Stochastic Nonlinear Model Predictive Control of an Uncertain Batch Polymerization Reactor ⋆

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Abstract: This paper presents a stochastic nonlinear model predictive control technique for discrete-time uncertain nonlinear systems with particular focus on the batch polymerization reactor application. We consider a nonlinear dynamical system subject to chance constraints (i.e. need to be satisfied probabilistically up to a pre-assigned level). This formulation leads to a finite-horizon chance-constrained optimization problem at each sampling time, which is in general non-convex and hard to solve. We propose a heuristic methodology to handle uncertainty for highly nonlinear systems. In our framework, the uncertainty propagation is modelled via a Markov chain and a randomization technique, the so-called scenario approach, is employed yielding a tractable formulation. The efficiency and limitations of the proposed methodology is illustrated through its application to an uncertain batch polymerization reactor model and a comparison with deterministic nonlinear model predictive control is presented.

Keywords: Stochastic NMPC, Randomized NMPC, Uncertain Batch Polymerization Reactor

1. INTRODUCTION

Model predictive control (MPC) is a powerful control approach for optimizing the performance of input constrained systems. Furthermore, it is one of the most commonly used methodology to control multivariable industrial systems. The key idea of MPC is to find an approximate solution for the original infinite horizon control problem by solving a finite horizon constrained optimal control problem at each sampling time, and then, implementing the control law in accordance to a receding horizon strategy [Prandini et al. (2012)]. The nonlinear counterpart of MPC, denoted hereafter by NMPC, offers opportunities to model sophisticated nonlinear features often arising in real world applications.

One challenging aspect of ensuring optimal operation of industrial systems while enforcing critical constraints is to address any uncertainty or disturbances that is present in real systems [Lucia et al. (2013)], [Margellos et al. (2013)]. Over the last decades, progress has been made toward formulating robust variants of MPC to address this issue, see [Bemporad et al. (2003)], [Bemporad and Morari (1999)], [Morari and Lee (1999)] and the references therein. The aim of a robust MPC is to provide guaranteed stability and recursive feasibility for all admissible values of the uncertain parameters, while the method should be computationally tractable. In this approach, the control cost is optimized against the worst-case disturbance realization which may lead to conservative results, since the disturbance distribution is not accounted for and all disturbance realizations are treated equally. For systems where the uncertainty is known to be in a bounded set this approach is very powerful [Oldewurtel et al. (2013)]. However, for many practical applications it is hard to specify an a-priori bounded disturbance set.

Recently, a different framework has been introduced to address this issue, namely, stochastic MPC where the constraints are addressed in a probabilistic sense, see [Oldewurtel et al. (2013)], [Schildbach et al. (2014)] and the references therein. Alternatively, it can be interpreted as a relaxation of robust MPC, in which the robust satisfaction of state constraints are traded probabilistically via chance constraints, allowing for a small constraint violation probability to reduce the conservatism of robust MPC. Unfortunately, the resulting optimization problem is non-convex and computationally expensive in general [Mohajerin Esfahani et al. (2015)], [Rostampour et al. (2013)].

A tractable approximation to the aforementioned optimization problem can be obtained through randomized MPC [Prandini et al. (2012)], [Schildbach et al. (2014)]. Randomized MPC is a sample-based approximation in which only finitely many uncertainty samples are considered [Calafiore and Campi (2006)], [Campi et al. (2009)]. The advantage of this approach is that no restriction on distribution of uncertainty is required and it is sufficient to assume that the uncertainties are independent and identically distributed (i.i.d) and the decision variables (for fixed uncertain variables) are convex. The randomized approach

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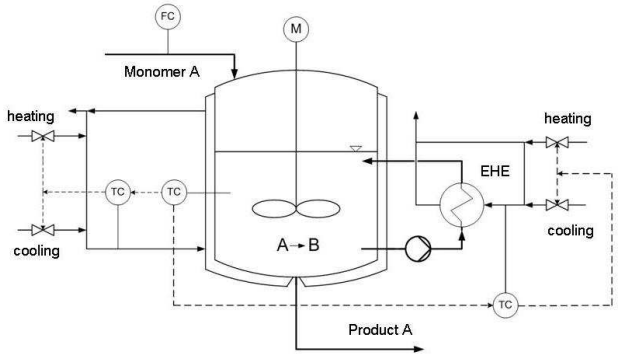

Fig. 1. Industrial batch polymerization reactor with an external heat exchanger (EHE).

has been extensively studied in literature for uncertain convex problems with efficient number of drawn samples.

