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Two-Phase Model Predictive Control and Its Application to the Tennessee Eastman Process

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Supporting Information

ABSTRACT: This paper considers a two-phase model predictive control (MPC) which utilize a parsimonious parametrization of the future control moves to decrease the number of the degrees of freedom of the optimization and, thereby, to reduce the computations. Namely, the future control actions of the dynamic optimization are split into two stages. In the first phase, the control moves are considered as individual degrees of freedom. In the second phase, which is defined as the period between the end of the first phase and the prediction horizon, the control actions are determined using a weighted sum of some open-loop controls selected at the MPC design stage. With this parametrization, the bounds on the manipulated variables need to be treated as linear constraints. Alternatively, this paper estimates the maximum and the minimum of the future control trajectory that allows one to limit the number of the constraints representing the bounds on the MPC inputs. Thus, an additional reduction of the computations is achieved. To test the two-phase MPC, an MPC-based control strategy for the Tennessee Eastman challenge problem is developed, and a comparison of the two-phase MPC with MPC using Laguerre functions and MPC with move blocking is presented.

1. INTRODUCTION

Model predictive control (MPC) is nowadays one of the leading industrial control techniques. The constrained MPC introduced in the late 1970s[1,2] enables keeping the process as close as possible to its constraints without violating them, which is normally required to maximize the process efficiency. Constrained MPC typically has the following main features: linear process constraints, a linear process model, and a quadratic objective, which results in a finite horizon formulation and quadratic programming (QP) optimization. During its development, MPC technology faced several major challenges. In particular, in the early 1990s it was discovered that hard constraints can cause feasibility problems, especially when large disturbances appear. Therefore most modern MPC products are designed to use soft output constraints in dynamic optimization.[3] Because of the finite horizon formulation, MPC faced stability problems. Attempts to achieve stability included different prediction and control horizon approach and the introduction of a terminal cost to the MPC objective. These methods were criticized in the study of Bitmead et al.[4] as "playing games" because there were no clear conditions guaranteeing stability. Therefore the stability of MPC was studied actively during the early 1990s (Keerthi and Gilbert[5] and Mayne and Michalska[6] were among the first studies exploring this question), and a comprehensive review of the studies was provided in Mayne et al.[7] Briefly summarized, the value of the MPC objective as a function of the plant state, which is also called the value function of MPC, is almost universally used as a natural Lyapunov function, and the stability can be ensured if the MPC possesses the recursive feasibility properties, which basically means that the control trajectory found by the previous MPC run is still feasible.

The computation requirements of MPCs are constantly growing due to both the increased complexity of control systems involving more variables and the increasing use of nonlinear models. That is why many researchers have concentrated their efforts on reducing online computations of MPC. In particular, the explicit MPC introduced by Bemporad et al.[8] precomputes the piecewise linear control law. However, because of the exponential explosion of the number of pieces as a function of the number of problem inputs, outputs, and constraints, this approach is only suitable for small-scale problems. A partial enumeration approach described by Pannocchia et al.[9] precomputes the optimal solutions for the most frequently occurring sets of active constraints. This approach combines the table storage method and the online optimization, which makes it suitable for large control problems. Rao et al.[10] proposed a modification of the interior-point algorithm exploring the structure of the QP tasks related to the MPC objective optimization.

The current study explores an alternative approach to reduce the computations which is based on improved parametrization of the future control trajectories. In particular, Wang[11,12] suggested using Laguerre functions to define the future control moves and provided some simple examples demonstrating the benefits of this approach compared with the traditional parametrization, considering each control move within the control horizon as an individual decision variable of the MPC optimization. It is straightforward to show that MPC with Laguerre functions possesses the recursive feasibility property,

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and therefore, the stability can be easily ensured. Numerous studies providing further comparison of the MPC parametrizations in terms of feasibility and optimality concluded that MPC using Laguerre functions outperforms the traditional approach[13−15] with the same degrees of freedom (dof). The same conclusion was made regarding a robust MPC.[16] The referred comparison studies, however, tend to evaluate the controllers on small-scale noiseless examples. An alternative approach to future control move parametrization is move blocking, in which the control trajectory is forced to stay constant over some steps. Despite working well in practice, this parametrization does not provide the recursive feasibility property, and, therefore, stability cannot be directly established. This limitation can be resolved by modifications of the move blocking technique, two of which were proposed by Cagienard et al.[17] and Longo et al.[18] An alternative parametrization of the MPC control trajectory is based on the observation that the terms of the MPC objective representing the first future steps are frequently much bigger compared with the terms related to a more distant future. In the result, the MPC objective is more sensitive to the first control actions compared to the latest ones. The two-phase MPC considered in the present work defines the first future control actions independently (the first phase), and the rest control moves are determined as a weighted sum of some open-loop controls selected at the MPC design stage (the second phase).

Compared to the traditional approach, considering each control action within the control horizon individually, three parametrizations described above reduce the number of dof needed to achieve good MPC performance, which results in considerable computational savings. However, the number of constraints has also a strong effect on the computational load. Both the MPC using Laguerrer functions and the two-phase MPC define the future control trajectory as a weighted sum of preselected functions, and, therefore, the lower and the upper bounds on the manipulated variables need to be treated as linear constraints. In this paper, the maximum and the minimum of the future control trajectory of the two-phase MPC are estimated, and the number of the constraints representing the bounds on the manipulated variables is greatly decreased. In the result, a considerable reduction of the computation time of the two-phase MPC is achieved.

In Zakharov et al.[19] the two-phase MPC was successfully tested on a small-scale grinding process with only two inputs and four outputs. The aim of the present study is to carry out comparative tests of the two-phase MPC and MPC with other parametrizations using a larger process which would provide an adequate ground for the comparison. In particular, the controls are evaluated with respect to both the feasibility, which is the capability to find a feasible solution during rapid transitions and large disturbances, and the performance, which is the ability to provide smooth trajectories of the process variables and to follow the set points accurately. The Tennessee Eastman challenge problem (TECP) was selected for the comparative study because of its high nonlinearity and the dynamics, including very fast and very slow responses, which result in the requirement of long control and prediction horizons. Moreover, some of the disturbances implemented in the process model can be used for additional control evaluation.

The paper is organized as follows: Section 2 introduces the proposed two-phase MPC and discusses its stability and implementation issues. A MPC based control strategy of the Tennessee Eastman process is presented in section 3, and the test results are provided in section 4. Finally, section 5 presents the conclusions.

