An Efficient Algorithm for Nonlinear Model Predictive Control of Large-Scale Systems Part II: Experimental Evaluation for a Distillation Column

Ein effizienter Algorithmus für die nichtlineare prädiktive Regelung großer Systeme Teil II: Experimentelle Erprobung an einer Destillationskolonne

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In the first part of this paper, that appeared in the last issue, an efficient approach for the online optimization in nonlinear model predictive control (NMPC), the so called real-time iteration scheme, was introduced. In the present second part we confirm experimentally the efficiency of the proposed strategy considering the control of a pilot-scale distillation column. In the experiments the column is used for the high-purity separation of a binary mixture of methanol and n-propanol. The differential-algebraic first principles model used for control is stiff and has more than 200 states. Despite the large state dimension the algorithm is able to provide newly optimized control inputs every 20 seconds on a standard PC. Even for rather large disturbances and without the need for much tuning the closed-loop shows good performance and does respect the required constraints. The presented results demonstrate that nonlinear model predictive control can even be applied for the control of large-scale systems and does lead to satisfying performance, if the outlined solution approach is used.

Im ersten Teil der vorliegenden Arbeit, der in der letzten Ausgabe **at** 12(2002) erschienen ist, wurde ein effizientes Verfahren für die Echtzeit-Optimierung in der nichtlinearen prädiktiven Regelung (NMPC) vorgestellt, das sogenannte Echtzeit-Iterations-Schema. Im vorliegenden zweiten Teil wird anhand der Regelung einer Destillationskolonne im Pilotanlagenmaßstab experimentell die Effizienz des vorgestellten Verfahrens bestätigt. In den Experimenten wird die Kolonne zur hochreinen Trennung eines binären Gemisches aus Methanol und n-Propanol verwendet. Das zur Regelung verwendete differentiell-algebraische Systemmodell ist steif und besitzt mehr als 200 Systemzustände. Trotz der hohen Systemordnung ist der Algorithmus in der Lage, auf einem Standard PC alle 20 Sekunden neuoptimierte Steuergrößen zur Verfügung zu stellen. Selbst für sehr große Störungen zeigt der geschlossene Kreis gutes Regelungsverhalten und erfüllt die geforderten Beschränkungen, wobei der notwendige Aufwand zur Einstellung der Reglerparameter minimal ist. Die präsentierten Ergebnisse zeigen, dass die nichtlineare prädiktive Regelung bei Verwendung des vorgestellten Verfahrens auch für große Systeme einsetzbar ist und zu guten Regelungsergebnissen führt.

Keywords: Nonlinear model predictive control, online-optimization, differential-algebraic equations, direct multiple shooting, distillation columns

Schlagwörter: Nichtlineare Prädiktive Regelung, Echtzeit-Optimierung, Differentiell-Algebraische Gleichungen, Direktes Mehrzielverfahren, Destillationskolonnen

1 Introduction

Online optimization of dynamic process models and nonlinear model predictive control (NMPC) have attracted increasing attention over the past decade [1; 4; 17; 26; 32]. Among the advantages of optimization based control are the flexibility provided in formulating the objective and the process model, the capability to directly handle equality and inequality constraints, and the possibility to treat unforeseen disturbances fast. It is in particular the availability of detailed nonlinear process models – that are increasingly being used for the *design* of industrial processes – which promises to make NMPC an appealing alternative to conventional control.

While linear model predictive control can be considered as somehow mature by now and is widely used in process industry applications [21; 27; 31], *nonlinear* MPC is still being perceived as an academic concept rather than a practicable control strategy. The difficulty of solving the arising optimal control problems in real-time is widely regarded as the principal obstacle to a practical application of NMPC. In a recent survey [32] it is pointed out that "speed and the assurance of a reliable solution in real-time are major limiting factors in existing applications." Reliable optimization methods for NMPC shall ideally be able to treat large-scale nonlinear first principle models as they are, without further need of modelling or model reduction.

