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Real-time Feasibility of Nonlinear Predictive Control for Large Scale Processes - a Case Study.

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Abstract

Despite many control theoretic and numerical advances, up to now there is no realistic feasibility study of modern nonlinear model predictive control (NMPC) schemes for the real-time control of large-scale processes. In this paper the application of NMPC to a nontrivial process control example, namely the control of a high-purity binary distillation column, is considered. Using models of different complexity and different control schemes, the computational load, resulting closed loop performance and the effort needed to design the controllers is compared. It is shown that a real-time application of modern NMPC schemes is feasible with existing techniques, even for a 164^{th} order model with a sampling time of 30 s, if a state of the art dynamic optimization algorithm and an efficient NMPC scheme are used.

1 Introduction

Over the last two decades linear model predictive control has emerged as a powerful and widely used control technique, especially in the process industry. Recently there is growing interest in model predictive control for *nonlinear* systems in academia and in the industrial process control community. By now several NMPC schemes have been proposed that generalize the state space formulation for linear MPC in a straightforward way. Recent advances in NMPC theory have also allowed to find NMPC with favorable system theoretic properties including guaranteed nominal closed loop stability (see for example [8, 1] for a review). In addition, there has been significant progress in the area of dynamic process optimization. Direct methods based on sequential quadratic programming (SQP), which require a discretization of the control trajectory to formulate a finite dimensional nonlinear program, are widely used for off-line optimization of dynamic processes. Recently, fast on-line optimization algorithms have been developed that exploit the specific structure of optimization problems arising in NMPC [2, 4, 1], and real-time application has been proven to be feasible for small-scale nonlinear processes [10].

However, despite the control theoretic and numerical advances, up to now there is no realistic feasibility study of NMPC for the real-time control of larger scale processes. Some people raise concern that none of the developed NMPC schemes would be suitable for real-world applications. In this paper a specialized dynamic optimization strategies for NMPC [9] along with up to date NMPC schemes [7, 14] is applied to the control of a nontrivial process control example. In particular, the control of a high purity binary distillation column for the separation of Methanol and n-Propanol is considered. For this process the computational and implementation complexity are compared utilizing models of different complexity, different NMPC schemes with guaranteed stability and different optimization strategies.

The paper is structured as follows. In Section 2 the considered high purity distillation column is briefly presented and the different models used are outlined. Section 3 contains a short outline of the used NMPC strategies, in particular quasi-infinite horizon (QIH) NMPC [7]. For the solution of the optimal control problem that has to be solved at every sampling time, the so called direct multiple shooting approach [6, 13] is used. This approach is reviewed in Section 4. Section 5 contains a comparison of the controller performance and the necessary computation time for different model sizes for the QIH-NMPC and "zero" terminal constraint NMPC scheme.

2 Distillation Control Application

In this paper the control of a high purity binary distillation column with 40 trays for the separation of Methanol and n-Propanol (see Fig. 1) is considered. The binary mixture is fed in the column with flow rate F and molar feed composition x_F. Products are removed at the top and bottom of the column with concentrations x_B and x_D and flowrates B and D, respectively. The column is considered in L/V configuration, i.e. the liquid flow rate L and the vapor flow rate V are the control inputs. The control problem is to maintain the specifications on the product concentrations x_B and x_D despite disturbances in the feed flow F and the feed concentration x_F. For

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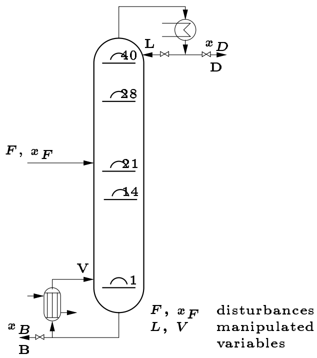

Figure 1: Scheme of the distillation column.

the controller design, models of different complexity are used. Modeling of the distillation column under the assumptions of constant relative volatility, constant molar overflow, no pressure losses, no energy balances and hydrodynamics leads to a 42^{nd} order ODE model. The states are the concentrations on the trays, in the boiler and the condenser. Based on this model a reduced 5^{th} order ODE model utilizing the so called wave propagation phenomena can be derived [15], that has as states the concentrations in the reboiler, condenser and feed tray as well as the wave positions for the stripping and rectifying section, respectively. The third model considered is a 164^{th} order model with 122 algebraic states (liquid flows, vapor flows and temperatures on each tray plus the temperatures in the condenser and reboiler) and 42 differential states (concentrations on the trays plus boiler and condenser). This model takes constant pressure losses from tray to tray and energy balances into consideration. All the models are derived such that they best reflect the dynamics of the distillation process.