2. TWO-PHASE MPC

2.1. Description of the Two-Phase MPC. This section describes the two-phase MPC designed to equalize the importance of every decision variable in terms of the MPC objective. The two-phase MPC was formulated for the linear discrete state space dynamics of a plant:

$$\begin{aligned}\mathbf{x}(k+1) &= A\mathbf{x}(k) + B\mathbf{u}(k)\\ \mathbf{y}(k+1) &= C\mathbf{x}(k+1)\end{aligned} \tag{1}$$

where $\mathbf{x}$ is an n-component state vector, $\mathbf{u}$ is an m component vector of the input variables, and $\mathbf{y}$ is a p-component vector of the measured plant outputs. For the sake of simplicity, it was assumed that there was no noise in both the dynamics and the measurements and that the state of the system was exactly known. In addition, the following linear constraints were imposed on the process inputs and process outputs:

$$\mathbf{u}^{\mathbf{l}} \le \mathbf{u}(k) \le \mathbf{u}^{\mathbf{u}} \tag{2}$$

$$\mathbf{y}^{\mathbf{l}} \le \mathbf{y}(k) \le \mathbf{y}^{\mathbf{u}} \tag{3}$$

On the basis of eqs 1−3 describing the dynamics and the constraints, an MPC optimization aims to minimize the objective function, which typically has the following form:

$$J_{N,K}(\mathbf{x}(0), \mathbf{u}(-1), \bar{\mathbf{u}}) = \sum_{k=1}^{K} L^{y}(y(k)) + \sum_{k=0}^{K-1} L^{u}(\Delta\mathbf{u}(k)) \tag{4}$$

where L^y and L^u are usually positive definite quadratic forms and a prediction horizon K longer than a control horizon N is usually used to stabilize the MPC. The previous control action $\boldsymbol{u}(-1)$ is needed to compute the increment of the control actions used on the right-side of eq 4.

Since constrained MPC was introduced to simplify the infinite horizon control problem, a longer control horizon is needed to approach the optimal solution. The traditional MPC treats the values of the first N control actions $\bar{\mathbf{u}} = (\mathbf{u}(0),\mathbf{u}(1), ..., \mathbf{u}(N-1))$ as decision variables of the optimization, and the constant value $\mathbf{u}(N-1)$ is usually applied after the control horizon. In the case of a long enough control horizon, the term $J_{N-k,K-k}(\mathbf{x}(k))$ approaches zero when k increases since MPC drives the plant state $\mathbf{x}(k)$ to the target steady state to minimize the objective (4). As a consequence, the relative contribution of the first control actions to the right-side of eq 4 is more important than the contribution of the latest control actions. However, the latest control actions within the control horizon increase the number of dof of the optimization in the same way as the first control actions do. For this reason, the traditional MPC parametrization requires relatively many dof to achieve good performance, and thus the MPC optimization is not computationally efficient. According to the two-phase MPC parametrization, new optimization variables were introduced in order to equalize the importance of every decision variable in terms of the objective. To be more specific, several nearest future control actions comprise the first phase, and the period between the end of the first phase and the prediction horizon was considered as a "second phase" of the dynamic optimization, in which two open-loop controls were used to define the control actions according to the following:

$$u_i(N+k) = \sum_{j=1}^{2} \alpha_i^j g_j(k) + u_i^*,$$
$$i = 1, ..., m;\ k = 0, ..., K - N - 1 \quad (5)$$

where $\mathbf{u}^*$ is the steady-state control defined by the set point value and the variables α_i^j, $j = 1, 2$, $i = 1, ..., m$ are considered optimization decision variables together with the first N control actions $\bar{\mathbf{u}}$. The steady control $\mathbf{u}^*$ can be calculated outside the MPC optimization or considered as its decision variable. The two open-loop controls $g_j(k)$ were defined using the following exponential function:

$$g_j(k) = \exp(-c_j k), \qquad k = 0, ..., K - N - 1 \quad (6)$$

where c_j are some nonnegative constants. According to eq 5, the same open-loop controls were used to define the future control values for all process inputs, but the separate weights α_i^j of these open-loop controls were used for different inputs. Figure 1 demonstrates a set of trajectories obtained as the weighted sum of two open-loop controls defined by eq 6, where the sum of the coefficients $\alpha^1 + \alpha^2$ equals unity.

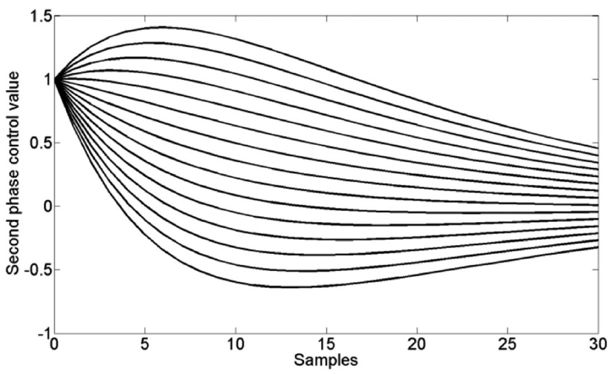

Figure 1. Weighted averages of the two open-loop controls defined by $c_1 = 0.15$ and $c_2 = 0.07$.

As a result, the second phase was available for minimization of the objective of the two-phase MPC in addition to providing its stabilization effect. Furthermore, the control actions related to the second phase could not be varied independently, and they were instead determined using the weighted sum of the open-loop controls which properly reflects the relative importance of the second-phase control actions compared to the control actions lying within the first phase.

2.2. Stability of the Two-Phase MPC. In this section, the stability of the developed MPC is explored using a method which has been previously used by many authors, including Chen and Shaw[20] and Primbs and Nevistic.[21] The following equation denotes the open-loop control produced by means of the two-phase MPC objective optimization at state $\mathbf{x}$ with the previous control action $\mathbf{u}$, the control horizon N, and the prediction horizon K as

$$k_{N,K}(\mathbf{x}, \mathbf{u}) = (k_{N,K}(\mathbf{x}, \mathbf{u}, 0), ..., k_{N,K}(\mathbf{x}, \mathbf{u}, K-1)) \quad (7)$$

In order to establish the stability of the MPC, it is enough to show that

$$J_{N,K}(\mathbf{x}^+, \mathbf{u}^+, k_{N,K}(\mathbf{x}^+, \mathbf{u}^+)) - J_{N,K}(\mathbf{x}, \mathbf{u}, k_{N,K}(\mathbf{x}, \mathbf{u})) + L^y(\mathbf{x}^+) + L^u(\mathbf{u}^+ - \mathbf{u}) \leq 0 \quad (8)$$

where

$$\mathbf{x}^+ = A\mathbf{x} + Bk_{N,K}(\mathbf{x}, \mathbf{u}, 0)$$
$$\mathbf{u}^+ = k_{N,K}(\mathbf{x}, \mathbf{u}, 0) \quad (9)$$

