{x}, \boldsymbol{y} : \\ \boldsymbol{x}_{k+1} = \boldsymbol{f}(\boldsymbol{x}_k, \boldsymbol{u}_k, \boldsymbol{d}), \\ \boldsymbol{y}_k = \boldsymbol{g}(\boldsymbol{x}_k), \\ \boldsymbol{y}_k \in \boldsymbol{Y}_k, \forall k \in \{1, \dots, N_e\} \end{array} \right\}. \tag{14}$$

Depicted in red in Fig. 2 is the set of parameters $\boldsymbol{D}_{\mathrm{e}}$ projected in the (d_1, d_2) space that generate trajectories satisfying $\boldsymbol{y}_k \in \boldsymbol{Y}_k$, $k = 1, \dots, N_e$.

Obtaining an exact characterization of the set $\boldsymbol{D}_{\mathrm{e}}$ is not possible in general, and one has to resort to approximation techniques to make the problem computationally tractable. We use a variant of the Set Inversion Via Interval Analysis (SIVIA) algorithm by Jaulin and Walter (1993)

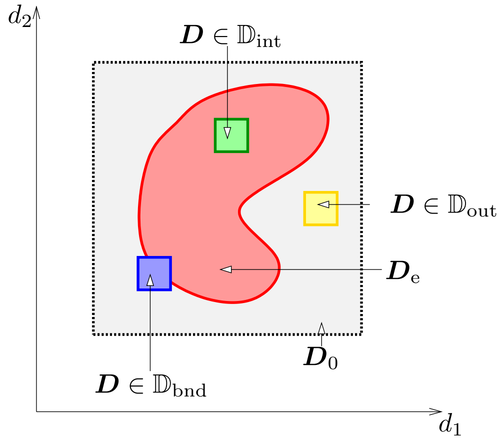

Fig. 2. Illustration of guaranteed parameter estimation concepts in the parameter space.

in order to approximate the solution set $\boldsymbol{D}_{\text{e}}$ as closely as possible. More concretely, the set $\boldsymbol{D}_{\text{e}}$ is approximated using the union of parameter sub-boxes that approximate its interior ($\mathbb{D}_{\text{int}}$) and over-approximate its boundary ($\mathbb{D}_{\text{bnd}}$). An illustration of such parameter sub-boxes is shown in Fig. 2 where $\mathbb{D}_{\text{out}}$ stands for the partition of parameter space guaranteed to have empty intersection with $\mathbb{D}_{\text{e}}$. Upon termination, this algorithm returns partitions $\mathbb{D}_{\text{int}}$ and $\mathbb{D}_{\text{bnd}}$ such that

$$\bigcup_{\boldsymbol{D}\in\mathbb{P}_{\text{int}}} \boldsymbol{D} \subseteq \boldsymbol{D}_{\text{e}} \subseteq \left(\bigcup_{\boldsymbol{D}\in\mathbb{D}_{\text{int}}} \boldsymbol{D}\right) \cup \left(\bigcup_{\boldsymbol{D}\in\mathbb{D}_{\text{bnd}}} \boldsymbol{D}\right) =: \boldsymbol{D}_{N_e}. \tag{15}$$

Further details on possible implementation variants of the described procedure can be found in Paulen et al. (2013a,b).

5. PROPOSED ALGORITHM

The main contribution of this paper is the presentation of a novel algorithm for the reduction of the uncertainty present in the model by applying robust optimal design of experiments and thus reducing the conservativeness introduced by a robust NMPC approach. The main motivation for proposing the novel OED criterion (11) is to estimate better the parameters that have a higher impact on the robust economic operation of the system. Since the Fisher information matrix provides only an approximation of the variance-covariance matrix of the estimated parameters, we propose the use of guaranteed parameter estimation to ensure more accurate approximation of the possible parameter values taking into account the measurement noise. We propose to apply the inputs generated via robust OED for a fixed number of steps N_e, then the maximum and minimum values of the estimated parameters obtained via guaranteed parameter estimation (set $\boldsymbol{D}_{N_e}$) are used to build a new scenario tree for multi-stage NMPC which is solved until the end of the control problem. The complete algorithm can be seen in Algorithm 1.

