

Robust Nonlinear Model Predictive Control of a Batch Bioreactor Using Multi-stage Stochastic Programming

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Abstract—This paper presents a robust nonlinear model predictive control scheme and its application to a batch bioreactor. The approach is based on the description of the uncertainty evolution as a scenario tree. This makes it possible to take explicitly into account the future disturbances and control inputs leading to a non-conservative approach that is not based on the tracking of a nominal solution. The main challenge of the approach is that the size of the resulting optimization problem grows exponentially with the prediction horizon and with the number of uncertainties. The potential of the approach is demonstrated by simulation examples of a nonlinear penicillin fermentation process where the proposed scheme can fulfill the state and the input constraints for all the possible values of several uncertain parameters, improving the performance of existing robust approaches such as tracking of the necessary conditions of optimality.

I. INTRODUCTION

Linear model predictive control (MPC) is an optimization based control scheme that has become one of the standard control strategies in the process industry. Increasingly also nonlinear model predictive control (NMPC) is being applied to challenging industrial processes. The reasons for the success of linear MPC are its ability to deal with strongly coupled multivariable plants and with constraints on input and states. Nonlinear MPC offers the possibility to use an economic criterion in the cost function in order to optimize directly the plant economics instead of tracking fixed references.

MPC solves an open loop optimization problem using a model of the plant at each sampling time. Feedback information enters only by the re-initialization of the optimizer at the next step with the new measurements, via the state update and the bias update. Therefore performance and stability depend strongly on the accuracy of the model that is employed in the optimization. As in many domains there is a significant plant-model mismatch, robustification of MPC is an important issue. MPC controllers should guarantee constraint satisfaction and have a satisfactory performance also in the presence of significant uncertainties which can be disturbances or model errors. There still is no general approach that can handle nonlinear systems and at the same time can be implemented in real-time, guarantees robust constraint satisfaction and shows a low degree of conservatism.

The most discussed robustification approach is min-max MPC, introduced in [1] where the optimization is performed for the worst case disturbance from a set. Min-max MPC can

be classified into open-loop and closed-loop approaches [2]. The first ones optimize over a sequence of optimal control inputs, and enforce that the constraints have to be satisfied for all possible values of the uncertainty. This ignores the fact that the controller will react to the uncertainty in the next steps. As no feedback is incorporated, open-loop robust controllers are known to be conservative and may lead easily to infeasibilities during the optimization (see [3]). In contrast, closed-loop min-max approaches optimize over a sequence of control policies, which is an infinite optimization problem that is very difficult to solve for general nonlinear systems. It can be simplified by optimizing only over a restricted type of control policies (e.g. affine policies) however resulting in suboptimality. This suboptimality can be bounded for linear time-varying systems as shown in [4].

In the last years, tube-based methods have received increasing attention in the robust MPC community as an alternative to min-max approaches. Tube-based MPC was presented for linear systems in [5] and later extended for the nonlinear case in [6]. It solves the nominal control problem and includes a so-called ancillary controller that makes sure that the evolution of the real uncertain system stays in a tube that is centered around the nominal solution. The cross-sections of this tube are positive invariant sets, what makes it possible to develop stability and recursive feasibility guarantees. Different improvements and modifications regarding the calculation of the ancillary controller and the cross-sections have been introduced in the literature leading to different computational complexities and degrees of conservativeness (see [7], [8], [9], [10]).

This paper proposes multi-stage NMPC as a promising alternative for the solution of a robust NMPC problem. The key idea behind multi-stage NMPC is that the evolution of the uncertainty is modeled by a scenario tree, in a similar manner as explained in [3]. In this way the fact that new information will be available at the next sampling times is taken explicitly into account, and also that the future control inputs can be adjusted according to this information to counteract the effect of the uncertainties. The idea to use multi-stage stochastic optimization for NMPC was introduced in [11] and in [12] and has been applied to semi-batch polymerization reactors in [13]. Similar ideas have been applied successfully to scheduling problems in [14] or for linear min-max MPC in [15], and in [16]. Assuming that the scenario tree describes the uncertainty perfectly, our approach represents the online decision problem exactly and therefore provides the best possible solution. The drawback of the approach is that it results in large optimization problems, the size of which

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grows exponentially with the prediction horizon and with the number of uncertainties and uncertainty levels.