Since

$$J_{N,K}(\mathbf{x}^+, \mathbf{u}^+, k_{N,K}(\mathbf{x}^+, \mathbf{u}^+)) - J_{N,K}(\mathbf{x}, \mathbf{u}, k_{N,K}(\mathbf{x}, \mathbf{u})) + L^y(\mathbf{x}^+) + L^{\mathbf{u}}(\mathbf{u}^+ - \mathbf{u}) = J_{N,K}(\mathbf{x}^+, \mathbf{u}^+, k_{N,K}(\mathbf{x}^+, \mathbf{u}^+)) - J_{N-1,K-1}(\mathbf{x}^+, \mathbf{u}^+, k_{N-1,K-1}(\mathbf{x}^+, \mathbf{u}^+)) \quad (10)$$

it is enough to finish the proof to show that

$$J_{J,K}(\mathbf{x}, \mathbf{u}, k_{N,K}(\mathbf{x}, \mathbf{u})) - J_{N-1,K-1}(\mathbf{x}, \mathbf{u}, k_{N-1,K-1}(\mathbf{x}, \mathbf{u})) \leq 0, \quad \forall\ \mathbf{x}, \mathbf{u} \quad (11)$$

or equivalently

$$J_{1,K-N+1}(\mathbf{x}, \mathbf{u}, k_{1,K-N+1}(\mathbf{x}, \mathbf{u})) \leq J_{0,K-N}(\mathbf{x}, \mathbf{u}, k_{0,K-N}(\mathbf{x}, \mathbf{u})) \quad (12)$$

On the right side of eq 12, the optimal control is selected among the second-phase controls defined by eqs 5 and 6. On the left side of the equation, the first control action is selected freely, and the rest of the control actions are defined by means of a second-phase control. To prove the two-phase MPC's stability, one must require the recursive feasibility property, which means that any second-phase control $\bar{\mathbf{v}} = (\mathbf{v}(0), ..., \mathbf{v}(N-K-1))$ considered without its first element must coincide with another second-phase control $\bar{\mathbf{w}}$:

$$\bar{\mathbf{v}}(k) = \bar{\mathbf{w}}(k-1), \qquad k = 1, ..., N - K - 1 \quad (13)$$

Condition 13 holds for the open-loop controls defined by eq 6 since

$$\alpha_i^j \exp(-c_j k) = \alpha_i^j \exp(-c_j) \exp(-c_j(k-1)) \quad (14)$$

Furthermore, the left side of eq 12 has one more term than the right-hand side. Therefore, to finish the proof, it is enough to ensure that the last term in the left-hand side turns to zero, which can be obtained by imposing the terminal constraints on the system state. In fact, it is enough to require that the optimal second-phase control on the left side of eq 12 achieves a rather small value in the last term instead of achieving the exact steady state. In particular, a long enough prediction horizon was used in this work, which is sufficient to provide sustainable stability to the controller without using the terminal constraints.

2.3. Implementation of the Bounds on the Input Varaibles of the Two-Phase MPC. The second-phase control actions $u_i(k)$ are linear functions of the optimization decision variables α_i^j. Thus, the MPC objective optimization continues to be a quadratic programming task. More specifically, the response of the decision variables α_i^j on the process outputs $y_l(k)$ can be obtained as a convolution of the open-loop controls $g_j(k)$ and the impulse response of the plant dynamics (eq 1), and the control error penalties and the output

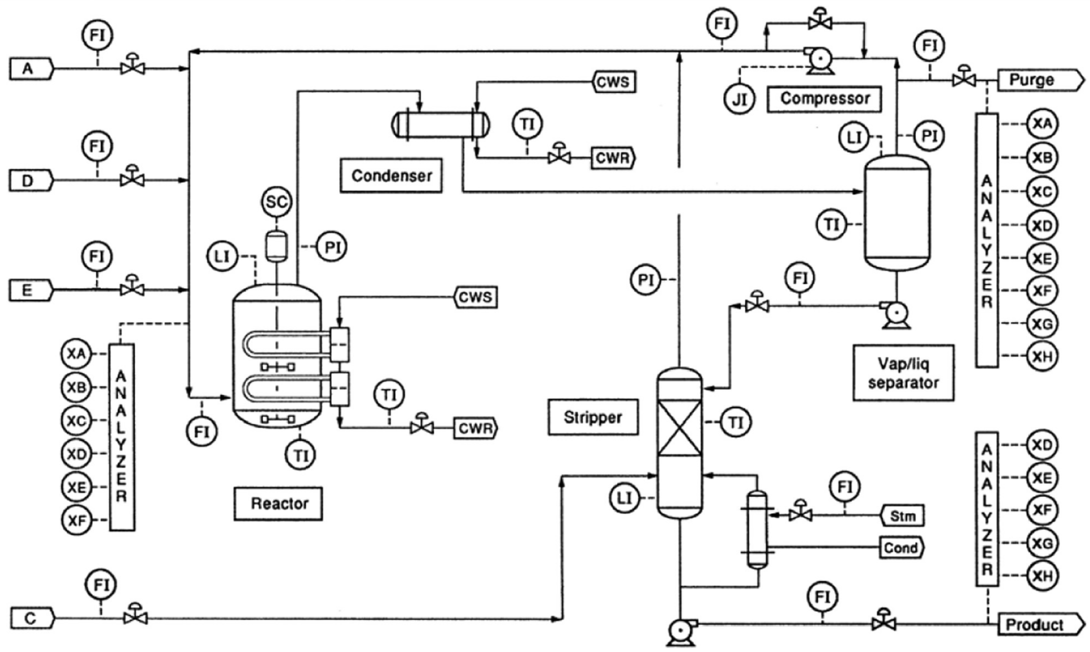

Figure 2. Tennessee Eastman challenge process, Downs and Vogel.[22]. Reproduced with permission from ref 22. Copyright 1993 Elsevier.

constraints can be implemented similarly to traditional MPC. The input bounds can be defined as follows:

$$u_i^l \le \Psi s_i \le u_i^u \tag{15}$$

where $s_i = [u_i(0), u_i(1), ..., u_i(N-1), u_i^*, \alpha_i^1, \alpha_i^2]$ are the decision variables of the MPC optimization and

$$\Psi = \begin{bmatrix} I_{N-1} & 0 & 0 & 0 \\ 0 & 1 & g_1(0) & g_2(0) \\ ... & ... & ... & ... \\ 0 & 1 & g_1(P-N) & g_2(P-N) \end{bmatrix} \tag{16}$$

Actually, N of the conditions in eq 15 define the bounds on the decision variables of the MPC optimization, whereas the rest of the $P - N$ conditions are treated as linear constraints. Alternatively, it is possible to estimate the maximum of the future control moves defined by eq 5. Assuming $c_1 < c_2$, $k = c_2/c_1$, and $k^* = (k-1)k^{-1/(k-1)}$. It is straightforward to show that

$$F(a, b) = \max_x a g_1(x) + b g_2(x) \le \begin{cases} 0, & \text{if } a + b < 0 \text{ and } a < 0 \\ k^*/ka, & \text{if } a + b < 0 \text{ and } a > 0 \\ a + b, & \text{if } a + b > 0 \text{ and } a > -kb \\ k^*((k - 1 + 1/k)a + (k-1)b), & \text{if } a + b > 0 \text{ and } a < -kb \end{cases} \tag{17}$$

Taking into account eq 17, the upper input constraints related to manipulated variable x_i hold if

$$\Phi s_i \le u_i^u \tag{18}$$

where

$$\Phi = \begin{bmatrix} I_{N-1} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & k^*/k & 0 \\ 0 & 1 & 1 & 1 \\ 0 & 1 & k^*(k - 1 + 1/k) & k^*(k-1) \end{bmatrix} \tag{19}$$

The lower input constraint can be handled symmetrically. In comparison of eqs 15 and 16, the number of linear constraints relating to a single manipulated variable drops from $2(P - N)$ to 6.