All the optimization problems reported in this work are solved using IPOPT (Wächter and Biegler, 2006) via CasADi (Andersson et al., 2012). The sensitivities entering in (11) are calculated using sIPOPT (Pirnay et al., 2012) and the guaranteed parameter estimation is implemented using GOLIB (`http://www3.imperial.ac.uk/environmentenergyoptimisation/software`) and library MC++ (`http://projects.coin-or.org/MCpp`).

Algorithm 1 Robust NMPC with uncertainty reduction

Input: $k = 0; N_e > 0; \boldsymbol{x}_0; \boldsymbol{D}_0$
1. **while** $k < N_e$ **do**
   1.1 Calculate $\dfrac{\partial \tilde{\mathcal{J}}^*}{\partial w(\boldsymbol{D})}$ with $\boldsymbol{D} = \boldsymbol{D}_0$.
   1.2 Solve the robust OED problem by minimizing (11) formulated as (6) in the framework of (5) with the prediction horizon $N_e - k$.
   1.3 Increment k, $k := k + 1$.

   end of while
2. Run guaranteed parameter estimation using the obtained measurements, getting $\boldsymbol{D}_{N_e}$ as a result.
3. Generate a new scenario tree using the guaranteed maximum and minimum values of the parameters from $\boldsymbol{D}_{N_e}$.
4. Run multi-stage NMPC by solving (5) with an economic cost function until the end of the control task.

6. CASE STUDY

We consider one of the traditional problems of optimal control of a chemical reactor. An exothermic chemical reaction $\text{A} + \text{B} \rightarrow \text{C}$ is run in a fed-batch reactor equipped with a cooling jacket. We use the setup of the experiment being closely similar to Srinivasan et al. (2003b) and Ubrich et al. (1999).

The reaction system is described by the following set of ODEs:

$$\frac{\mathrm{d}c_{\text{A}}}{\mathrm{d}t} = -kc_{\text{A}}c_{\text{B}} - \frac{u}{V}c_{\text{A}}, \qquad c_{\text{A}}(0) = c_{\text{A},0}, \tag{16}$$

$$\frac{\mathrm{d}c_{\text{B}}}{\mathrm{d}t} = -kc_{\text{A}}c_{\text{B}} + \frac{u}{V}(c_{\text{B,in}} - c_{\text{B}}), \qquad c_{\text{B}}(0) = c_{\text{B},0}, \tag{17}$$

$$\frac{\mathrm{d}c_{\text{C}}}{\mathrm{d}t} = kc_{\text{A}}c_{\text{B}} - \frac{u}{V} - c_{\text{C}}, \qquad c_{\text{C}}(0) = 0, \tag{18}$$

$$\frac{\mathrm{d}V}{\mathrm{d}t} = u, \qquad V(0) = V_0, \tag{19}$$

where c_i represents concentration of the substance i, k stands for the reaction rate, V is the volume of the reactor, and u represents the feed flowrate of reactant B with concentration $c_{\text{B,in}}$=10 mol L^{-1}. The considered initial conditions $c_{\text{A},0}$, $c_{\text{B},0}$ and V_0 take values of 2 mol L^{-1}, 0.46 mol L^{-1} and 0.7 L respectively.