3 NMPC with Guaranteed Stability

In the following a short review of the used NMPC schemes is given. We consider the stabilization of setpoints of the following index-one DAE system:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t)), \qquad \mathbf{x}(0) = \mathbf{x}_0 \tag{1a}$$

$$\mathbf{0} = \mathbf{g}(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t)), \tag{1b}$$

with the differential variables $\mathbf{x}(t) \in \mathbb{R}^n$, algebraic variables $\mathbf{z}(t) \in \mathbb{R}^p$ and inputs $\mathbf{u}(t) \in \mathbb{R}^m$. The setpoints $(\mathbf{x}_s, \mathbf{z}_s, \mathbf{u}_s)$ satisfy $\mathbf{0} = \mathbf{f}(\mathbf{x}_s, \mathbf{z}_s, \mathbf{u}_s)$, $\mathbf{0} = \mathbf{g}(\mathbf{x}_s, \mathbf{z}_s, \mathbf{u}_s)$. The considered distillation column models fit in this framework. Due to safety considerations and physical limitations it is additionally often required that constraints on the inputs and differential variables of the form $\mathbf{h}(\mathbf{x}, \mathbf{z}, \mathbf{u}) \geq \mathbf{0}$ must be satisfied. In Section 5 two NMPC schemes are employed, the so called zero terminal constrained NMPC scheme [14] and the quasi-infinite horizon NMPC [7] scheme.

In predictive control, at each "sampling" time an open loop optimal control problem is solved. The first part of the resulting optimal input is implemented and the optimization is repeated once new state information is available. For the purpose of this paper the following, in comparison to [7] slightly modified QIH-NMPC open loop optimization problem, that has to be solved at every sampling instance is considered:

NMPC Problem:

Solve
$$\min_{\bar{\mathbf{u}}(\cdot)} J_s(\bar{\mathbf{x}}(\cdot), \bar{\mathbf{u}}(\cdot)) \tag{2}$$

with:
$$J_s(\bar{\mathbf{x}}(\cdot), \bar{\mathbf{u}}(\cdot)) = \int_t^{t+T_p} (\|\bar{\mathbf{x}}(\tau) - \mathbf{x}_s\|_Q^2 + \|\bar{\mathbf{u}}(\tau) - \mathbf{u}_s\|_R^2) d\tau + E_s(\bar{\mathbf{x}}(t+T_p)) \ , \tag{3}$$

subject to:
$$\dot{\bar{\mathbf{x}}}(\tau) = \mathbf{f}(\bar{\mathbf{x}}(\tau), \bar{\mathbf{z}}(\tau), \bar{\mathbf{u}}(\tau)), \quad \bar{\mathbf{x}}(t) = \mathbf{x}(t) \tag{4a}$$

$$\mathbf{0} = \mathbf{g}(\bar{\mathbf{x}}(\tau), \bar{\mathbf{z}}(\tau), \bar{\mathbf{u}}(\tau)) \tag{4b}$$

$$\mathbf{h}(\bar{\mathbf{x}}(\tau), \bar{\mathbf{z}}(\tau), \bar{\mathbf{u}}(\tau)) \geq \mathbf{0} \quad \tau \in [t, t+T_p] \tag{4c}$$

$$r(\bar{\mathbf{x}}(t+T_p)) \geq 0. \tag{4d}$$

Internal controller variables are denoted by a bar. In the cost function the state and input deviation from their operating points are weighted by matrices Q and R. The term $E_s(\cdot)$ is called the terminal penalty term. It is given by $E_s(\bar{\mathbf{x}}) = \|\bar{\mathbf{x}} - \mathbf{x}_s\|_{P_s}^2$, i.e. P_s weights the terminal state deviation from its setpoint. The terminal constraint with $r(\bar{\mathbf{x}}) = \alpha - E_s(\bar{\mathbf{x}})$ restricts the predicted state at the end of the prediction horizon to lie in an ellipsoid around the setpoint: $\{\bar{\mathbf{x}} | \ \|\bar{\mathbf{x}} - \mathbf{x}_s\|_{P_s}^2 \leq \alpha\}$. The subscript $\cdot_s$ denotes that the terminal region and terminal penalty term in general depend on the chosen setpoint. The system input during the sampling time δ is given by the optimal input $\bar{\mathbf{u}}^\star(\cdot)$ that is the solution of the NMPC Problem at time t: $\mathbf{u}(\tau) = \bar{\mathbf{u}}^\star(\tau)$, $\tau \in [t, t+\delta)$.