NMPC of batch processes has been widely studied in the literature [17], usually based on a shrinking horizon approach so that the properties at the end of the batch that have to be controlled can be included directly in the optimization problem. However, this may result in some cases in a large prediction horizon, leading to intractable optimization problems. In this work a standard receding horizon approach is used, with a constant prediction horizon smaller than the batch time. The loss of optimality caused by this approximation is investigated for a batch bioreactor presented in [18] and the advantages of multi-stage NMPC for the control of the system in the presence of several uncertainties are illustrated in a comparison with standard NMPC and with a different robustification approach (tracking of the necessary conditions of optimality) also proposed in [18]. In addition, a comparison between two state-of-the-art nonlinear programming solvers, IPOPT [19] and SNOPT [20], is included for the solution of the resulting optimization problems.

After this introductory section, the paper is organized as follows. The proposed robust multi-stage NMPC scheme is introduced in Section 2. In Section 3, the model under consideration is presented together with the results of the standard NMPC controller when there are no uncertainties or disturbances. Section 4 includes the results obtained with multi-stage NMPC under several uncertainties. Finally, the conclusions and directions of future work are presented in Section 5.

II. MULTI-STAGE NMPC

As stated previously, the key idea of multi-stage NMPC is the modeling of the uncertainty by a tree of discrete scenarios (see Fig. 1). Each path from the root node x_0 to one of the leaf nodes is called a scenario. At each call of the optimization, the decision at the root node is computed, taking into account explicitly the uncertainty about the future evolution, as well as the presence of future decisions (recourse variables) that utilize the additional information gained as the evolution progresses along the branches. In this way, feedback information is incorporated in the open-loop optimization problem solved at each sampling time, reducing the conservativeness of the approach. For the correct modeling of the real-time decision problem, decisions at the nodes that are based upon the same information must be equal. This is imposed by the so-called *non-anticipativity* constraints. They force all control inputs that branch at one node to be the same (i.e., in Fig. 1 $u_0^1 = u_0^2 = u_0^3$, $u_1^1 = u_1^2 = u_1^3$, ...).

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

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

where each state vector x_{k+1}^j at stage $k+1$ and position j in the scenario tree depends on the parent state $x_k^{p(j)}$ at stage k , the control input u_k^j and the corresponding

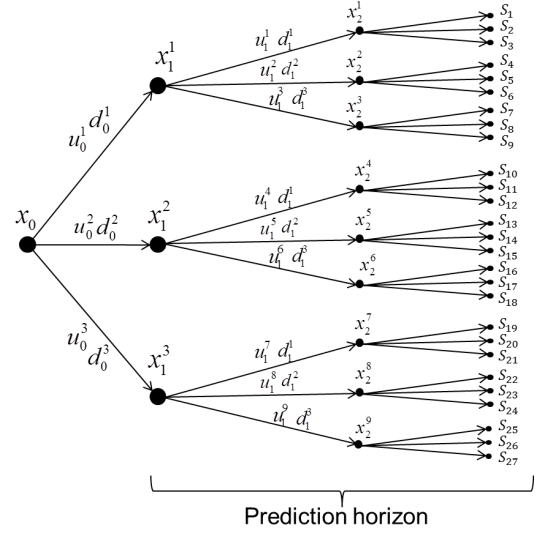


Fig. 1. Scenario tree representation of the uncertainty evolution for multi-stage NMPC.

realization r of the uncertainty $d_k^{r(j)}$ (for example in Fig.1, $x_2^6 = f(x_1^2, u_1^6, d_1^3)$). For simplicity, it is considered that the tree has the same number of branches at all nodes, defined by $d_k^{r(j)} \in \{d_k^1, d_k^2, \dots, d_k^s\}$ for s different possible values of the uncertainty. Finally, for the ease of notation, the set of occurring indices (j, k) in the scenario tree is denoted by I . S_i denotes scenario number i .