We propose a stochastic NMPC strategy for an uncertain batch polymerization reactor. To this end, a finite horizon nonlinear optimization problem with chance constraints at each step is formulated. In order to have a tractable scheme in the proposed framework we deploy a sample-based approximation in the spirit of randomization techniques to replace the chance constraints at each step by a number of hard constraints where each constraint represents one realization of the uncertain parameter. We set up a Markov chain to model the uncertainty of the batch polymerization reactor and deploy the model to generate scenarios accordingly. Finally, we illustrate the efficiency and limitations of the proposed framework via a numerical study of uncertain batch polymerization reactor and a comparison with deterministic NMPC is presented.

The layout of this paper is as follows: In Section 2 we introduce a general stochastic NMPC framework for the industrial problem of uncertain batch polymerization reactor model. In Section 3 a tractable methodology is developed while using a heuristic approximation of chance constrained optimization problem. To investigate the efficiency and practical feasibility of the discussed methodology, in Section 4 the proposed framework is applied to an uncertain batch polymerization reactor model and then, a comparison with deterministic NMPC is presented. The paper is concluded in Section 5.

2. PROBLEM STATEMENT

2.1 Model Description

Consider an uncertain batch polymerization reactor system which is shown in Figure 1. Monomer is fed into the reactor and it turns into a polymer via a very exothermic chemical reaction. The reactor consists of a jacket and an External Heat Exchanger (EHE) that can both be used to control the temperature inside the reactor. A model of the process can be derived by using the following continuous-time system dynamics.

- Energy balances for the temperature of reactor ($\mathbf{T}_\mathrm{r}$), mixture in EHE ($\mathbf{T}_\mathrm{ek}$), coolant leaving EHE ($\mathbf{T}_\mathrm{awt}$), jacket ($\mathbf{T}_\mathrm{j}$) and vessel ($\mathbf{T}_\mathrm{s}$):

$$\dot{\mathbf{T}}_\mathrm{r} = \frac{1}{c_{p,r}m_{ges}}(\dot{\mathbf{m}}_\mathrm{f}c_{\mathrm{p,f}}(T_\mathrm{f}-\mathbf{T}_\mathrm{r})+\Delta H_\mathrm{r}k_{r_1}m_{\mathrm{m,r}} - k_\mathrm{k}A(\mathbf{T}_\mathrm{r}-\mathbf{T}_\mathrm{s})-\dot{m}_\mathrm{awt}c_{\mathrm{p,r}}(\mathbf{T}_\mathrm{r}-\mathbf{T}_\mathrm{ek}))\ , \tag{1a}$$

$$\dot{\mathbf{T}}_\mathrm{ek} = \frac{1}{c_{\mathrm{p,r}}m_\mathrm{awt}}(\dot{m}_\mathrm{awt}c_{\mathrm{p,w}}(\mathbf{T}_\mathrm{r}-\mathbf{T}_\mathrm{ek}) - \alpha(\mathbf{T}_\mathrm{ek}-\mathbf{T}_\mathrm{awt})+k_{r_2}\mathbf{m}_\mathrm{m}m_\mathrm{awt}\frac{\Delta H_\mathrm{r}}{m_\mathrm{ges}})\ , \tag{1b}$$

$$\dot{\mathbf{T}}_\mathrm{awt} = (\dot{\mathbf{m}}_{\mathrm{awt,kw}}c_{\mathrm{p,w}}(\mathbf{T}^\mathrm{in}_\mathrm{awt}-\mathbf{T}_\mathrm{awt}) - \alpha(\mathbf{T}_\mathrm{awt}-\mathbf{T}_\mathrm{ek}))/(c_{\mathrm{p,w}}m_{\mathrm{awt,kw}})\ , \tag{1c}$$

$$\dot{\mathbf{T}}_\mathrm{j} = \frac{1}{c_{\mathrm{p,w}}m_{\mathrm{m,kw}}}(\dot{m}_{\mathrm{m,kw}}c_{\mathrm{p,w}}(\mathbf{T}^\mathrm{in}_\mathrm{j}-\mathbf{T}_\mathrm{j}) + k_\mathrm{k}A(\mathbf{T}_\mathrm{s}-\mathbf{T}_\mathrm{j}))\ , \tag{1d}$$

$$\dot{\mathbf{T}}_\mathrm{s} = \frac{1}{c_{\mathrm{p,s}}m_\mathrm{s}}(k_\mathrm{k}A(\mathbf{T}_\mathrm{r}-\mathbf{T}_\mathrm{s})-k_\mathrm{k}A(\mathbf{T}_\mathrm{s}-\mathbf{T}_\mathrm{j}))\ , \tag{1e}$$