In Part I of the paper we presented an efficient algorithm for optimization in NMPC, the so called *real-time iteration scheme*. The approach is based on an iterative solution method for dynamic optimization, namely the direct multiple shooting technique [6; 22; 23], which is able to treat system models described by *differential algebraic equations* (DAE) and has been successfully used in many applications [5; 11; 24]. In the context of NMPC, where a sequence of neighboring optimization problems is treated, solution information of the previous problem can be exploited efficiently by an *initial value embedding* strategy for initialization of the current problem. Building on the favourable properties of direct multiple shooting and the initial value embedding – which have already been observed and compared for various NMPC schemes [15; 29] – the *real-time iteration scheme* [8; 10] only performs one optimization iteration per sampling instant. The calculated approximated solutions can be shown to stay close to the exact optimal solutions, while the sampling time is reduced to a minimum, the cost of only one solution iteration, and feedback can be obtained much more frequently. Furthermore, the calculations of each real-time iteration can be split up in a preparation phase and a feedback phase. Since the feedback phase is much faster than the preparation phase, the delay between the measurement and the resulting input is reduced considerably.

In its actual implementation, the real-time iteration scheme is realized as part of the optimal control package MUSCOD-II [12; 22], which offers several advantages in the context of practical online optimization. Among these are the possibility to provide the DAE model equations as generic C or Fortran-Code or in the gPROMS modelling language [24; 30], to make use of efficient state-of-the-art DAE solvers (e.g. DAESOL [3]), or to employ an existing parallelization in the portable MPI standard [24] in time critical cases.

In this paper we experimentally verify the applicability of the real-time iteration scheme for NMPC considering the control of a pilot-plant distillation column located at the Institute for System Dynamics and Control Engineering of the University of Stuttgart. The distillation column has been the subject of a number of theoretical and experimental studies for dynamic modelling [18; 25] and control [16; 19; 20; 33; 34; 36]. Here, we show that the real-time iteration NMPC scheme can be applied to this process and achieves good control performance, without much tuning. The presented results demonstrate that nonlinear model predictive control can even be applied nowadays for the control of large-scale systems and leads to satisfying performance if the real-time iteration scheme is used.

This part of the paper is structured as follows: In Sect. 2 we describe the pilot-plant distillation column and we outline the model used for optimization. The controller setup and the open-loop optimal control problem are described in Sect. 3, and the experimental results are presented in Sect. 4.

2 Description of Process and Model

We consider the control of a pilot-plant distillation column. In the configuration considered here the column is used for the high purity separation of a binary mixture of Methanol and n-Propanol. It has a diameter of 0.10 m and a height of 7 m and consists of 40 bubble cap trays. The overhead vapor is totally condensed in a water cooled condenser which is open to atmosphere. The reboiler is heated electrically. A flowsheet of the distillation system is shown in Fig. 1. The preheated feed stream enters the column at the feed tray as saturated liquid. It can be switched automatically between two feed tanks in order to introduce well defined disturbances in the feed concentration.

In the considered configuration, the manipulated variables are the heat input to the reboiler Q and the reflux flow rate L_{vol}. The control aim is to maintain high purity specifications defined in terms of the distillate and boiler product concentrations x_{D} and x_{B} despite disturbances in the volumetric inlet feed stream F_{vol} and the inlet feed concentration x_{F}. Furthermore, constraints on the maximum and minimum allowable bottom and distillate volumetric streams B_{vol} and D_{vol} as well as on the maximum heat input to the boiler must be satisfied.

The column is controlled by a distributed control system (DCS) that is used for the lower level control. Basic control loops for the levels, the flow rates, and the heat input are realized on the DCS. To allow the consideration of