The reaction is run under isothermal conditions where the inlet cooling jacket temperature is assumed to be adjusted to maintain the temperature in the reactor at $T = 70°C$. The respective evolution of the temperature of cooling medium inside the jacket obeys:

$$T_j(t) = T - \frac{(-\Delta H)kc_{\text{A}}(t)c_{\text{B}}(t)V(t)}{\alpha A(t)}, \tag{20}$$

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

In order to prevent an uncontrollable behavior of the reaction under a cooling failure (*thermal runaway*), the maximum attainable temperature is restricted to:

$$T_{cf} = T(t) + \min_{i\in\{A,B\}} c_i \frac{(-\Delta H)}{\rho c_p} \leq T_{\max}, \tag{21}$$

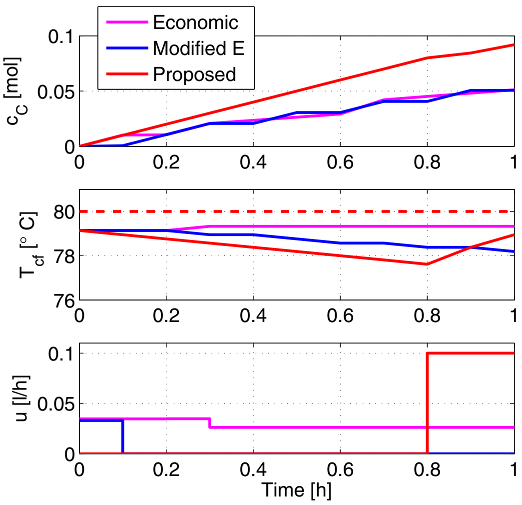

Fig. 3. Concentration c_C, temperature T_{cf} and control input u obtained from running robust optimal OED for different design criteria.

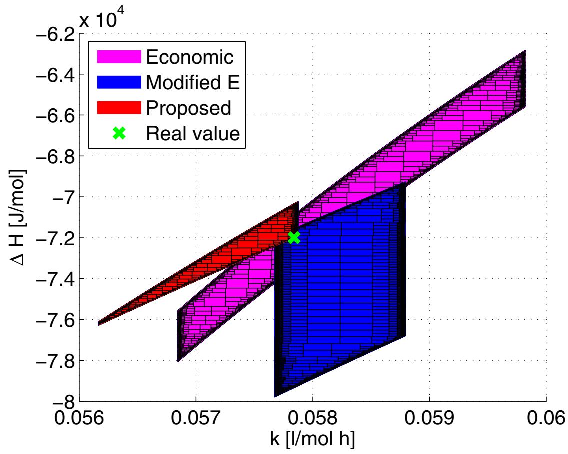

Fig. 4. Sets of guaranteed parameter estimates resulting from the measurements and control inputs obtained from optimal OED for different design criteria.

where ρ denotes the density and c_p the heat capacity 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 ($u_{\min} \leq u \leq u_{\max}$) as well.

The control task is to achieve a desired mass of the product C as fast as possible, $n_C = c_C V \geq n_{C,\text{des}}$. In this work we approximate the minimum time problem by a maximization of the mass of product C (n_C) over a finite prediction horizon, since simulation studies showed that the results obtained are almost equivalent. All the values of parameters present in the model and constraints are taken from Srinivasan et al. (2003b). It is considered that the parameters k and ΔH are uncertain and have constant but unknown values in the range $\pm 30\%$ with respect to their nominal values. The measured quantities (c_A, c_B and T_j) are subject to the noise $\boldsymbol{E}_{c_i} = [-0.05, 0.05]$ and $\boldsymbol{E}_{T_j} = [-0.5, 0.5]$ which is simulated using the appropriate rounding of the value of simulated outputs for the purpose of reproducibility of the results obtained here.

In the remainder of the paper, we show the results of applying Algorithm 1 to the presented case study. The first step is the robust optimal dynamic experiment design. In order to achieve robust performance and satisfaction of the constraints for all the possible values of the uncertainty ($\pm 30\%$), the OED problem is formulated as in (5) using a scenario tree that contains the maximum, minimum and nominal value of the uncertain parameters with a robust horizon equal to 1. The OED problem is solved in a shrinking horizon fashion for $N_e = 10$ steps and a sampling time $T_s = 0.1$ h. The results for three different OED criteria are shown in Fig. 3. The economic design uses as objective function the maximization of the concentration of product C (n_C), the Modified E design minimizes the OED criterion defined in (10) and the proposed algorithm minimizes the criterion (11).