Remark 1 *The main focus of the paper lies in an assessment of the computational complexity of NMPC for real-time control. Concerning stability we only remark that if the terminal penalty E_s, the terminal region and the weighting matrices are chosen suitably, stability of the closed loop system can be guaranteed in the case of no model plant mismatch. Stability results for the given configuration and suitable procedures to obtain E_s and the terminal region can be easily derived combining results from [7, 12, 11].* $\diamondsuit$

The setup for the zero terminal constrained NMPC scheme follows the NMPC problem given. The difference is, that the final predicted state is forced to be at the setpoint, i.e. the well known terminal equality constraint $\bar{\mathbf{x}}(t+T_p) - \mathbf{x}_s = \mathbf{0}$ is used to guarantee stability. In comparison to the QIH-NMPC approach, the control horizon has often to be increased significantly to allow feasibility of the optimization problem. This leads, in comparison to the QIH-NMPC approach in general to a drastical increase in the computational time necessary for the solution of the corresponding optimization problem and to degraded controller performance. In Section 5 the performance and computational complexity of both approaches is compared for the control of the distillation process.

4 Direct Multiple Shooting for NMPC

Using direct multiple shooting [6], the optimal control problem at time t for the current system state $\mathbf{x}(t)$

can be solved in the following way: First the predicted control trajectory $\bar{\mathbf{u}}(\cdot)$ is discretized. In this paper it is assumed that the controls are piecewise constant on each of the $N = \frac{T_p}{\delta}$ predicted sampling intervals: $\bar{\mathbf{u}}(\tau) = \bar{\mathbf{u}}_i$ for $\tau \in [\tau_i, \tau_{i+1})$, $\tau_i = t + i\delta$. Secondly, the DAE solution is decoupled on these intervals by considering the initial values $\bar{\mathbf{s}}_i^x$ and $\bar{\mathbf{s}}_i^z$ of differential and algebraic states at the times τ_i as additional optimization variables. The solution of such a decoupled initial value problem is denoted by $\bar{\mathbf{x}}_i(\cdot)$, $\bar{\mathbf{z}}_i(\cdot)$; it obeys the following *relaxed* DAE formulation on the interval $[\tau_i, \tau_{i+1})$:

$$\dot{\bar{\mathbf{x}}}_i(\tau) = \mathbf{f}(\bar{\mathbf{x}}_i(\tau), \bar{\mathbf{z}}_i(\tau), \bar{\mathbf{u}}_i) \tag{5a}$$

$$\mathbf{0} = \mathbf{g}(\bar{\mathbf{x}}_i(\tau), \bar{\mathbf{z}}_i(\tau), \bar{\mathbf{u}}_i) - \mathbf{g}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i) \tag{5b}$$

$$\bar{\mathbf{x}}_i(\tau_i) = \bar{\mathbf{s}}_i^x, \quad \bar{\mathbf{z}}_i(\tau_i) = \bar{\mathbf{s}}_i^z \tag{5c}$$

The subtrahend in (5b) is deliberately introduced to allow an efficient DAE solution for initial values and controls $\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i$ that violate temporarily the consistency conditions $\mathbf{0} = \mathbf{g}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i)$ during the solution iterations [5, 13, 16]. The objective contribution of the Lagrange term on $[\tau_i, \tau_{i+1})$ is – like the DAE solutions $\bar{\mathbf{x}}_i(\tau)$, $\bar{\mathbf{z}}_i(\tau)$ – completely determined by $\bar{\mathbf{s}}_i^x$, $\bar{\mathbf{s}}_i^z$, $\bar{\mathbf{u}}_i$:

$$J_{si}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i) = \int_{\tau_i}^{\tau_{i+1}} (\|\bar{\mathbf{x}}(\tau) - \mathbf{x}_s\|_Q^2 + \|\bar{\mathbf{u}}(\tau) - \mathbf{u}_s\|_R^2) d\tau.$$