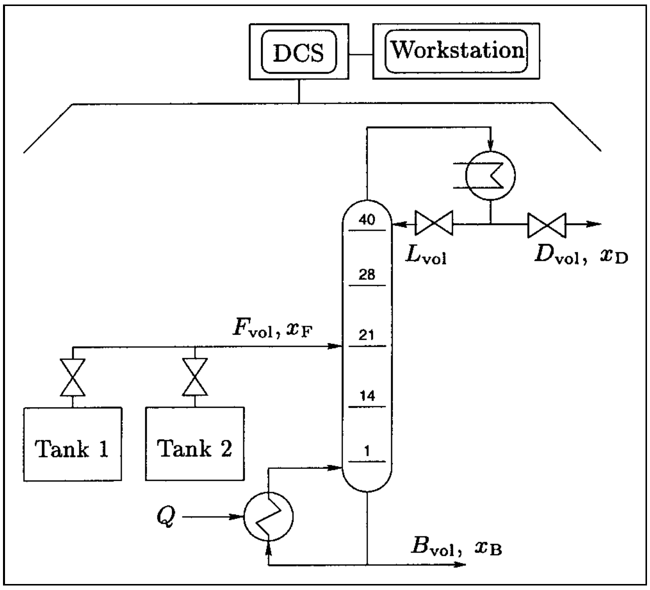

Figure 1: Flowsheet of the distillation column.

computationally more involved control schemes the DCS is connected to a LINUX workstation with a 1 GHz AMD Athlon processor. All higher level control algorithms, in particular the state estimator and the real-time iteration scheme, are implemented on this workstation.

2.1 System Model

Depending on the modelling assumptions different kind of models [18; 25; 28; 35] can be obtained for the dynamics of the distillation column. In first numerical tests, where the feasibility of the real-time iteration scheme was verified by simulations, a 164th order model of the process was used [15; 29]. The practical applicability was confirmed in a first series of closed-loop experiments [13]; however, the observed closed-loop performance suffered from oscillations which are probably due to neglected hydrodynamic effects that have *not* been captured by the 164th order model.

In this paper, we therefore use a slightly refined equilibrium stage model that includes hydrodynamics, resulting in a considerably stiffer and larger system model which is considered to capture the main features of the column dynamics. The model [8] is based on the following assumptions: total condenser, negligible vapor holdup, variable liquid holdup, constant pressure drop along the column, perfect mixing; the mixture is at equilibrium temperature; Murphree efficiency is applied for each tray.

The model is described by means of material and energy balances, hydrodynamic effects, equilibrium relationships for each tray and for the reboiler and the condenser. The resulting model consists of 82 differential equations and 122 algebraic equations. The differential states $x(t)$ include the molar liquid holdups and the methanol concentrations on each tray plus in the reboiler and the condenser. The algebraic states $z(t)$ include liquid flows, vapor flows and temperatures on each tray in addition to temperatures in the reboiler and condenser. The input to the system is given by $u = (L_{\text{vol}}, Q)^T$. The overall resulting DAE system has index one and fits into the structure assumed in the first part of the paper.

2.2 Identification of Unknown System Parameters

Some of the model parameters – e.g. tray holdups, Murphree coefficients, pressure losses – have been estimated by parameter identification. To obtain suitable data sets for the identification step changes in the feed rate F_{vol} and concentration x_{F}, the reflux rate L_{vol}, and heat input Q were performed. Measurements of *all* tray temperatures were taken for least squares fitting of the simulated to the observed behavior.

2.3 Treatment of Feedstream Disturbances

For the controller design we consider the feed flow F_{vol} and feed concentration x_{F} as external disturbance inputs. In the prediction, it is assumed that they will not change. To consider them in the dynamic optimization and state estimation we augment the differential state vector by the two trivial differential equations $\dot{F}_{\text{vol}} = 0$ and $\dot{x}_{\text{F}} = 0$. This formulation conveniently allows to react to changes by the initial value embedding. Note that offset free control is obtained by implicitly determining the steady state in the dynamic optimization as explained in the following section.

3 Controller Setup

The control aim is to maintain the specifications on the product concentrations x_{B} and x_{D} in reboiler and condenser despite disturbances. As usual in distillation control, the product concentrations are not controlled directly – instead, an inferential control scheme which controls the deviation of the concentrations on tray 14 and 28 from a given setpoint is used. These two concentrations are much more sensitive to changes in the system than the product concentrations. If the concentrations on tray 14 and 28 are kept sufficiently constant one can assume that the product purities are also safely maintained. As concentrations are difficult to measure, we control instead the tray *temperatures*, which correspond directly to the concentrations via the Antoine equation. The desired temperatures on tray 14 and 28 are denoted in the following by T_{14}^{ref} and T_{28}^{ref}. Furthermore, the setpoint of the controls is denoted by u_S.