3. DESCRIPTION OF THE MPC-BASED CONTROL OF THE TENNESSEE EASTMAN CHALLENGE PROCESS (TECP) DEVELOPED FOR THE TWO-PHASE MPC TESTING

In this section, the Tennessee Eastman process is briefly introduced and the MPC based control strategy developed for the two-phase MPC testing is presented.

3.1. Description of the TE. The TECP was first published by Downs and Vogel,[22] and their paper describes the model for this process. The model was created for the development, study, and evaluation of process control technology. The authors state that the TECP is well-suited for a variety of studies of both plantwide and multivariable control. The nature of the process is classified as open loop unstable and consists of the following five units: an exothermic two-phase reactor, a vapor−liquid flash separator, a condenser, a recycle-compressor, and a reboiled stripper. Figure 2 illustrates the process diagram of the TECP. A summary of the real process can be found in Downs and Vogel,[22] and it is presented here very shortly to clarify the operation of this process.

Among the reactions occurring within the process, two simultaneous gas−liquid exothermic reactions producing two products from four reactants are shown in the reaction equations that follow:

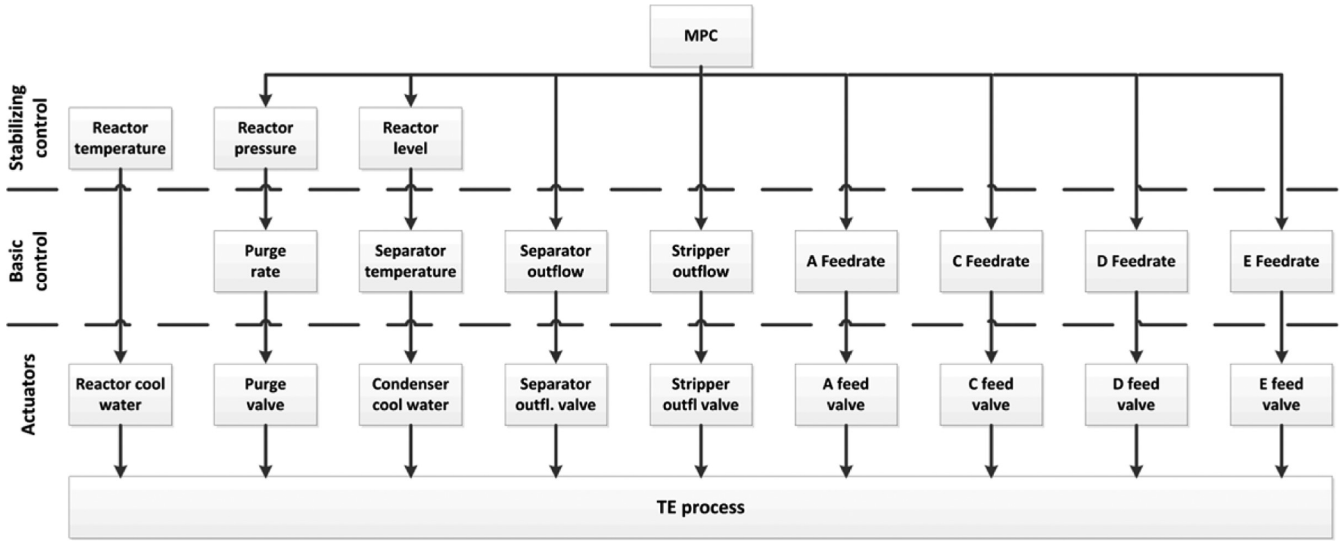

Figure 3. MPC-based control of the TECP.

$$A(g) + C(g) + D(g) \rightarrow G(l) \qquad \text{(product 1)}$$

$$A(g) + C(g) + E(g) \rightarrow H(l) \qquad \text{(product 2)}$$

All of the reactions involved in the process are irreversible and exothermic whereas the reaction rates are a function of the temperature through the Arrhenius equation. The gaseous reactants are fed to the reactor, where they react and form the liquid products. These gas-phase reactions are catalyzed by means of a nonvolatile catalyst that is dissolved in the liquid phase. The reactor is cooled by an internal cooling bundle, and the products leave the reactor as vapor along with unreacted feeds. The catalyst does not leave the reactor together with the product. The product stream leaving the reactor is condensed in a cooler and isolated in a vapor–liquid separator in a successive stage downstream. The uncondensed components are recycled back through a centrifugal compressor to the reactor's feed stream, whereas the condensed components are led to a product stripping column where unreacted reactants are removed by feed stream four. The final products G and H leave the base of the stripper and are separated in a downstream refining section, not included in the base problem description.

According to Downs and Vogel,[22] the objectives of the plant control are as follow: to maintain process variables at desired values, to keep process operating conditions within the constraints, to minimize variability of the product rate and the product quality during the disturbances, to minimize movement of valves which affect other processes (A and C feed flows) and to recover quickly and smoothly from disturbances and production rate and product mix changes. In particular, the composition of the purge flow, the recirculation rate and the temperature in the tanks are usually controlled to achieve and maintain the desired operating conditions, including the composition of the reactor content. Since the number of the listed process outputs is bigger compared to the number of process inputs, which are available to manipulate the process conditions, various control strategies are possible. In addition, the level of the tanks and the pressure in the reactor are frequently controlled to keep them within the safety limits.

3.2. Description of the MPC-Based TECP Control.

A number of different control strategies for the TE are introduced and discussed in the literature. As the basis for the development of an MPC based control, the model of the process provided by Ricker[23] and the decentralized control developed by Larsson et al.[24] were used in the current study. The decentralized control strategy includes the following five stabilizing loops: control of the reactor pressure and the reactor temperature and control of the reactor, separator, and stripper levels. The reactor level, reactor temperature, and reactor pressure control loops are able to follow the respective set points fairly well. However, the reactor pressure control loop may saturate due to the limited capacity of the purge valve, which may result in a process shutdown. To achieve smoother production rate, the separator level and the stripper level loops were not tuned to track the set points tightly, and significant control errors may occur during transitions.