- Mass balances for the water ($\mathbf{m}_\mathrm{w}$), monomer ($\mathbf{m}_\mathrm{m}$) and product (polymer) ($\mathbf{m}_\mathrm{p}$) of the process:

$$\dot{\mathbf{m}}_\mathrm{w} = \dot{\mathbf{m}}_\mathrm{f}w_{\mathrm{w,f}}\ , \tag{1f}$$

$$\dot{\mathbf{m}}_\mathrm{m} = \dot{\mathbf{m}}_\mathrm{f}w_{\mathrm{m,f}} - k_{r_1}m_{\mathrm{m,r}} - k_{r_2}m_\mathrm{awt}\frac{\mathbf{m}_m}{m_\mathrm{ges}}\ , \tag{1g}$$

$$\dot{\mathbf{m}}_\mathrm{p} = k_{r_1}m_{\mathrm{m,r}} + \rho_1 k_{r_2}m_\mathrm{awt}\frac{\mathbf{m}_\mathrm{m}}{m_\mathrm{ges}}\ , \tag{1h}$$

where $\dot{\mathbf{m}}_\mathrm{f}$, $\mathbf{T}^\mathrm{in}_\mathrm{j}$, $\mathbf{T}^\mathrm{in}_\mathrm{awt}$ are the feed flow, coolant temperature at the inlet of the jacket and EHE control variables,

$$k_{r_1} = k_0\exp\left(\tfrac{-E_a}{R(T_\mathrm{r}+273.15)}\right)\left(k_{\mathrm{u1}}(1-\tfrac{\mathbf{m}_\mathrm{p}}{\mathbf{m}_\mathrm{p}+\mathbf{m}_\mathrm{m}})+k_{\mathrm{u2}}\tfrac{\mathbf{m}_\mathrm{p}}{\mathbf{m}_\mathrm{p}+\mathbf{m}_\mathrm{m}}\right),$$

$$k_{r_2} = k_0\exp\left(\tfrac{-E_a}{R(T_\mathrm{ek}+273.15)}\right)\left(k_{\mathrm{u1}}(1-\tfrac{\mathbf{m}_\mathrm{p}}{\mathbf{m}_\mathrm{p}+\mathbf{m}_\mathrm{m}})+k_{\mathrm{u2}}\tfrac{\mathbf{m}_\mathrm{p}}{\mathbf{m}_\mathrm{p}+\mathbf{m}_\mathrm{m}}\right)$$

are reaction ratios inside reactor and EHE, respectively. $m_\mathrm{ges} = \mathbf{m}_\mathrm{w}+\mathbf{m}_\mathrm{m}+\mathbf{m}_\mathrm{p}$ corresponds to the total mass, $m_{\mathrm{m,r}} = \mathbf{m}_\mathrm{m} - \mathbf{m}_\mathrm{m}\frac{m_\mathrm{awt}}{m_\mathrm{ges}}$ is the current amount of monomer inside the reactor and $k_\mathrm{k} = (\mathbf{m}_\mathrm{w}k_\mathrm{ws}+\mathbf{m}_\mathrm{m}k_\mathrm{ms}+\mathbf{m}_\mathrm{p}k_\mathrm{ps})/m_\mathrm{ges}$ denotes the heat transfer coefficient of the mixture inside the reactor. The reaction ratios k_{r_1}, k_{r_2} represent the nonlinear terms of the system. All undefined variables are constant parameters that represent process operational limits of the involved quantities. For detailed descriptions the reader is referred to [(Lucia et al., 2014, Table 1)].

By following a model proposed by [Lucia et al. (2014)], there is a safety constraint due to the temperature ($\mathbf{T}_\mathrm{adiab}$) that the reactor would achieve in the case of cooling failure which can be modelled by an additional differential state as follows:

$$\dot{\mathbf{T}}_\mathrm{adiab} = \frac{\Delta H_\mathrm{r}}{m_\mathrm{ges}c_{\mathrm{p,r}}}\dot{\mathbf{m}}_\mathrm{m} - (\dot{\mathbf{m}}_\mathrm{w}+\dot{\mathbf{m}}_\mathrm{m}+\dot{\mathbf{m}}_\mathrm{p})(\frac{\mathbf{m}_\mathrm{m}\Delta H_\mathrm{r}}{m^2_\mathrm{ges}c_{\mathrm{p,r}}})+\dot{\mathbf{T}}_\mathrm{r}\ . \tag{1i}$$

Due to the fact that the batch reactor has two different working phases (feeding and holding) and is considered to be finished only when the desired amount of polymer is produced an additional state is defined by [Lucia et al. (2014)] that accounts for the accumulated material that has been fed by

$$\dot{\mathbf{m}}_\mathrm{acc} = \dot{\mathbf{m}}_\mathrm{f}\ . \tag{1j}$$

One of the important sources of the uncertainty in real-life problems is a mismatch between the real system parameters and the model parameters. Due to this reason, the most crucial parameters of the model are considered to be

uncertain and varying with respect to their nominal value. Particularly, the specific reaction enthalpy ΔH_{r} and the specific reaction rate k_0 is assumed to be stochastic variables with respect to each time instant. To generate a time series random variable (scenarios) for the uncertainties, we developed a Markov chain-based model that produces a scenario taking into account the temporal correlation of the uncertainty.