The stage cost L used in the NMPC open-loop objective is formulated as the integral of a least squares term (for simplicity no units are assumed)

$$L(z, u, u_S) := \left\| \begin{bmatrix} T_{14} - T_{14}^{\text{ref}} \\ T_{28} - T_{28}^{\text{ref}} \end{bmatrix} \right\|_2^2 + 0.05\, \|u - u_S\|_2^2 ,$$

where the second term is introduced for regularisation purposes only since the used control is not of key relevance.

3.1 Open-Loop Optimal Control Problem

The terminal penalty term E appearing in the general NMPC formulation presented in Part I of the paper is often introduced in NMPC for stability and performance purposes [1; 7; 14; 26]. Slightly deviating from the problem formulation in Part I, we will approximate a suitable terminal penalty term by dividing the prediction horizon into a control horizon $[0, T_c]$ and a (long) prediction interval $[T_c, T_p]$ on which the controls are fixed to the setpoint values u_S, similar as proposed in [7; 15]. The objective contribution of the prediction interval provides an upper bound of the neglected future costs that are due after the end of the control horizon, if T_p is choosen sufficiently long. For the experiments we use a length of $T_p - T_c = 36\,000$ seconds that leads to sufficiently good performance in all experiments.

The resulting open-loop NMPC optimal control problem to solve at each sampling instant is given by:

$$\min_{u(\cdot),x(\cdot),u_S} \int_0^{T_p} \left\{ \left\| \begin{bmatrix} T_{14} - T_{14}^{\text{ref}} \\ T_{28} - T_{28}^{\text{ref}} \end{bmatrix} \right\|_2^2 + 0.05\, \|u - u_S\|_2^2 \; d\tau \right\} \tag{1}$$

subject to the model DAE

$$\begin{aligned} B(\cdot)\dot{x}(\tau) &= f(x(\tau), z(\tau), u(\tau)) \\ 0 &= g(x(\tau), z(\tau), u(\tau)) \quad \text{for} \quad \tau \in [0, T_p]\,. \end{aligned}$$

Where the initial values for the differential states are given by:

$$x(0) = x(t_k).$$

The state and control inequality constraints are formulated by

$$h(x(\tau), z(\tau), u(\tau)) \geq 0 \quad \tau \in [0, T_p]\,,$$

where

$$h(x, z, u) := \begin{bmatrix} D(x, z, u) - D_{\min} \\ B(x, z, u) - B_{\min} \\ u - u_{\min} \\ u_{\max} - u \end{bmatrix}$$

define the lower bounds for the fluxes $D(x, z, u)$ and $B(x, z, u)$ that are determined according to the model assumptions, which should always maintain small positive values, and lower and upper bounds for the controls.

The steady state control u_S is determined implicitly by the requirements that u is constant on the long prediction interval

$$u(\tau) = u_S \quad \text{for } \tau \in [T_c, T_p]\,,$$

together with the final state constraint

$$\begin{bmatrix} T_{14}(T_p) - T_{14}^{\text{ref}} \\ T_{28}(T_p) - T_{28}^{\text{ref}} \end{bmatrix} = 0\,.$$

An alternative formulation of the steady state condition can be found in [8].

3.2 On-Line State Estimation

To perform the prediction at every recalculation time t_k the full state information must be available. In practice, however, not all states can be measured directly. In the given setup we assume that only the three temperatures T_{14}, T_{21}, T_{28} and the feedflow F_{vol} can be measured directly and are available for control purposes. To obtain an estimate of the 82 differential system states and of the feed disturbance x_F a variant of an Extended Kalman Filter (EKF) is used.