This leads to the following large, but specially structured nonlinear programming (NLP) problem:

NLP Problem:

Solve
$$\min_{\bar{\mathbf{u}}_i, \bar{\mathbf{s}}_i} \sum_{i=0}^{N-1} J_{si}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i) \quad + E_s(\bar{\mathbf{s}}_N^x) \tag{6}$$

subject to:
$$\bar{\mathbf{s}}_0^x = x(t), \tag{7a}$$

$$\bar{\mathbf{s}}_{i+1}^x = \bar{\mathbf{x}}_i(\tau_{i+1}), \qquad i = 0, 1, \dots N-1, \tag{7b}$$

$$\mathbf{0} = \boldsymbol{g}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i), \qquad i = 0, 1, \dots N, \tag{7c}$$

$$\mathbf{h}(\bar{\mathbf{s}}_i^x, \bar{\mathbf{s}}_i^z, \bar{\mathbf{u}}_i) \geq \mathbf{0}, \qquad i = 0, 1, \dots N, \tag{7d}$$

$$r_s(\bar{\mathbf{s}}_N^x) \geq 0. \tag{7e}$$

This large structured NLP problem in the variables $(\bar{\mathbf{s}}_0^x, \bar{\mathbf{s}}_0^z, \bar{\mathbf{u}}_0, \dots)$ is solved by a specially tailored *partially reduced* SQP algorithm [13, 4, 3].

4.1 An Initial Value Embedding Strategy

Subsequent optimization problems differ only by different initial values $\mathbf{x}(t)$, that are imposed via the initial value constraint (7a): $\bar{\mathbf{s}}_0^x = \mathbf{x}(t)$. Accepting an initial violation of this constraint, the complete solution trajectory of the previous optimization problem can be used as an initial guess for the current problem. Furthermore, all problem functions and derivatives (as well as an approximation of the Hessian matrix) have already been found for this trajectory and can be used in the new problem, so that the first QP solution can be performed *without any additional DAE solution* [4, 10]. Please note that the given approach differs significantly from a conventional warm start technique which uses only the *controls* of the previous solution, but initializes the NLP variables by integrating the DAE with $\mathbf{x}(t)$ as initial value. In contrast to this, the first QP solution of this approach gives an increment to the NLP variables that satisfies not only the new initial value constraint (as this constraint is *linear*), but delivers also a first correction to the control trajectory. In the case of a linear system with quadratic cost this first correction would already be the solution, in the nonlinear case it allows to perform the first function evaluation of the new problem at a point that is closer to the solution manifold than the conventional initial guess.

Usage of this optimization strategy that is specially tailored to the NMPC problem structure leads to significant computational savings, as is demonstrated in the following section.

5 Computational Complexity and Controller Performance

In the following an application of the outlined NMPC schemes and the direct multiple shooting method to the control of the high purity distillation column as described in Section 2 is given. Especially the computational and implementation complexity as well as the resulting controller performance for different model sizes, optimization concepts and NMPC schemes are compared. For all simulations it is assumed that the real plant is given by the 164^{th} order model. The 5^{th}, 42^{nd} and 164^{th} order models respectively are used for the controller predictions. Notice that in the case of a controller using the 164^{th} order model there is no model plant mismatch. Since the goal is to compare NMPC controller performance and computation time (and not performance of state estimation schemes), it is assumed that the full plant state is known. In the case of the 42^{nd} order model used in the NMPC controller, the concentrations of the 164^{th} order model are directly used for state feedback. In case of the 5^{th} order model the boiler, condenser and feed tray concentrations as well as the positions of the wave inflection points are needed. To obtain these 5 states a least squares fit of the form stable wave profile to the 42 concentrations of the 164^{th} order simulation model is used.