Define the complete vector of state and control variables to be

$$x = [\mathbf{m}_{\mathrm{w}}, \mathbf{m}_{\mathrm{m}}, \mathbf{m}_{\mathrm{p}}, \mathbf{T}_{\mathrm{r}}, \mathbf{T}_{\mathrm{ek}}, \mathbf{T}_{\mathrm{awt}}, \mathbf{T}_{\mathrm{j}}, \mathbf{T}_{\mathrm{s}}, \mathbf{T}_{\mathrm{adiab}}, \mathbf{m}_{\mathrm{acc}}]$$

and $u = [\dot{\mathbf{m}}_{\mathrm{f}}, \mathbf{T}^{\mathrm{in}}_{\mathrm{awt}}, \mathbf{T}^{\mathrm{in}}_{\mathrm{j}}]$, respectively. We consider a vector $\delta = [k_0, \Delta H_{\mathrm{r}}]$ that contains the uncertain variables of system model. Using a more compact notation, the continuous-time dynamics formulation of the uncertain nonlinear system (1) can be written as

$$\dot{x} = f(x, u, \delta) \ , \tag{2}$$

where the states and control variables of the real process system (2) are also subject to the following constraints.

$$x_{\min} \leq x \leq x_{\max} \ ,$$
$$u_{\min} \leq u \leq u_{\max} \ ,$$

where $x_{\min}, u_{\min}$ and $x_{\max}, u_{\max}$ correspond to the lower and upper limitation of the state and control variables, respectively. We refer the reader to [(Lucia et al., 2014, Table 2 and Table 4)] for the detailed description about upper, lower bounds of the state and the control variables as well as the initial conditions.

2.2 Stochastic Control Problem

In order to solve the NMPC problem, we employ direct multiple-shooting, where the control and the state trajectories are discretized to form a finite-dimensional nonlinear program (NLP). This method handles inequality and terminal constraints robustly and it has been implemented by using the CasADi toolbox [Andersson et al. (2012)] in Python.

Consider the discrete-time nonlinear dynamics formulation of the aforementioned uncertain system in a compact format as

$$x_{t+1} = F(x_t, u_t, \delta_t) \ , \tag{3}$$

where $x_t \in \mathbb{R}^{10}$ is the state vector, $u_t \in \mathbb{R}^3$ the control input vector, $\delta_t \in \Delta \subseteq \mathbb{R}^2$ the random variable (uncertainty) defined on a probability space Δ. It is assumed that Δ is endowed with the Borel $\sigma-$algebra $\mathfrak{B}(\Delta)$ and $\mathbb{P}$ is a probability measure defined over Δ. $f : \mathbb{R}^{10} \times \mathbb{R}^3 \times \mathbb{R}^2 \to \mathbb{R}^{10}$ is assumed to be a measurable function with respect to each $\delta_t \in \Delta$. However, it is important to note that for our study we only need a finite number of instances of δ_t, and we do not require the probability space Δ and the probability measure $\mathbb{P}$ to be known explicitly. For further technical details on this aspect the reader is referred to [(Mohajerin Esfahani et al., 2015, Section 3.3)].

Consider a full prediction horizon that contains T time steps, and a subscript 't' in our notation is introduced to characterize the value of the quantities for a given time instance $t = \{1, 2, \cdots, T\}$ within the horizon. We denote x_0 as the initial value of the states, and define x_t and u_t to be the state and input vector at time t of the horizon, respectively. It is assumed that the entire state vector of the system is available at each time instant, since one can eliminate all future state variables depending on the observed initial real plant state by using (3). We are interested in generating an input sequence $\{u_1, \cdots, u_T\}$ to control the nonlinear system (2) that are to be chosen from a set of feasible inputs $\mathbb{U} \subseteq \mathbb{R}^3$ (constraint set of control variables).

The minimization of the objective function is subject to keeping the state inside a feasible set $\mathbb{X} \subseteq \mathbb{R}^{10}$ (constraint set of state variables) for a given fraction of all time steps which maybe too conservative, and result in a poor performance. Specifically, this is the case when the best performance of an economic objective is achieved close to the boundary of $\mathbb{X}$. Due to the imperfect models (uncertainty source), constraint violations will be then unavoidable [Engell (2007)]. To avoid infeasibility of the state constraints when the disturbance has unbounded support, we consider the state variables to be *probabilistically feasible* by means of chance constraint on the state

$$\mathbb{P}_{\boldsymbol{\delta}} \left[x_{t+i|t} \in \mathbb{X} \ , \ \forall \ i \ \right] \geq 1 - \epsilon \ , \tag{4}$$

where $\epsilon \in (0, 1)$ is the admissible constraint violation parameter. Note that the index of $\mathbb{P}_{\boldsymbol{\delta}}$ denotes the dependency of $x_{t+i|t}$ on the string of random scenarios $\{\delta_0, \delta_1, \cdots, \delta_{T-1}\}$, which are independent and identically distributed (i.i.d.).