In contrast to an ordinary EKF the implemented estimator [8] can incorporate additional knowledge about the possible range of states and parameters in form of bounds. This is necessary as the tray concentrations need to be constrained to physical meaningful values in the interval $[0, 1]$. A comparison of estimated and measured temperature profiles can be found in Fig. 5 – note that only the temperatures T_{14}, T_{21} and T_{28} are available to the state estimator.

3.3 Coupling with the Process Control System

The overall closed loop NMPC setup is shown in Fig. 2. The three processes – data acquisition, state estimation and real-time optimization – were running independently and communicating only via input and output files in such a way that a breakdown of one component did not cause an immediate breakdown of the others. Missing new inputs were automatically replaced by old values. This construction made the whole system sufficiently stable against variations in computation and data transfer times.

The EKF operates with a sampling time of 10 seconds. The length T_c of the control horizon and the control discretization are chosen such that the computation time for one real-time iteration does not exceed the relevant time scale of the system dynamics or of the occurring disturbances. Based on numerical experiments on the available workstation and on the requirement that one real-time iteration should not exceed 20 seconds, we found that $T_c = 600$ seconds with 5 control intervals each of 120 seconds length is a good choice. Note that the control interval length of 120 seconds is 6 times longer than the desired sampling time of 20 seconds – conceptionally this does not pose any difficulty.

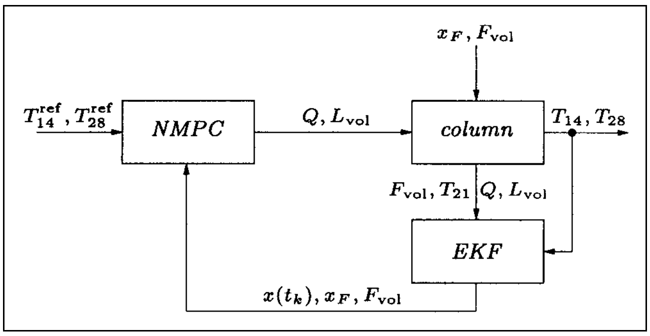

Figure 2: Closed-loop NMPC setup.

4 Experimental Results

The NMPC scheme has been tested on various scenarios [8; 13]. Here, only two scenarios, a step change in the feed flow rate F_{vol}, and a large disturbance scenario where the column was driven with too low reflux flow for over ten minutes are presented.

4.1 Feed Flow Change

The closed loop response of the scheme to a step change in F_{vol} is shown in Fig. 3. In the left column the closed loop result of the proposed real-time iteration scheme is shown. The right column shows the closed loop performance of an existing PI control scheme [13], which is usually employed to control the column. It consists of two single-input/single-output PI loops, one of which uses the heat input Q to control the temperature T_{14}, whereas the other uses the reflux L_{vol} to control the temperature T_{28}.

For the shown results starting from a steady state, the feedflow is increased at $t = 1000$ seconds by 20%. The NMPC controller based on the real-time iteration scheme is able to complete the transition to the resulting new steady state in less then 1000 seconds after the feed flow change, with a maximum deviation in T_{28} of 0.3°C. This compares well with the PI performance, which has a maximum deviation of 0.8°C, and needs much longer to complete the transition to the new steady state. In principle the performance of the PI controller could be improved using an additional feedforward term based on the feedflow information leading to slightly better results. The NMPC controller also compares well with other existing control strategies based for example on exact I/O-linearization [16] and linear multivariable controller designs [2] such as H_∞ minimization, Direct Nyquist Array, Characteristic Locus method and H_2 minimization.