A. Mathematical Formulation

Once the necessary notation has been introduced, a general formulation of the optimization problem that has to be solved can be written as follows:

$$\min_{\tilde{u}} \tilde{J} \quad (2a)$$

subject to:

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

$$x_k^j \in \mathbb{X}, \quad \forall (j, k) \in I, \quad (2c)$$

$$u_k^j \in \mathbb{U}, \quad \forall (j, k) \in I, \quad (2d)$$

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

where $\tilde{J} = \left(\sum_{i=1}^N (\omega_i J_i)^\alpha \right)^{1/\alpha}$. ω_i denotes the probability of each scenario S_i . There are N different scenarios and the cost of each one is denoted by J_i and can be written as:

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

where $L(x_{k+1}^j, u_k^j)$ is the stage cost. The non-anticipativity constraints in (2e) force all the control inputs u_k^j branching at the same parent node $x_k^{p(j)}$ to be the same. With this general formulation, if $\alpha = 1$ the resulting optimization problem represents the multi-stage NMPC approach, whereas if $\alpha = \infty$ is chosen, the optimization problem yields a closed-loop

min-max approach in which feedback is taken explicitly into account. In addition, if the number of scenarios is $N = 1$, the problem is reduced to standard NMPC.

B. Implementation details

A simultaneous implementation of NMPC is chosen in this work, that is, both states and control inputs are discretized and included in the resulting Nonlinear Programming problem (NLP) as optimization variables. Most of the models for process control are described by a set of ODEs which can be written as:

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

In this work the dynamics of the system are included as nonlinear constraints using a simple implicit Euler discretization, since it provides a sufficient accuracy and results in a fast solution of the NLP. If the accuracy provided by this discretization method is not enough, more elaborated approaches can be applied to multi-stage NMPC [21] such as multiple-shooting approach (see [22]) or pseudospectral collocation (see [23]). Using the same notation as in (1), the discretized model can be written as:

$$x_{k+1}^j = x_k^{p(j)} + h(\Phi(x_{k+1}^j, u_k^j, d_k^{r(j)})), \quad (5)$$

where h is the chosen sampling time. After the discretization, the resulting optimization problem is a standard NLP that can be solved with any available solver. The NLP can be written as follows:

$$\min_{x^{\text{opt}}} f(x^{\text{opt}}) \quad (6a)$$

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

$$c_l \leq c(x^{\text{opt}}) \leq c_u, \quad (6c)$$

where x^{opt} is the augmented optimization vector. It includes all the states (nodes) and control inputs as indicated in Fig. 1, i.e., $x^{\text{opt}} = [x_0, x_1^1, x_1^2, \dots, x_{N_p}^N, u_1^1, u_1^2, \dots, u_{N_p}^N]$. The cost function f is formulated as in (2). The bounds on the optimization variables (6b) represent the constraints on states and inputs and the nonlinear constraints (6c) include the discretized model for all the nodes of the tree, the *non-anticipativity* constraints, and the initial conditions. The special structure and high sparsity of the problem can be exploited explicitly leading to a large improvement on the solution times as presented in [24], but this is part of our future work and therefore it is not discussed in this paper.

As stated previously, the main drawback of multi-stage NMPC is that the size of the NLP that has to be solved at each time step grows exponentially with the prediction horizon, with the number of uncertainties and with the levels of the uncertainty considered in the design of the scenario tree. A simple strategy to cut the exponential growth of the problem with the prediction horizon is to consider that the tree branches only up to a certain stage (called the robust horizon) and after this point, the uncertainty is assumed to be constant for the rest of the prediction horizon. An example of a scenario tree with a robust horizon equal to 2 and a prediction horizon of 4 steps is shown in Fig. 2.