2.3 Stochastic NMPC

Consider $\boldsymbol{\delta} := (\delta_0, \delta_1, \cdots, \delta_{T-1}) \in \Delta^T$ to be a sequence of i.i.d. random scenarios and $\boldsymbol{u} := (u_0, u_1, \cdots, u_{T-1}) \in \mathbb{U}^T$ as a sequence of the planned input. The predicted state for i steps into the future is denoted by $x_{t+i|t} = \varphi(x_t, \tilde{\boldsymbol{u}}, \tilde{\boldsymbol{\delta}})$ according to (3), where x_t is assumed to be the current state, $\tilde{\boldsymbol{u}} := (u_0, \cdots, u_t)$ and $\tilde{\boldsymbol{\delta}} := (\delta_0, \cdots, \delta_t)$. The main goal is to maximize the amount of production (polymer) of the batch reactor over a finite time horizon while satisfying states and inputs constraints, and taking into account that the uncertainty manifests itself in the form of random variable. Moreover, we define a set-point tracking term for the desired reactor temperature to ensure that the produced polymer has the required properties. We define

$$-\mathbf{m}_{\mathrm{p},t+i|t} + \gamma(\mathbf{T}_{\mathrm{r},t+i|t} - T_{\mathrm{set}})^2 = \ell \left(x_{t+i|t} = \varphi(x_t, \tilde{\boldsymbol{u}}, \tilde{\boldsymbol{\delta}}) \right) \ ,$$

where T_{set} is the desired reactor temperature and γ is a cost coefficient for the tracking term. $\ell(\cdot)$ is a stage cost function that reflects our control purpose, i.e., maximizing the amount of polymer and set-point tracking of the reactor temperature. Consider the stochastic objective function as follows:

$$J(x_t, \boldsymbol{u}, \boldsymbol{\delta}) := \sum_{i=1}^{T} \ell(x_{t+i|t} = \varphi(x_t, \tilde{\boldsymbol{u}}, \tilde{\boldsymbol{\delta}})) \ , \tag{5}$$

where J is a random variable. In order to obtain a deterministic objective function, we consider the $\mathbb{E}\left[J(x_t, \boldsymbol{u}, \boldsymbol{\delta})\right]$.

Now we can formulate a chance constrained finite horizon optimal control problem for each time step t:

$$\min_{\boldsymbol{u} \in \mathbb{U}} \quad \mathbb{E}\left[J(x_t, \boldsymbol{u}, \boldsymbol{\delta})\right] \qquad \text{subject to:} \tag{6a}$$

$$\mathbb{P}\left[x_{t+i|t} \in \mathbb{X} \ , \ \forall \ i = \{1, \cdots, T\} \ \right] \geq 1 - \epsilon \ . \tag{6b}$$

The solution of (6) is the optimal planned input sequence $\boldsymbol{u}^* := (u_0^*, u_1^*, \cdots, u_{T-1}^*)$. Based on the stochastic NMPC algorithm the current input is set to $u_t := u_0^*$ and we proceed in a receding horizon fashion. This means (6) is solved at each time step 't' by using the current measurement of the state x_t. Due to the presence of chance constraints, the feasible set is, in general, non-convex and hard to determine explicitly. In the following section, we describe a tractable formulation to solve (6) by using a sample-based approximation [Calafiore and Campi (2006)].

3. HEURISTIC METHODOLOGY

To solve the chance constrained optimization problem proposed in Section 2.3, we resort to an approximation approach. In order to avoid introducing arbitrary assumptions on $\mathbb{P}$ and its moments, we follow a randomized approach. The randomized approach is a tool to approximate chance constraints and substitute the chance constraints with a finite number of pointwise constraints at independently generated scenarios of the uncertain parameter. The number of scenarios 'S' remains a crucial parameter and has to be selected carefully to achieve the desired level of approximation of the chance constraints.

In [Calafiore and Campi (2006)] the so-called 'scenario approach' is developed to provide a lower bound for the number of scenarios that should be extracted to establish the desired probabilistic guarantees with high confidence. The limitation of this approach is that the theoretical bound only holds for convex problems, i.e., when the cost and the constraint functions are convex in the decision variable for each realization of uncertainty. This setting was later extended in [Mohajerin Esfahani et al. (2015)] for a class of non-convex problems, but unfortunately our problem here does not fall into this category. Besides, on the practical side, the number of scenarios suggested by theory grows linearly in the dimension of decision variables and often goes beyond our computational capabilities. This hampers the applicability of the method to large scale systems, see [Rostampour et al. (2013)] for more detailed explanation to an application in power grids. Due to the non-convexity of the system (3), the theoretical results in the scenario approach literature does not apply here.