As usual in distillation control, x_B and x_D are not controlled directly. Instead an inferential control scheme which controls the deviation of the concentrations on tray 14 and 28 from the setpoints is used. Since for the standard setpoint conditions the turning point positions of the waves approximately correspond to these trays, one can expect good control performance with respect to x_B and x_D. Even small changes in the inflow or feed conditions lead to significant changes in the wave positions and thus of the concentrations on trays 14 and 28. However, the changes in the product concentrations x_B and x_D are in general quite small, compare Fig. 2. Due to these considerations only the concentration deviations from the setpoint on trays 14 and 28 are penalized in the cost-function (3), i.e. Q is semidefinite and only

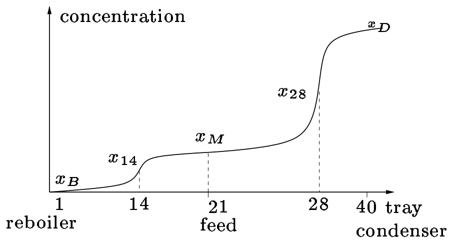

Figure 2: Concentration wave profile.

the diagonal elements 14 and 28 are nonzero and set to 1. The deviation of the inputs from their setpoint values is not penalized, i.e. $R = \mathbf{0}$ [1]. The goal is to achieve good controller performance under disturbances in the feed stream. To increase comparability it is assumed that the disturbances in the feed concentration can be measured and thus are known by the controller. The terminal region and the terminal penalty matrix P in the QIH-NMPC approach are calculated according to a similar procedure as described in [11]. Note that the terminal region and terminal penalty have to be adjusted accordingly to the setpoint, which is an implicit function of the feed-concentration and is determined automatically during the calculations.

To estimate the computational burden, simulations with different control horizons and with the two NMPC schemes as described in Section 3 are performed. The computations are carried out using a tailored version of MUSCOD-II for NMPC [9], which is based on the multiple shooting approach with initial value embedding as described in Section 4. All computations are carried out on a Compaq Alpha XP1000 workstation. The sampling time is chosen to be $\delta = 30s$. For all simulations the following disturbance scenario is used: at $t = 110s$ a step change of -10 % in the feed concentration x_F occurs. The feed concentration stayed constant up to $510s$, where a feed concentration change by +15 % is assumed. The last change in x_F occurs at $t = 810s$, back to the original steady state.

In Table 1 the maximum and average CPU times necessary to solve one open-loop optimization problem for the QIH-NMPC scheme are shown (KKT tolerance: 10^{-6}). One can see that the proposed QIH strategy, using the appropriate tool for optimization is feasible for the 5^{th} and 42^{nd} order models for horizon lengths of $N = 5, 10$ and 20. Even in the case of the 164^{th} order DAE model used in the NMPC controller real-time application is feasible, if one limits the horizon length to $N = 5$. Notice that the CPU time only grows "linear" with the control horizon length N. In Fig. 3 the performance of the QIH controller using the 3 different models are compared for

[1] To guarantee stability, (1) has to be observable by $\mathbf{y} = Q^{1/2}\mathbf{x}$. For the chosen Q this condition is satisfied. However, for the calculation of the terminal region a nonsingular R is necessary. Since for stability E_s has to upper bound the infinite horizon cost [7], one can thus use for the calculation of the terminal region a different, nonsingular R. However, this might degrade the control performance.

Table 1: Comparison of the necessary CPU time using MUSCOD-II and QIH-NMPC (in sec.)

model	N=5 (150 s)		N=10 (300 s)		N=20 (600 s)	
size	max	avrg	max	avrg	max	avrg
5	0.4	0.1	1.9	0.3	5.8	0.6
42	0.9	0.4	2.1	0.8	6.8	2.0
164	18.8	1.9	36.6	4.5	47.5	5.2

a control horizon of $N = 5$. Not surprisingly, the best performance is obtained using the 164^{th} order model for optimization. The slight steady state offset in the case of the 5^{th} and 42^{nd} order models is due to model/plant mismatch. Both models behave nearly similar, since they are based on the same modeling assumptions. In all cases, one can observe that the top and bottom concentrations are kept in a narrow high purity band, which is certainly more than satisfying. One conclusion which can be drawn up to here is, that even the use of the 5^{th} order model leads to satisfying performance while only a very low computational load is necessary. However, to obtain a reduced order model suitable for control is often not easy. In this case, the use of higher order models, like the 42^{th} order model or even the 164^{th} order model can be necessary. Thus the control horizon must be decreased enough to assure real-time feasibility.