The MPC based control strategy used in the current study considered the reactor level and the reactor pressure set points as manipulated variables of the MPC because of the clear effect of the reactor operating conditions on the whole process. In addition, the feed flow rates of the raw materials were also considered as manipulated variables of the MPC. Following the control strategy proposed in Larsson et al.,[24] the controlled variables of the MPC were the production rate, the concentration of G in the product, the concentration of C in the purge, and the recirculation flow rate. In addition, the MPC must prevent saturation of the reactor pressure control loop, and, therefore, the purge rate was also considered as a controlled process output.

In the current study, it was decided to switch off the separator level and the stripper level loops in the MPC based control and to instead consider the separator level and the stripper level as controlled variables of the MPC. The reason for this is that a constrained MPC is able to handle the process safety limits more efficiently than the PI loops can. In addition, the separator and the stripper levels can be varied by the MPC to produce smoother fluctuations of the production rate during the plant transitions. The separator outflow and the stripper outflow rates were considered as the manipulated variables of the MPC to enable efficient control of the levels of these tanks.

The resulting MPC based control strategy is summarized in Figure 3, and the manipulated and the controlled variables of the MPC are listed in Table 1 and Table 2, together with the related constraints, the suppression move penalty coefficients,

Table 1. Controlled Variables of the MPC

controlled variable of the MPC	nominal value	low limit	high limit	control error penalty
concn of C in the purge, %	21.6			50
recirculation rate, kscmh	32.2			50
concn of G in product, %	54.0			50
separator level, %	50	35	65	1
stripper level, %	50	35	65	1
production rate, m^3/h	22.85			200
purge rate, kscmh	0.23	0.05	0.6	0

Table 2. Manipulated Variables of the MPC

manipulated variable of the MPC	nominal value	low limit	high limit	suppression move penalty
E feed flow, kg/h	4 435.6	0	8 335.6	0.2
striper underflow, m^3/h	25.11	0		200
separator underflow, m^3/h	22.85	0	-	200
reactor level SP, %	65	50	80	200
reactor pressure SP, KPa	2 800	2 700	2 900	20
D feed flow, kg/h	3 663.5	0	5 813.5	0.2
A + C feed flow, kscmh	9.28	0	15.08	4 000
A feed flow, kscmh	0.23	0	0.73	40 000

and the control error penalty coefficients. The hard constraints imposed on the separator and the stripper levels are normal operation limits, and the hard constraints are imposed on the purge rate to avoid saturation of the reactor pressure loop and prevent plant shutdown. The control error penalty coefficients for the separator and the stripper levels have relatively small values to enable smoothing the production rate fluctuations by varying the tank levels. On the other hand, the penalty coefficients for the production rate and the component G in the product have relatively large values. The suppression move penalties are defined according to the scale of the manipulated variables of the MPC. The sampling time of 0.2 h was selected to capture the dynamics of the fastest input−output models. Since there are many very slow input−output responses, some of which are even longer than 20 h, a prediction horizon of 50 samples corresponding to 10 h of simulation time was used.

3.3. Identification of the TE Model for the MPC. Because of the highly nonlinear process dynamics, the identification of an accurate process model based on the process data is a difficult task. Due to the process nature, a linear model fails to describe some of the process phenomena even qualitatively. In particular, an increase in the A and C feed rates without supplying more D and E reactants may increase the production rate up to a certain extent. However, further increase will only cause an explosive growth of the purge rate without any further production rate increase due to exhaustion of the D and E components in the reactor. These phenomena cannot be described properly by a linear process model, and it was noted that including the squared A and C feed rates in the model inputs results in much better model accuracy in a wide range of process operations.

Since it was difficult to achieve proper accuracy in the process model identified from the data, the state estimation is a critical stage for reliable prediction of the process outputs and an efficient MPC implementation in general. There are some measurements not included to the MPC inputs and outputs which may provide additional valuable information about the process state and therefore increase prediction accuracy. In particular, some of the reactor state variables are determined by the MPC inputs. However, neither the MPC inputs nor the outputs describe the reactor content composition, which correlates strongly with the composition of the purge flow. In

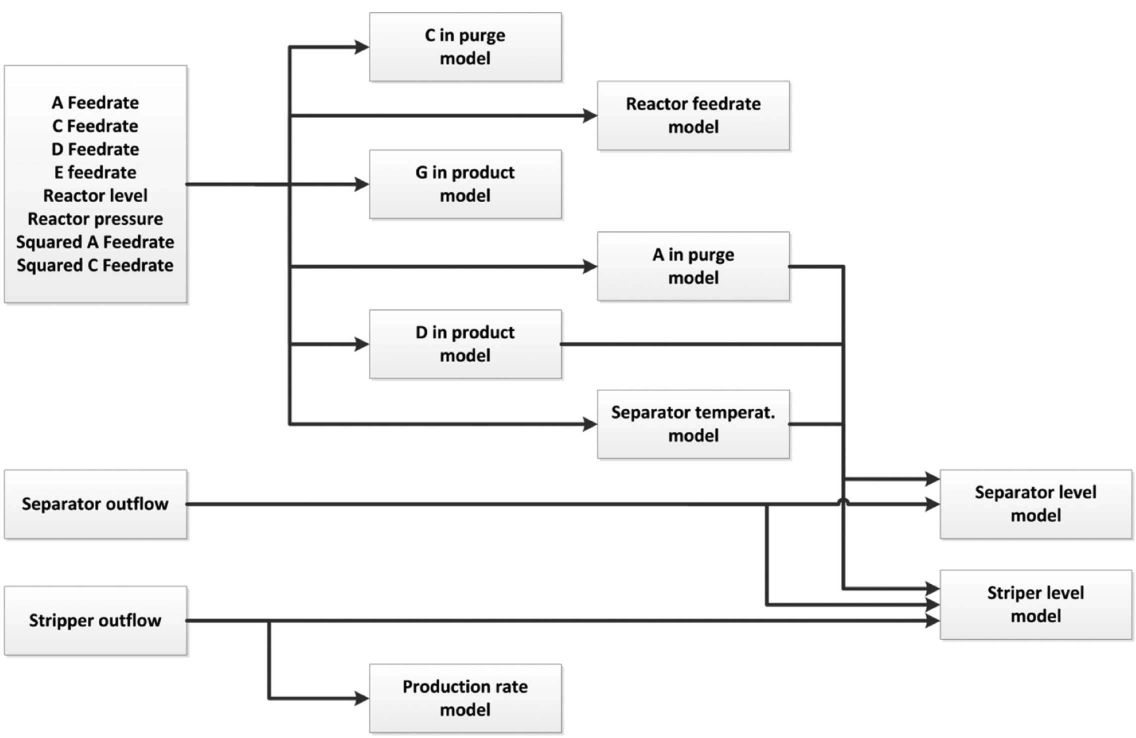

Figure 4. Structure of the TECP model containing a concentration of A in the purge, the concentration of D in the purge, and the separator temperature as the state variables.