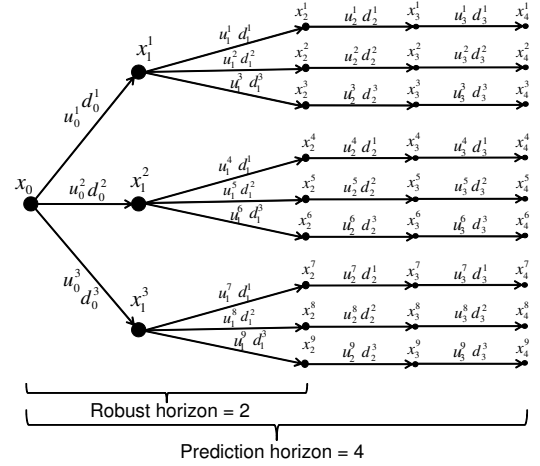


Fig. 2. Scenario tree representation of the uncertainty evolution for multi-stage NMPC.

Finally, one of the main challenges of this approach is to obtain a scenario tree that is manageable but that at same time represents truthfully the uncertainty of the system. This problem is called scenario generation and has been investigated in the stochastic programming community over the past years (see the review in [25]). This is an important area of future work. In this paper we assume that a suitable scenario tree is given or can be obtained easily with engineering insight about the problem under consideration. As a guideline, one should include extreme scenarios in order to achieve robust constraint satisfaction and intermediate scenarios to increase the performance of the controller.

III. NOMINAL NMPC OF A BATCH BIOREACTOR

The main goal of this work is to show the potential of the presented multi-stage NMPC to control a batch bioreactor under uncertainty. As a first step, this section shows that a receding horizon NMPC approach with finite prediction horizon is suitable for the optimal control of the end-batch properties of a nonlinear penicillin fermentation process. The model, presented in [18], can be described by the following nonlinear differential equations:

$$\begin{aligned} \dot{X} &= \mu(S)X - \frac{u}{V}X, \\ \dot{S} &= -\frac{\mu(S)X}{Y_x} - \frac{vX}{Y_p} + \frac{u}{V}(S_{\text{in}} - S), \\ \dot{P} &= vX - \frac{u}{V}P, \\ \dot{V} &= u, \end{aligned} \quad (7)$$

where $\mu(S) = \frac{\mu_m S}{K_m + S + (S^2/K_i)}$, X represents the concentration of biomass, S the concentration of substrate, P is the concentration of product and V the volume. The control input u is the feed flow rate of S . The values for the different parameters, such that the inlet substrate concentration S_{in} , the kinetic parameters μ_m, K_m, K_i, v and the yield coefficients Y_x, Y_p as well as more information about the process can be

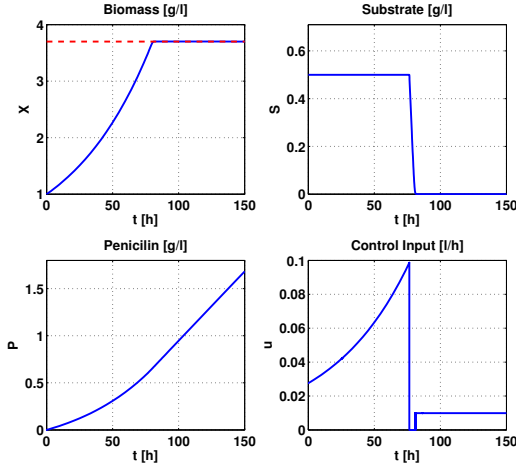


Fig. 3. Nominal optimal trajectory calculated analytically.

found in [18]. The parameters Y_x and S_{in} are uncertain. Y_x is in the range 0.3 – 0.5 and it is assumed to be constant through the whole batch. The inlet substrate concentration S_{in} is normally distributed ($S_{in} \sim \mathcal{N}(200, 25)$), truncated at 2σ and it is assumed to vary every hour.