Consider the following tractable formulation of (6), called Randomized NMPC:

$$\min_{\boldsymbol{u}\in\mathbb{U}} \sum_{\boldsymbol{\delta}^k\in\boldsymbol{W_0}} J(x_t, \boldsymbol{u}, \boldsymbol{\delta}^k) \qquad \text{subject to} \tag{7a}$$

$$x_{t+i|t} = \varphi(x_t, \boldsymbol{u}, \boldsymbol{\delta}^l) \in \mathbb{X}\ , \ \begin{cases} \forall\ i = \{1, \cdots, T\} \\ \forall\ \boldsymbol{\delta}^{(l)} \in \boldsymbol{W_1} \end{cases}, \tag{7b}$$

where $\boldsymbol{W_0} := \{\boldsymbol{\delta}^1, \cdots, \boldsymbol{\delta}^{S_0}\}$ is a set of 'S_0' number of scenarios that is used to empirically approximate the cost function J and $\boldsymbol{W_1} := \{\boldsymbol{\delta}^{(S_0+1)}, \cdots, \boldsymbol{\delta}^{(S_0+S_1)}\}$ is a set of 'S_1' number of scenarios to empirically enforce the state constraints for the full predicted stages $i = \{1, \cdots, T\}$. (S_0, S_1) are non-negative integers and $S = (S_0 + S_1)$ full horizon uncertainty scenarios are drawn independently with respect to Δ^T. We assumed for every realization of uncertainty a feasible solution is admitted.

Applying a receding horizon policy in the MPC framework, the problem in (7) must be solved at each time step with an updated initial state x_t and the current input $u_t := u_0^\star$ is set to the first element of the feasible solution $\boldsymbol{u}^* := (u_0^*, u_1^*, \cdots, u_{T-1}^*)$. The proposed procedure is summarized in Algorithm 1. Note that the user defined scenario sizes

Algorithm 1 Randomized NMPC

1: Fix $S_0 \in [1, \infty)$ to approximate the cost function and $S_1 \in [1, \infty)$. When S_1 goes to infinity, the level of constraint violation 'ϵ' goes to zero.
2: Generate $S = (S_0 + S_1)$ scenarios of $\boldsymbol{\delta}$ (uncertain variables) corresponding to Δ^T.
3: Solve (7) and determine a feasible solution $\boldsymbol{u}^*$.
4: Apply the first input of solution $u_t := u_0^\star$ to the uncertain real system (2).
5: Measure state (x_t): **if** $(\mathbf{m}_{p,t})$ is the desired quantity **then** stop.
6: Go to step 2.

S_0 and S_1 can be seen as tuning variables to approximate the cost function and to enforce the constraints for the predicted stages, respectively.

For sake of comparison, we consider a deterministic NMPC strategy where in the problem (7) we replace $\boldsymbol{\delta}$ with a nominal value, i.e. the forecast or expected value of uncertain terms for the full horizon. The procedure is summarized in Algorithm 2.

Algorithm 2 Deterministic NMPC

1: Fix $\boldsymbol{\delta} = (\delta_0^n, \delta_1^n, \cdots, \delta_{T-1}^n)$ in the problem (7).
2: Solve (7) and determine a feasible solution $\boldsymbol{u}^*$.
3: Apply the first input of solution $u_t := u_0^\star$ to the uncertain real system (2).
4: Measure state (x_t): **if** $(\mathbf{m}_{p,t})$ is the desired quantity **then** stop.
5: Go to step 2.

It is worth mentioning that one may consider a robust NMPC strategy where it needs to characterize the worst-case realization of $\boldsymbol{\delta}$ for each predicted stage using vertices of predetermined bounds for each element of δ. This leads to a set of all possible worst-case scenarios for $\boldsymbol{\delta} \in \boldsymbol{W}_{\text{worst}}$. Finding the worst-case scenario in particular for a nonlinear system is in general intractable. As an attempt to address this issue, one may only focus on extreme points of the uncertainty set. If we assume a rectangular uncertainty set at each sampling step, then there are two possible worst-cases (upper and lower bounds) for each uncertain element (2^2 vertices). This leads to 2^{2T} possible worst-case scenarios over the prediction horizon, and as such encounters the curse of dimensionality and renders the robust variant of the problem (6) intractable.

4. CASE STUDY

4.1 Uncertainty Model

In this section we concentrate on the development of an uncertainty model that enables us to generate scenarios (uncertainty samples), while taking its temporal correlation into account. We assume that the uncertainty is a discrete-time stochastic process, in which the outcome of a given state can affect the outcome of the next state.