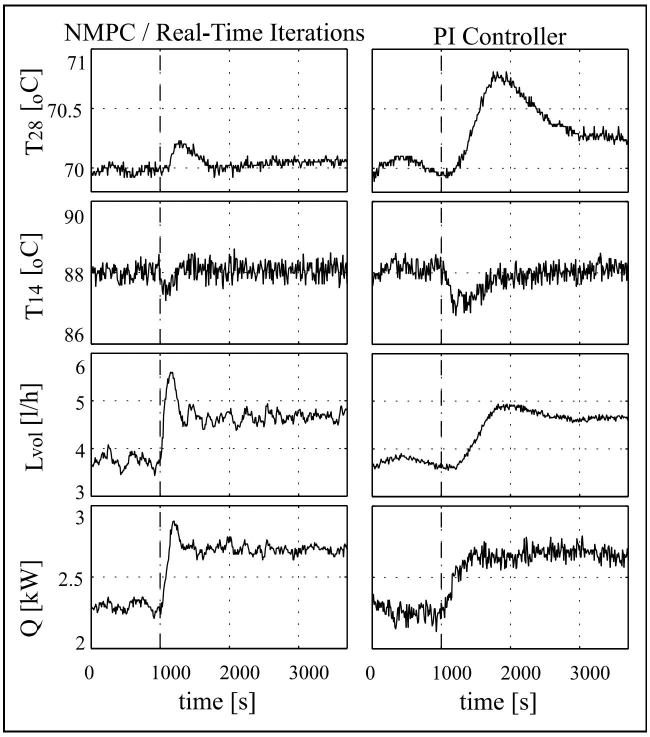

Figure 3: Feed flow change: Comparison of real-time iteration NMPC with a conventional PI controller for a feed flow step change by 20 % at $t = 1000$ seconds.

4.2 Large Disturbance Scenario

In the following we consider the behavior of the closed-loop with respect to a large deviation from the desired steady state caused by a disturbance, see Fig. 4. For this purpose we consider the following scenario: starting with a steady state for an increased feed flow rate (by 20%), we reduce at $t = 700$ seconds simultaneously the feed-flow (back to its nominal value) and the reflux, from $L_{\mathrm{vol}} = 5.3\,\mathrm{l/h}$ down to $L_{\mathrm{vol}} = 2\,\mathrm{l/h}$, while maintaining the heating power constant at the (high) value $Q = 2.9\,\mathrm{kW}$. These inputs, that are maintained constant for 800 seconds, heat the column up and move the temperature profile far away from the nominal operating conditions, as can be seen in Fig. 5, where the distorted temperature profile at time $t = 1500\,\mathrm{s}$ is shown.

Only at $t = 1500\,\mathrm{s}$ the NMPC feedback is switched on. While Q drops immediately down to its minimum value of 1.5 kW, L_{vol} is *not* increased to its maximum value, which from first sight seems to be the best measure to cool the column. However, this would result in valve saturation; it

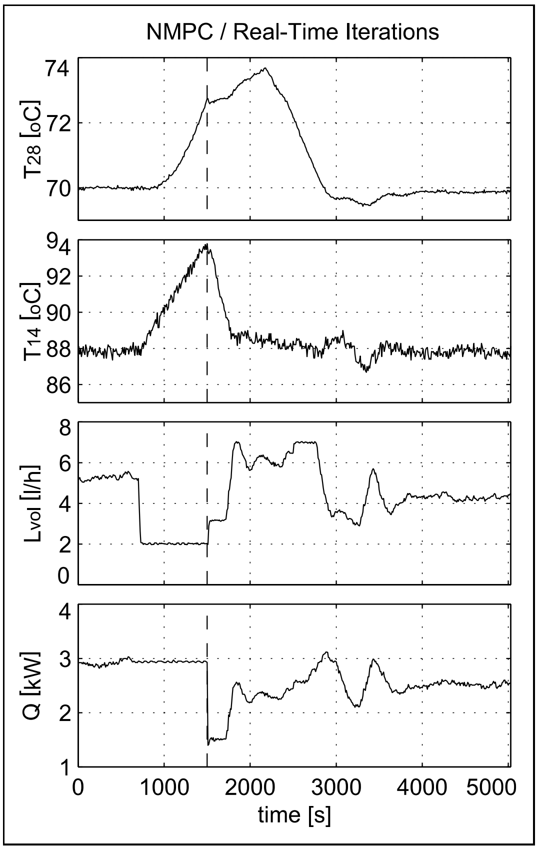

Figure 4: Large disturbance scenario. Closed-loop response. Feedback starts only at time $t = 1500$ seconds.