The control task is to maximize the concentration of the product P at the fixed final time $t_f = 150$ hours. The input is bounded between $u_{min} = 0$ l/h and $u_{max} = 1$ l/h, and there is an upper bound $X_{max} = 3.7$ g/l on the biomass concentration that is physically motivated by the limitations in the transfer of oxygen that usually occur at high biomass concentrations.

The nominal optimal solution of this example yields an optimal value of the penicillin concentration at final time of $P^*(t_f) = 1.68$ g/l. It can be obtained analytically as described in [18] and it is shown in Fig. 3.

The optimization problem to be solved at each sampling time for the NMPC controller can be written as:

$$\min_{\bar{u}} \sum_{i=1}^N (\omega_i J_i) \quad (8a)$$

subject to:

$$\text{model in (7)}, \quad (8b)$$

$$X_k^j \leq X_{max}, \quad \forall (j, k) \in I, \quad (8c)$$

$$u_{min} \leq u_k^j \leq u_{max}, \quad \forall (j, k) \in I, \quad (8d)$$

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

where the model described in (7) is discretized using an implicit Euler approach with a sampling time $h = 1$ hour. Since in this section only the nominal NMPC problem is solved, the number of scenarios is $N = 1$, the uncertain parameters have their nominal values ($Y_x = 0.5$ and $S_{in} = 200$), there are no non-anticipativity constraints and the cost of the nominal scenario is defined as:

$$J_i = \sum_{k=0}^{N_p-1} x_{k+1}^j Q x_{k+1}^j + \Delta u_k^j R \Delta u_k^j, \quad \forall x_{k+1}^j, u_k^j \in S_i, \quad (9)$$

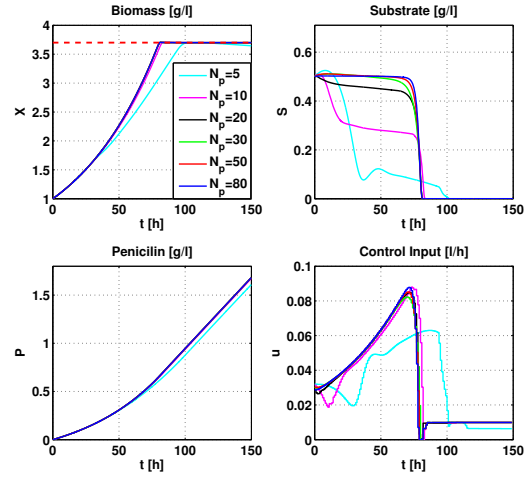


Fig. 4. Simulation of nominal NMPC for different prediction horizons.

where

$$Q = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } R = 0.5.$$

That is, the penicillin concentration is maximized and the control movements are penalized in the cost function in order to obtain a smoother control input.

Nominal NMPC is applied by solving the problem described in (8) at each sampling time $T_s = 1$ hour. The results for different prediction horizons can be seen in Fig. 4. It is clear that a short prediction horizon ($N_p = 5$) leads to a solution that is far from the optimal one but with an increasing prediction horizon, the solution gets closer to the optimal analytic solution.

A summary of the results for different prediction horizons including the average computation time per iteration is presented in Table I. The resulting NLP is solved with IPOPT via MATLAB using a 4-core Intel i5 processor at 2.67 GHz with 4 Gb of RAM running Windows. For comparison purposes, the computation times needed to solve the problem with SNOPT via TOMLAB/MATLAB are also shown. In both cases, the analytic Jacobian of the nonlinear constraints and gradient of the cost function are provided to the optimizer and the Hessian is approximated internally by IPOPT and SNOPT using a limited-memory quasi-Newton method. In addition, the same feasibility and optimality tolerances are used (1×10^{-6}) and the warm-start option of both solvers is utilized. The solution obtained by both solvers is nearly the same in all cases and therefore only the solutions obtained by IPOPT are shown in Fig. 4. SNOPT seems to be slightly faster for small problems but with increasing number of optimization variables it is slower than IPOPT.