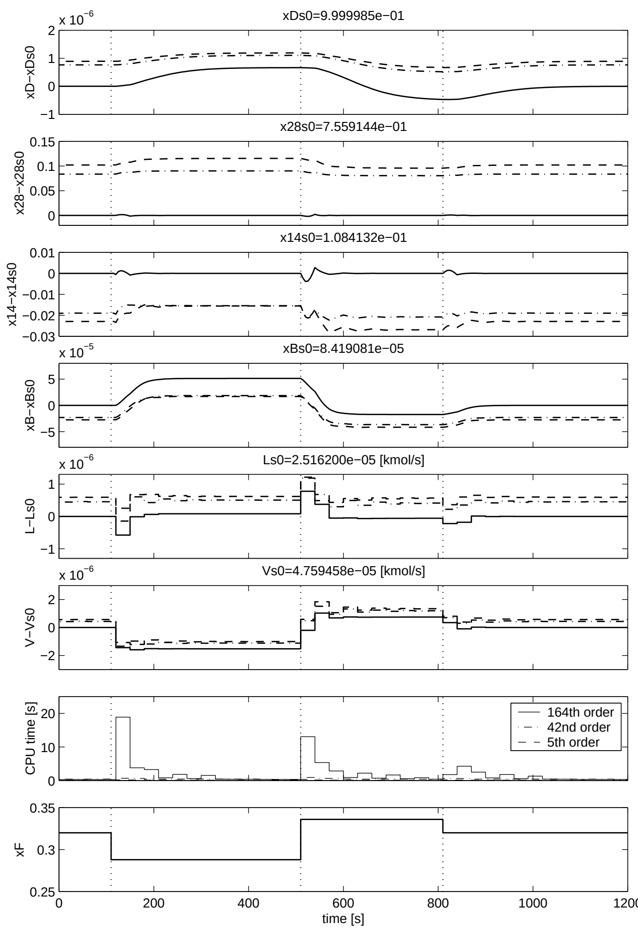

Figure 3: Behavior of the closed loop to feed disturbances.

To show the advantage of an efficient NMPC approach like QIH-NMPC, simulations with the zero terminal constraint NMPC scheme are performed for comparison. Usually a much longer control horizon is necessary to allow feasibility of the zero terminal constraint. For the 5^{th} order model a control horizon of $N=20$ ($T_p=600\ s$) is sufficient and the maximum CPU time increases to 6.8 s (average CPU time = 0.7 s). In the case of the 42^{nd} order model a control horizon of $N=50$ ($T_p=1500\ s$) is necessary. The maximum CPU time increases to 131.5 s (average CPU time=21.0 s). However, the used optimization algorithm shows excellent robustness, even in the case of rather large disturbances. The differences in control performance between the QIH and the "zero" terminal constraint NMPC are not significant.

Remark 2 *Another possibility to further reduce the computational burden is to use the initial value embedding strategy and to perform only the first SQP iteration of each open-loop optimization problem, which can even deliver an* immediate *state feedback [4, 3]. For the given simulation examples the maximum CPU time is significantly reduced in all cases. In case of the QIH-NMPC scheme using the* 164^{th} *order DAE model, for a control horizon of N=20 (600 s) the maximum CPU time is 8.2 s (average CPU time=3.4 s).* ◇

For an additional comparison simulations using the optimization toolbox of Matlab are performed. For the QIH approach with a horizon length of $N = 5$ the optimization problem with the 5^{th} order model requires a maximum CPU time of 103.4 s (average CPU time=48.8 s), while for the 42^{nd} order model a maximum CPU time of 207.8 s (average CPU time=122.1 s) is necessary, which is 200-400 times slower than the corresponding MUSCOD-II-results in Table 1.

As one can see, the computational complexity necessary for a real-time application of modern NMPC approaches depends on the used optimization strategy, the NMPC scheme, the horizon length and the system model used. The use of a well suited reduced order model can significantly lower the necessary computational time. However, often such a model is not available. In this case, as can be seen from the simulations, a real-time application is still possible even for rather large models based on first principle modeling.

6 Conclusions

In this paper we have focused on the question whether modern NMPC schemes can be used for the control of large scale processes utilizing a specialized optimization algorithm like MUSCOD-II and efficient NMPC schemes like QIH-NMPC. We considered the control of a high purity distillation column by using control models of different complexity. We have shown that in this case a suitable reduced order model can lower the computational burden significantly while not jeopardizing the closed loop performance. However, where such a model is not easily available, even the use of a 164^{th} order model is feasible for real-time control.

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