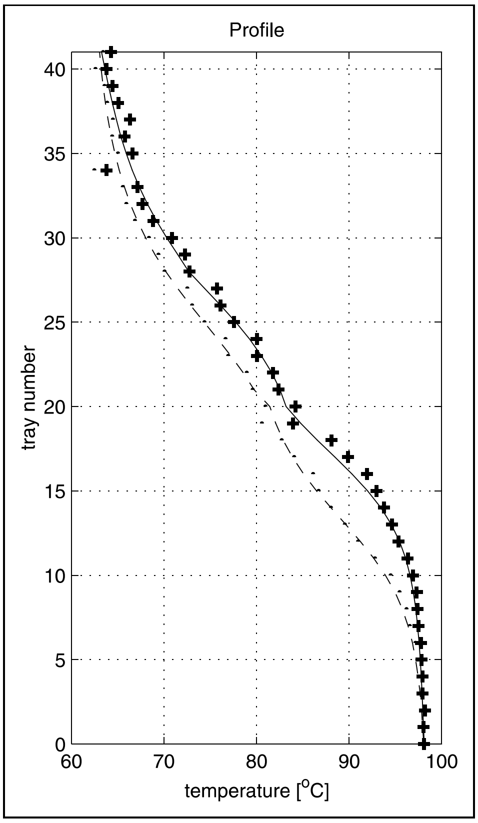

Figure 5: Large disturbance scenario. The real temperature profile at $t = 1500$ (+) is compared to the estimated profile (solid) and to the desired steady state profile (dots/dashed).

is the formulated path constraint $D \geq D_{\min}$ which impedes the immediate increase of L_{vol}.

Note that the PI controller fails to drive the system back to the steady state as strong oscillations occur due to valve saturation.

Computation Times: The computation times necessary for the feedback and preparation phase of the real-time scheme have been recorded for each recalculation instant and can be found in Fig. 6. The time measurements were done externally (from a MATLAB environment), i.e., they are not CPU times in the strict sense, but represent an estimate for the overall times that the computations required under the given CPU load conditions.

Note that due to the fact that the sampling rate for communication with the DCS was 10 seconds, the immediate response may in our realization have taken up to 10 seconds until it arrives at the distillation column, depending on the phase difference of the optimizer and the data transfer system.

Optimal Solution: To estimate the quality of the real-time iteration scheme and the model used for prediction it is interesting to compare the experimental closed-loop with the simulated optimal open-loop trajectories as plotted in Fig. 7.

The left column shows the experimental closed-loop results for the large disturbance scenario presented before. The right column shows the theoretically optimal open-loop trajectories obtained off-line for the state at $t = 1500$ seconds. It can be seen that the experimental closed-loop trajectories show considerable similarity with the theoretically optimal solution. This shows on the one hand that the model cap-

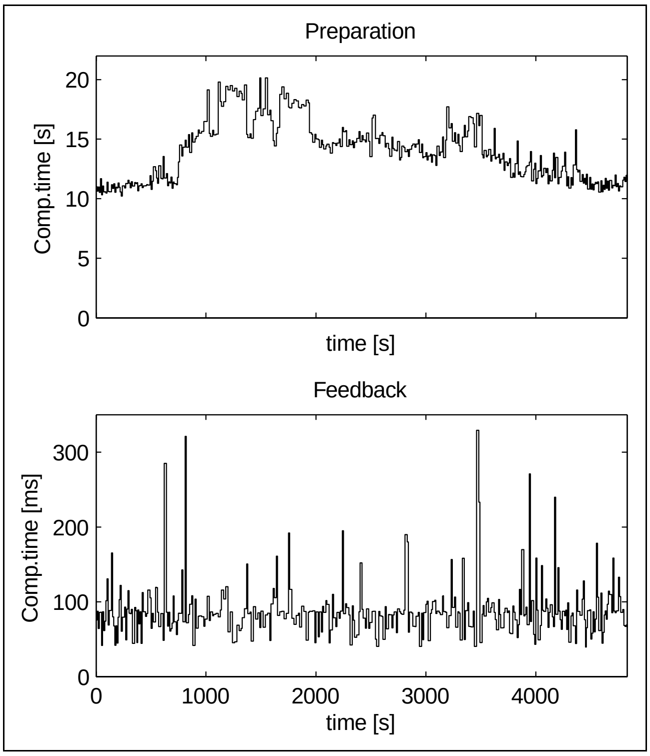

Figure 6: Computation times for preparation phase and for feedback phase, during the large disturbance experiment (cf. Fig. 4). Note the different scales of the graphs.