TABLE I
PERFORMANCE COMPARISON OF NOMINAL NMPC WITH NO
UNCERTAINTY FOR DIFFERENT PREDICTION HORIZONS.

Prediction horizon	Penicillin conc. [g/l]	Number of opt. variables	Comp. time/iter. [ms]	
			IPOPT	SNOPT
5	1.61	29	21	13
10	1.67	54	32	21
20	1.68	104	64	54
30	1.68	154	86	62
50	1.68	254	126	135
80	1.68	404	188	330

IV. ROBUST MULTI-STAGE NMPC OF A BATCH BIOREACTOR

In this section, multi-stage NMPC is applied to the same example in the presence of uncertainties in Y_x and in S_{in} . The first step for applying multi-stage NMPC is to design a suitable scenario tree. In this case 9 scenarios are chosen. This results from combining the 3 different values for each uncertain parameter ($Y_x = \{0.3, 0.4, 0.5\}$ and $S_{in} = \{150, 200, 250\}$). In addition, the scenario tree is branched only in the first stage, that is, the robust horizon is chosen to be 1, because it provides good results while preventing the exponential growth of the tree with the prediction horizon, which is chosen to be $N_p = 30$. Fig. 5 shows the performance of the nominal NMPC controller designed in the previous section when it is applied to the system under uncertainties using different values of Y_x in the model of the optimizer. The different trajectories show the solution for different values of the uncertain parameters. The sampling time used for all the simulations is $T_s = 1$ hour. There are constraint violations for the cases when the value of Y_x used in the optimizer is not the worst case ($Y_x = 0.5$), but even if the value is chosen to be the worst case, the constraint violations due to the variations on S_{in} cannot be avoided. In contrast to this behavior, if multi-stage NMPC is applied solving at each sampling time the problem in (8) with 9 scenarios the controller automatically implements a back-off constraint that can prevent the violations (see Fig. 6). Note that this is an illustrative example with the focus on the principle of the approach rather than on the magnitude of the resulting constraint violations using nominal NMPC.

A summary of the performance of nominal (using $Y_x = 0.5$ in the model of the optimizer), and multi-stage NMPC can be seen in Table II together with the results obtained using tracking of the necessary conditions of optimality (NCO tracking) that were reported in [18]. Multi-stage NMPC outperforms nominal NMPC because it avoids the constraint violations (indicated as c.v. in Table II) that occur for all the cases of the the uncertainty and has even a better performance when the value of the parameter in the model of the optimizer ($Y_x = 0.5$) and in the plant are different (Plant $Y_x = 0.3$). In comparison with NCO tracking, whereas both satisfy the constraints for all the cases, multi-stage NMPC

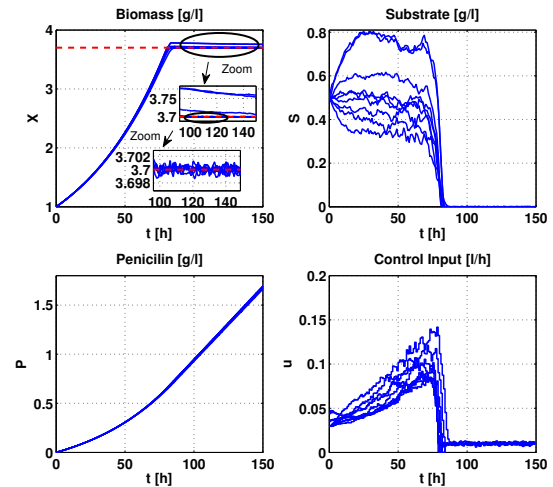


Fig. 5. Simulation of nominal NMPC for different values of the uncertain parameters and different values of Y_x used in the model of the optimizer.