After $N_e = 10$ steps, guaranteed parameter estimation is run where the obtained sets of guaranteed parameter estimates are shown in Fig. 4. We are interested in the projections of the resulting set on the parameter axes, because these determine the generation of the (new) scenario tree for the solution of problem (5). As expected, the robust OED with an economic cost yields the biggest ranges of the parameters which justifies the utilization of dual control for this case study. The modified E design gives smaller ranges and the proposed OED criterion (11) yields a smaller range for ΔH and a bigger range for the parameter k. As expected, all the sets contain the 'true' values of the parameters that in this case were assumed to be 20% bigger than the nominal value.

Due to the novel scaling of the Fisher matrix introduced in (11), ΔH can be estimated with a higher accuracy and this results in a superior performance compared to the OED using other criteria (see Fig. 5) when multi-stage NMPC is run with the new scenario tree based on the parameter estimates and with an economic cost function (maximization of n_C). The reason for this is that ΔH has a higher impact on the robust economic operation of the plant, since it influences directly the constraint on the temperature T_{cf}. As can be seen in Fig. 5, the economic optimal operation of the plant consists in driving the system as close as possible to the temperature constraint T_{cf}. Multi-stage NMPC calculates automatically a back-off to ensure that the constraint is not violated for any value of the uncertainty. If the range of the uncertainty that has to be taken into account is wider, then the necessary back-off is bigger and the resulting economic performance decreases. In this case, the lower bound on the uncertain parameter ΔH is the most important factor for the back-off. Therefore the dual control-like procedure that uses the OED with modified E design criterion gives a performance similar to the performance achieved by sole robust economic cost optimization despite yielding a narrower range of parameter uncertainty. The algorithm proposed in this paper achieves a batch time reduction by 1.5 hours which stands for a 7.5 % improvement over running robust NMPC with economical cost and the same procedure for estimation of the uncertainty.

7. CONCLUSION

A novel strategy for robust NMPC with improved performance via uncertainty reduction was presented. A new

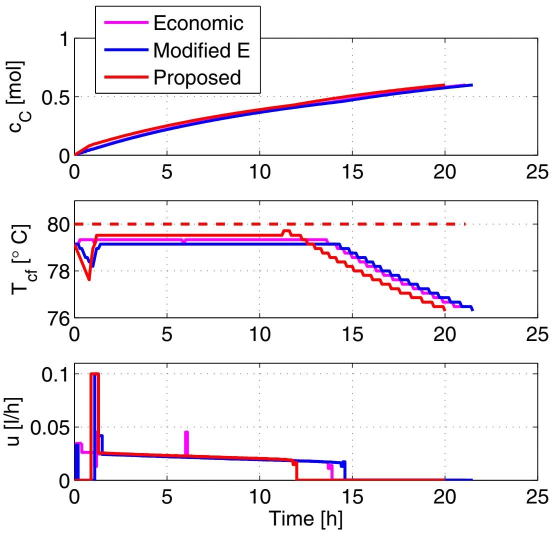

Fig. 5. Concentration c_C, temperature T_{cf} and control input u obtained from running multi-stage NMPC with a scenario tree generated with parameter bounds obtained by the guaranteed parameter estimation for different OED design criteria.

criterion for optimal OED is proposed in order to prioritize the more accurate estimation of the parameters that have a higher influence on the robust economic operation of the system. In order to avoid the unreliable approximation on the parameter ranges associated with typical OED approaches, a guaranteed parameter estimation approach is used to obtain the bounds of the uncertain parameters. The obtained bounds are used to build a new scenario tree with reduced uncertainty and a better economic performance is achieved. Simulation results of a chemical reactor show the potential of the approach and the possible improvements compared to a typical OED design and to a standard robust economic operation of the plant.

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