This type of process is called a Markov chain. Consider a finite number of states, where the process starts in one of these states and moves successively from one state to another, and define the probabilities for the transitions between states. To generate various uncertainty realizations, the transition probability matrix is constructed, which is initialized via a nominal value of the uncertainty for the starting state. This method offers an excellent fit for both the probability density function and the autocorrelation function of the generated time series. It is assumed to have two independent models for each random variable $(\Delta H_r, k_0)$. To generate a random scenario, we first initialize the state of the first stage and then it will jump to the next state with high probability and this will continue until the last stage. In case of having the same probability of transition, a random decision will be made.

4.2 Simulation Setup

As described before, to solve the optimal control problem we employed CasADi by using direct multiple-shooting for the discretization of the aforesaid continuous-time dynamical system. For the multiple shooting approach we used the explicit Runge-Kutta integration scheme. In particular, in this work all NLP optimization problems are solved using IPOPT [Wächter and Biegler (2006)] which uses first and second order exact derivative information provided automatically by CasADi [Andersson et al. (2012)]. The real system plant (2) is simulated with the calculated control input using also the explicit Runge-Kutta integration scheme. The uncertain elements of the real system are generated randomly from uniform distribution of predetermined interval for each simulation. All proposed optimization problems are solved in Python on a standard MacBook Pro with an Intel i-5 processor at 2.5GHz with one core and 4 GB of RAM.

4.3 Simulation Results

Consider a simulation study derived based on the following parameters that are chosen based on physical knowledge of the process. The sampling time of the NMPC controller $\tau = 15s$ and with a prediction horizon of $T = 15$ steps. The cost coefficient for tracking term is chosen to be $\gamma = 10^4$. The criteria that the batch process is considered to be finished is the amount of product (polymer) that has been produced ($\mathbf{m}_{\mathrm{p},t+T|t} = 20680\ [kg]$) and the set-point tracking of the reactor temperature is $T_{\mathrm{set}} = 90\ [^\circ C]$. We assumed the nominal values of $k_0^{\mathrm{n}} = 7.0$, $\Delta H_{\mathrm{r}}^{\mathrm{n}} = 950.0$, and taking a value from $k_0 \sim \mathcal{U}(4.0, 10.0)$, $\Delta H_{\mathrm{r}} \sim \mathcal{U}(850.0, 1050.0)$, randomly.

Figure 2 contains six sub-figures from top to bottom that represent the following results: The first three are state trajectories that are reactor temperature ($\mathbf{T}_{\mathrm{r},t}$), monomer mass ($\mathbf{m}_{\mathrm{m},t}$) and product mass ($\mathbf{m}_{\mathrm{p},t}$), respectively. The rest are optimal control inputs that are feed flow ($\dot{\mathbf{m}}_{\mathrm{f},t}$), jacket temperature ($\mathbf{T}_{\mathrm{j},t}$) and EHE temperature ($\mathbf{T}_{\mathrm{awt},t}$), respectively. The obtained results for the implementation of the deterministic NMPC strategy are denoted by 'Red' color using Algorithm 2. 'Green' and 'Blue' colors both represent the results obtained via randomized NMPC with a different number of scenarios. We consider same scenarios that contribute to the cost function and the states constraints. Namely, we generate S scenarios instead of using different tuning parameters in Algorithm 1. 'Green' color represents the case where $S = 4$ and 'Blue' color shows the case with $S = 100$.

	Computational time	Batch time
Deterministic NMPC	00:15 Minutes	01:51 Hour
Randomized NMPC ($S = 4$)	01:00 Hour	02:29 Hour
Randomized NMPC ($S = 100$)	more than 5 Days	05:19 Hour

Table 1. The computational and batch process time of different control strategy.

Since the quality of product (polymer) is related to the reactor temperature (sub-figure one), we consider that as the set-point tracking term in our objective function (5). We examine a violation level of $T_{set} \pm 1.5[^\circ C]$ a posteriori. As it is clearly shown, using randomized NMPC resulted in a feasible solution and inside the desired bound for the reactor temperature. The result of deterministic NMPC strategy is, indeed, an infeasible (undesired) reactor temperature, since the observed ($\mathbf{T}_{r,t}$) is outside of the desired bounds. Furthermore, the two different results (Blue and Green) of randomized NMPC depict that taking into account more possible random scenarios ($S = 100$) the reactor temperature almost perfectly tracked the desired T_{set} and thus, lead to better performance.

Sub-figure two presents the monomer mass at each sampling time whereas the polymer mass is shown in sub-figure three. From these two figures, it is clearly visible that better set-point tracking of the reactor temperature results in longer batch process time. The reason is due to the fact that there is always a trade-off between the quality of product and how fast the batch process is done. Table 1 illustrates the computational time and batch process time of the different strategies.