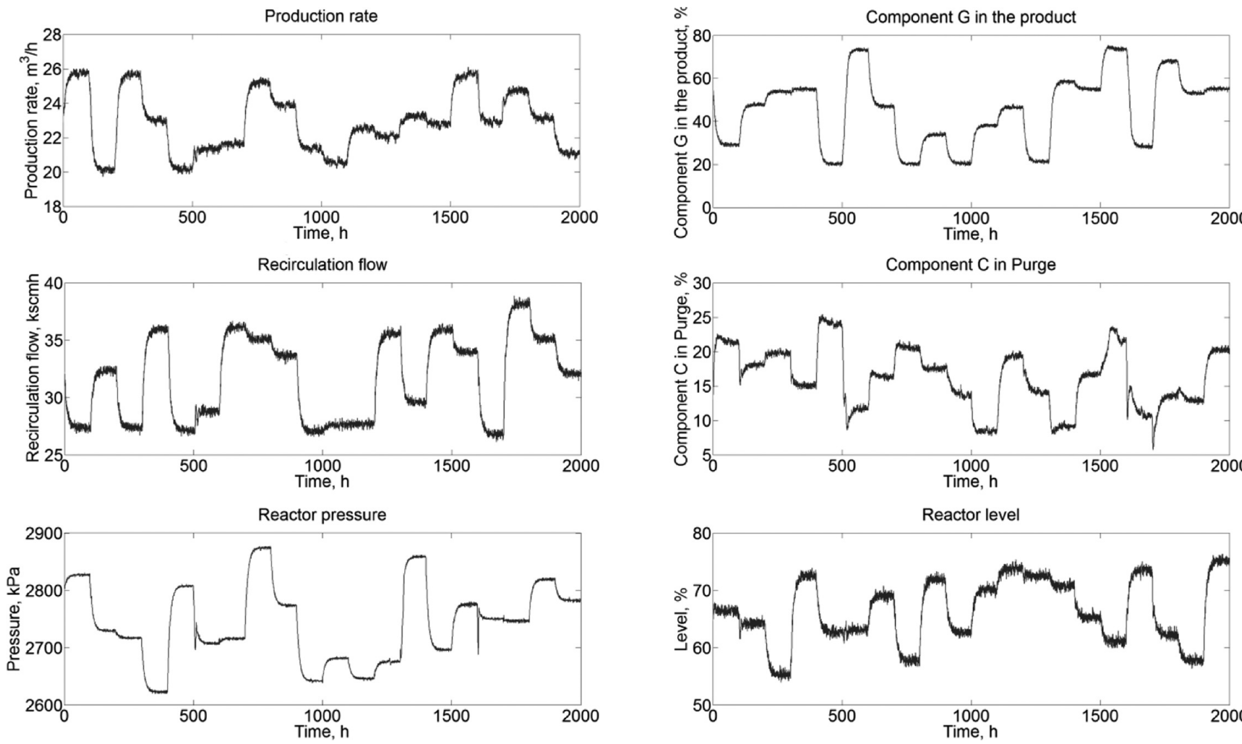

Figure 5. Part of the data used for the model identification.

addition, the separator temperature is another key state variable affecting the product condensation rate in the separator. To achieve better state estimation and thereby more accurate model prediction, the aforementioned variables were incorporated into the process model as states by identifying the model as presented in Figure 4. In other words, most of the process outputs were predicted directly from the model inputs, and the inputs to the separator level and the stripper level models were the process states (separator temperature and concentrations of A and D in the purge flow) which were predicted from the process inputs.

Process data for the model identification were generated by simultaneously exciting the set points of the decentralized control strategy proposed by Larsson et al.[24] with a sequence of steps of random magnitudes. Some of the controlled variables of the decentralized strategy (which are mostly the outputs of the MPC based control) are shown in Figure 5, presenting about one-third of the data used for identification. It is worth noting that the magnitude of the steps was high enough to cover the whole operating range of the MPC. The matrixes defining the model according to eq 1 are provided in the Supporting Information. Before the MPC objective optimization, the process model is linearized at the conditions defined by the control value obtained at the previous MPC run.

To achieve offset free tracking, the variables representing the bias of each model output (including the separator temperature and components A and D in the purge) were introduced to the model. The Kalman filter was obtained assuming the process noise, the measurement noise, and the noise affecting the model bias have the variance provided in Table 3. Using these Kalman filter parameters, the estimations of the recirculation rate, the purge flow rate, and especially the concentration of C in the purge flow are relatively slow and inaccurate. However, the penalty weights assigned to the listed variables are rather small, and the respective set points are not followed precisely.

Table 3. Variance of the Process Noise, Measurement Noise, and the Noise Related to the Model Bias Used for the Kalman Filter

	variance of the process noise	variance of the measurement noise	variance of the model bias noise
separator temp	0.005 2, 0.005 3, 0.001 5, 0.007 2	0.084	0.001 7
concn of C in the purge	0.000 11	0.10	0.000 16
recirculation rate	0.001 7	0.12	0.000 78
concn of G in product	0.006 7, 0.007 4	0.12	0.002 5
component A in purge	0.005 4	0.11	0.002 2
component D in purge	0.011	0.13	0.004 5
separator level	0.073	0.12	0.000 26
stripper level	0.026	0.12	0.000 13
production rate	0.000 98	0.10	0.000 24
purge rate	0.049	0.048	0.007 8

Because of this, the filtering quality does not deteriorate the controller performance much. On the other hand, more aggressive Kalman filter settings can result in strong oscillations, an example of which is given in Figure 6. An increase of the suppression move penalty weights which is sufficient to prevent oscillations leads to a too sluggish response of the output variables. For this reason, the filtering settings provided in Table 3 were used in all simulations.

4. RESULTS OF THE SIMULATIONS

The aim of the present section is to compare the proposed two-phase MPC against two other predictive control techniques utilizing parsimonious parametrization of the future control

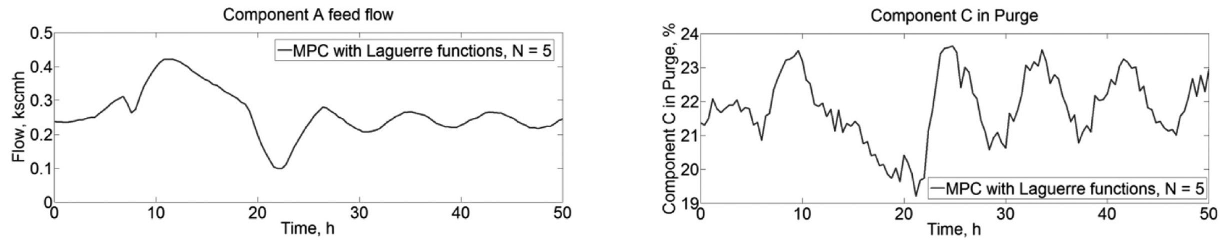

Figure 6. Oscillations in the signals produced by the MPC with Laguerre functions using a more aggressive filter configuration.