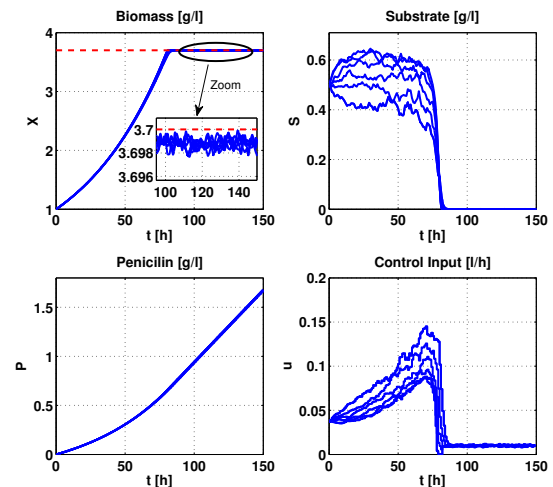


Fig. 6. Simulation of multi-stage NMPC for different values of the uncertain parameters.

has a better performance. This can be explained by the fact the NCO tracking approach tries to track the nominal optimal solution and avoids the constraint violations by the use of a precalculated back-off constraint. However, this back-off constraint may be conservative and the nominal optimal solution is not the optimal solution for the uncertain system. Finally, Table III shows a comparison of the computation times needed to solve the resulting NLP. For this example IPOPT is clearly faster than SNOPT and the difference increases with the size of the problem.

It is important to note that the proposed multi-stage NMPC is able to satisfy the constraints also for the values of the uncertainty that are not included in the scenario tree, if the scenarios are chosen properly. In addition, it can handle systematically different types of uncertainty such as constant uncertain parameters or normally distributed disturbances.

TABLE II
PERFORMANCE COMPARISON BETWEEN STANDARD NMPC,
MULTI-STAGE NMPC AND NCO TRACKING.

Plant Y_x	Penicillin concentration at final time [g/l]		
	Nominal NMPC	Multi-stage NMPC	NCO tracking
0.5	1.68 (c.v)	1.68	1.68
0.45	1.68 (c.v)	1.68	1.68
0.4	1.68 (c.v)	1.68	1.67
0.35	1.67 (c.v)	1.67	1.67
0.3	1.66 (c.v)	1.67	1.66

TABLE III
AVERAGE COMPUTATION TIME PER ITERATION USING SNOPT AND
IPOPT FOR DIFFERENT SCENARIO TREES.

Prediction horizon	Robust horizon	Number of opt. variables	Comp. time/iter [s]	
			IPOPT	SNOPT
30	1	1354	1.33	3.12
50	1	2254	2.78	10.63
70	1	3154	5.25	27.23

V. CONCLUSION

This work presents how the feedback information present in the receding horizon strategy of model predictive control can be considered explicitly in then open-loop optimization problem solved at each sampling time, leading to a non-conservative control of a system under uncertain parameters and disturbances. Multi-stage NMPC is a general framework that includes nominal NMPC and closed-loop min-max as particular cases. The main assumption of multi-stage NMPC is that the evolution of the uncertainty can be described by a scenario tree. In contrast to other methods such as tube-based MPC or NCO tracking, the proposed approach is not based on tracking the nominal optimal solution, but it makes possible that the optimal trajectory depends on the realization of the uncertainties, leading to a better performance. In addition, no back-off constraint is necessary in order to achieve robust constraint satisfaction. The results and the advantages of the approach are evaluated using simulation studies of a batch bioreactor, that shows that the approach provides a real-time implementable robust controller of the nonlinear process with improved performance with respect to existing controllers.

Future work will be focused on the generation of a suitable scenario tree for problems with many uncertainties and in the efficient solution of the resulting large optimization problems.

VI. ACKNOWLEDGEMENTS

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