5. CONCLUSIONS

In this paper we formulated a stochastic nonlinear model predictive control problem for an uncertain nonlinear system, in particular a batch polymerization reactor. We proposed a heuristic framework to approximate chance constrained finite horizon optimization with a large-scale deterministic optimization problem at each sampling time. Due to the limitation arising from non-convexity of the considered system, we cannot directly employ randomized algorithms that are developed for convex problems.

To circumvent this limitation, one can employ tools from statistical learning literature, in particular the notion of Vapnik-Chervonenkis (VC) dimension. The VC-dimension is a useful 'complexity measure' in many classical control problems. However, calculating this bound for the system function (3) may be a difficult task and we will pursue this viewpoint in our subsequent work.

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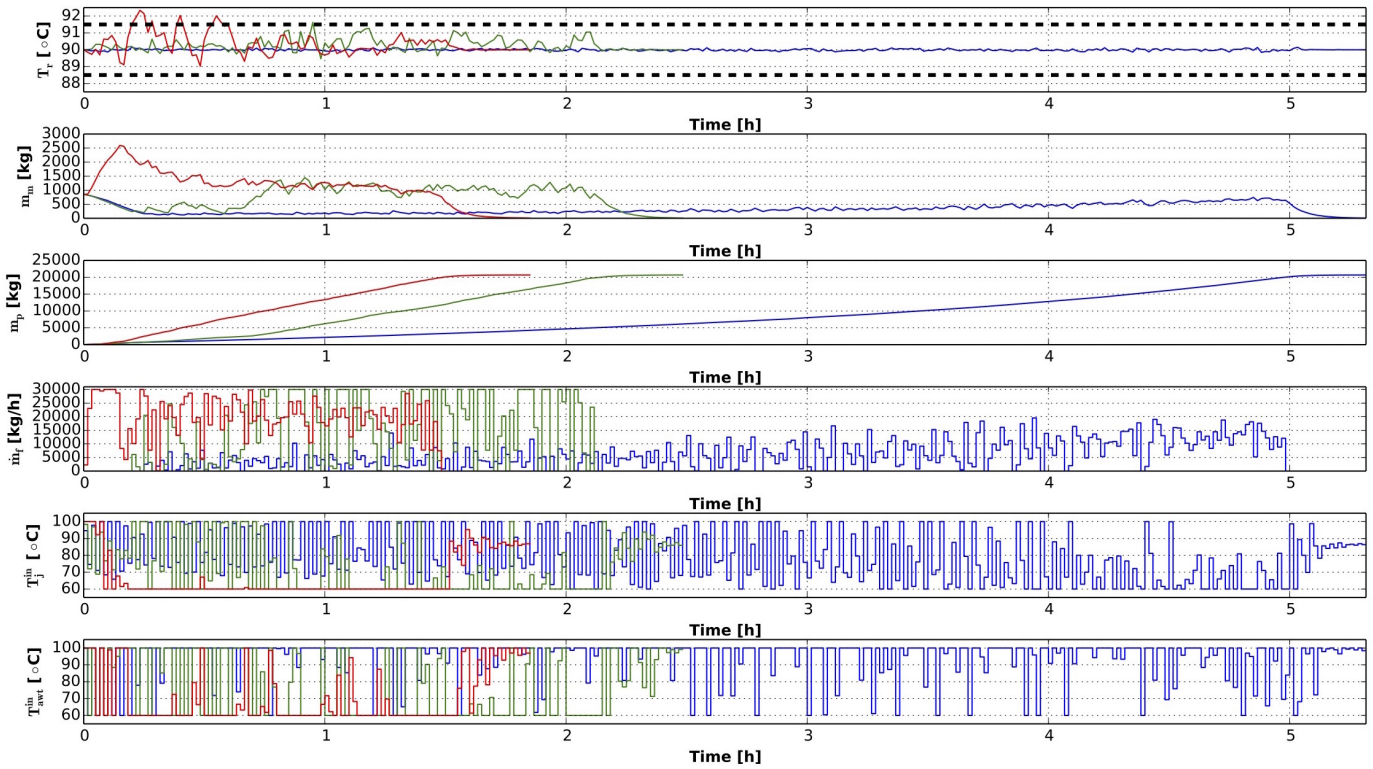

Fig. 2. From top to bottom: reactor temperature, monomer mass, product (polymer) mass, feed (monomer) flow, jacket temperature and EHE temperature. The first three from top are state trajectories and the rest are control inputs trajectories. Red color denotes the results of implementation of deterministic NMPC as stated in Algorithm 2. Green color represents the results obtained via randomized NMPC with just four different scenarios for uncertainties using Algorithm 1. Blue color represents the results obtained via randomized NMPC with a hundred of different scenarios for uncertainties using Algorithm 1.

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