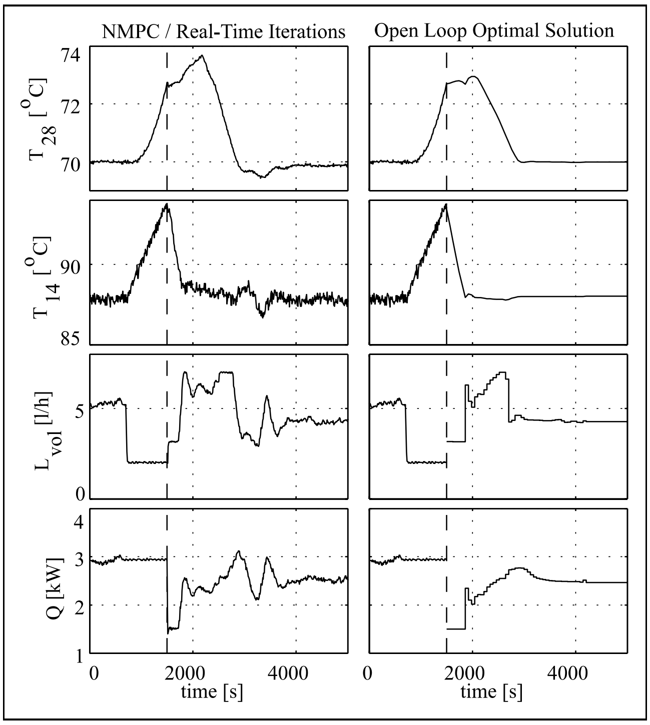

Figure 7: Large disturbance scenario. Left: Closed-loop response, as in Fig. 4. Right: Theoretically optimal open-loop solution.

tures sufficiently well the behaviour of the real apparatus, and on the other hand that the real-time iteration NMPC scheme delivers a good approximation to the optimal feedback control law.

The computation of the optimal trajectory with the off-line multiple shooting method required 23 major SQP iterations with a CPU time of 3356 seconds, where the control horizon was chosen to consist of 45 multiple shooting intervals, each of 30 seconds length. Note that the computation time for this problem is in the same order as the whole process duration.

4.3 Discussion

It was shown that the proposed real-time iteration NMPC control scheme is not only feasible for a practical large scale application, it also delivers good closed-loop performance. The key advantage is that the application did not require much tuning, and a standard distillation model can be used for control; the most time consuming step in the controller setup is, however, the unavoidable parameter estimation and model validation.

5 Conclusions

In Part I of this paper we have presented a new numerical approach to NMPC, the so called *real-time iteration* scheme. The scheme is based on the direct multiple shooting method, which in particular allows to treat highly nonlinear and unstable systems [9], and employs an *initial value embedding* for optimal transition from one optimization problem to the next. The algorithm is implemented within the dynamic optimization package MUSCOD-II, which allows to provide the DAE model equations either in the gPROMS modelling language [24] or as generic C or Fortran-Code.

In Part II, the algorithm was applied experimentally for the control of a binary distillation process, considering a DAE model with 82 differential and 122 algebraic state variables for optimization. The experimental results obtained confirm the computational efficiency of the scheme and the straightforward application if a suitable system model is available. As shown, even for rather large disturbances the real-time iteration NMPC scheme is able to safely return the system state to the desired setpoint.

The experimental study demonstrates that NMPC is a feasible control alternative; it does not need much tuning and can directly employ nonlinear first principle models. Due to the computational efficiency of the real-time iteration scheme, even large-scale models can be treated. Thus often time consuming simplifications of models for use in online control can be avoided.

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