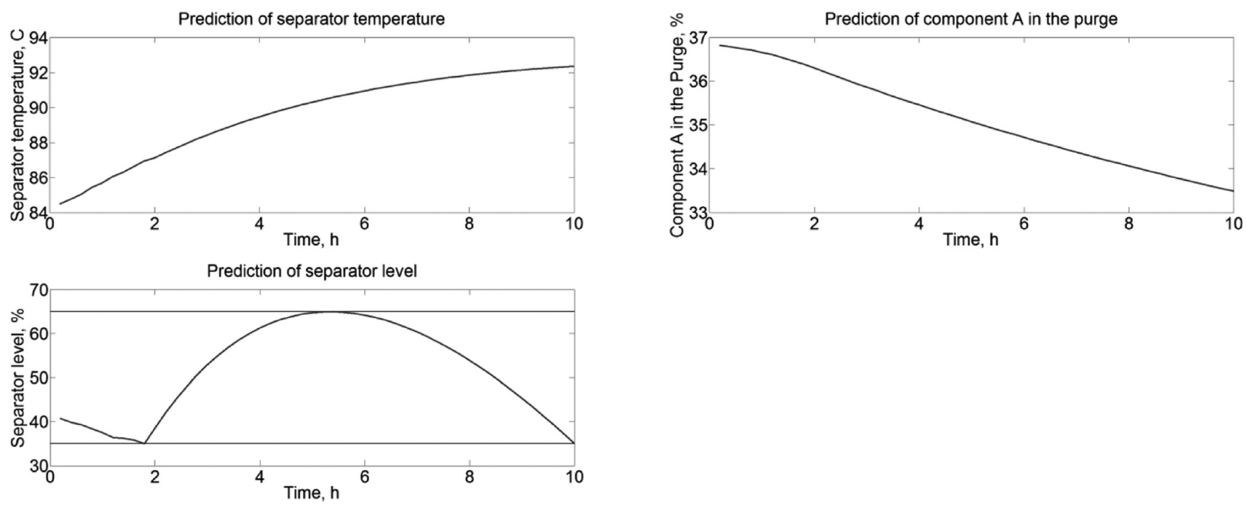

Figure 7. Prediction of three process variables made by the MPC with blocking at the beginning of the second transition (20.2 h of the simulation time).

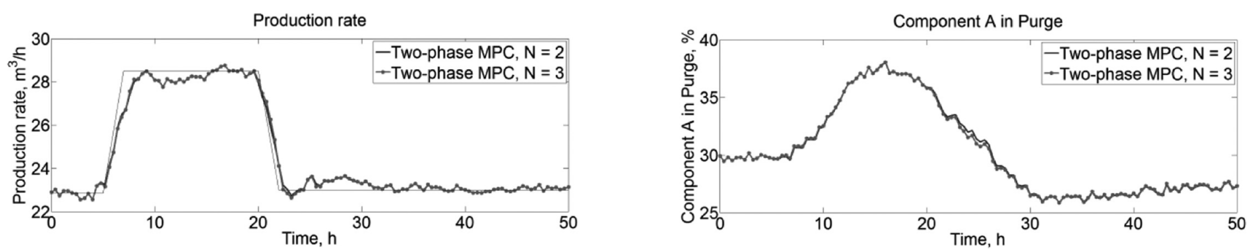

Figure 8. Comparison of the results of the two-phase MPCs with the control horizon of two and three samples.

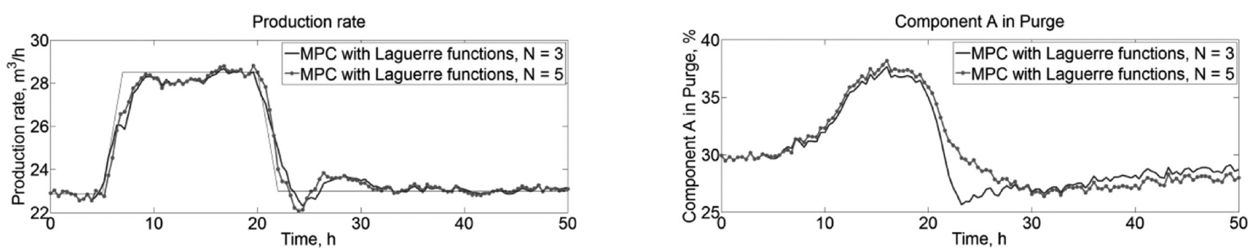

Figure 9. Comparison of the results of the MPCs using three and five Laguerre functions.

moves. Namely, the MPC with blocking used for the comparison study has the control horizon of nine samples and the blocking factors of [**1**,**1**,**2**,**2**,**3**]. Two configurations of the MPC using Laguerre functions were considered, in which 3 and 5 degrees of freedom are assigned to each manipulated variable. In both cases, the parameter a defining the decay rate of the functions is set to 0.85. Finally, the two-phase MPC with the control horizon of two and three samples was tested, and the decay parameters were set to $c_1 = 0.2$ and $c_2 = 0.3$ in both configurations. The bounds on the manipulated variables were implemented according to eqs 18 and 19. In fact, the selected controllers introduce approximately the same amount of dof (from 4 to 6 for each manipulated variable), in order to adequately compare different parametrization approaches. Furthermore, all predictive controllers share the same sampling time of 0.2 h and the same prediction horizon of 50 samples corresponding to 10 h of simulation time. The same objective function with the parameters defined in Tables 1 and 2 is minimized by all MPCs.

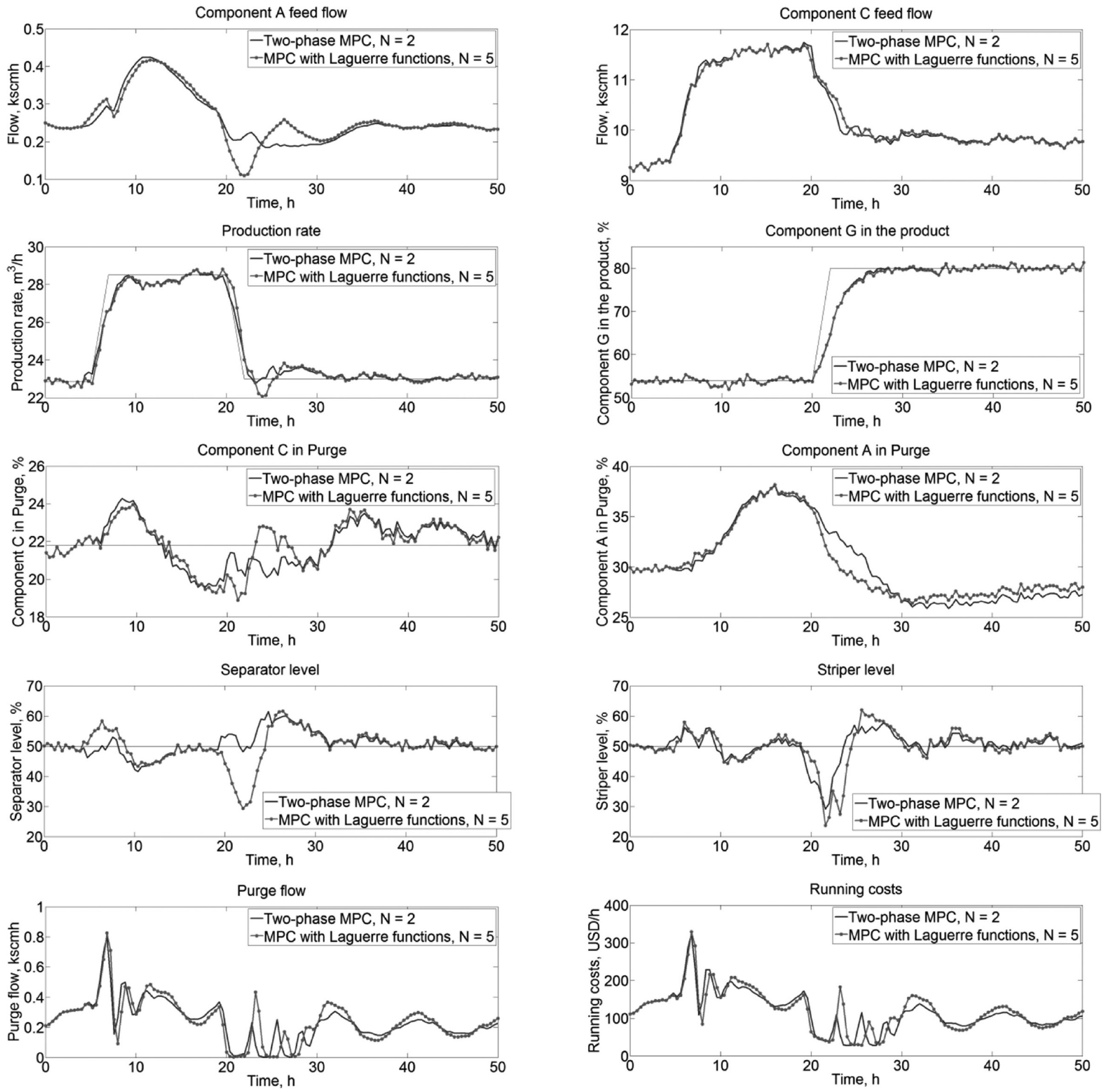

Figure 10. Case study 1: Simulation results for the two-phase MPC (N = 2) and MPC with Laguerre functions (N = 5).

Table 4. Average Computation Time and the Running Cost of the MPCs in Case Study 1

MPC name	no. of decision variables	av calculation time, s: transition 1	av calculation time, s: transition 2	av running costs: transition 1	av running costs: transition 2
MPC with blocking, N = 6	48	0.109		177.4	
Laguerre MPC, N = 3	24	0.165	0.197	164.9	97.7
Laguerre MPC, N = 5	40	0.228	0.285	171.8	92.0
two-phase MPC, N = 2	32	0.131	0.133	174.0	86.4
two-phase MPC, N = 3	40	0.128	0.147	173.7	86.7

Downs and Vogel[22] proposed steps in the production rate, the product composition, the reactor pressure, and component B in the purge to test control strategies. The production rate and the product composition were varied in the first case study. In the proposed control strategy, the reactor pressure is controlled by a SISO control loop, and a step in this variable was not considered for this reason. Since component B in purge is not an output variable in the considered control strategy, the second case study induced changes in the recirculation flow rate and component C in the purge, which both strongly affect the composition of the purge rate in general, instead of the last of the step tests proposed by Downs and Vogel.[22] Finally, the controllers performance was evaluated in the presence of random variations of the composition of the A and C feed

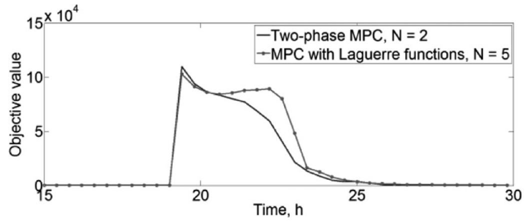

Figure 11. Objective of the MPC optimization during the second transition period.

stream, which is defined as IDV(8) in Downs and Vogel.[22] According to Ricker and Lee,[25] this is one of the most difficult disturbances to handle.

The simulation results are described as follows. First, it is reported which of the controllers (if any) was unable to perform the required transitions, and the suitable numbers of dof were selected for the two-phase MPC and the MPC utilizing Laguerre functions. The results of the selected controllers are compared in terms of deviations of the output variables from the respective set points, variations of the purge flow, smoothness of the raw material feed flow rates, and the running costs of the plant. In the first comparative study, the controller performance is also compared by checking the trajectories of the optimization objective, wherein a decreasing curve indicates that the transition went smoothly.

4.1. Results of the Production Rate and the Product Composition Variation Tests. The first scenario contained two transitions. During the first transition, the production rate set point was linearly increased from the nominal value, which is 22.84 m^3/h, to 28.5 m^3/h between 5 and 7 h of simulation time. In the second transition period, taking place from 20 to 22 h of the simulation time, the content of component G in the product was switched from its nominal value of 54 to 80%. The production rate was simultaneously changed back to 23 m^3/h, because the increased production rate is infeasible for 80:20 product composition. In both episodes the set points were manipulated very rapidly in order to provide a proper ground for MPCs feasibility and performance evaluation.

The only controller that failed to complete the transitions is the MPC with blocking, which was unable to find a feasible solution of the optimization at the beginning of the second transition period. In this case study, the separator level constraints are the most difficult to fulfill, which is confirmed by the prediction of the trajectories of three process variables made by the MPC at the beginning of the second transition; see Figure 7. The separator temperature and the concentration of component A in the purge, having respectively negative and positive effects on the condensation rate in the separator, both possess very slow dynamics. For this reason, driving these variables to the target steady values takes over 10 h of simulation time, which is the prediction horizon of the MPC. The optimization of the MPC with blocking, however, is only able to consider a constant separator outflow between 2 and 10 h of the simulation time, and, therefore, it has insufficient capability to keep the separator level within the constraints. In particular, Figure 7 shows the prediction of the separator level obtained by the MPC optimization just before it started to be infeasible. In the result, the MPC with blocking was able to perform the second transition neither in 2 nor in 5 h.

Before the comparison of the two-phase MPC and the MPC using Laguerre functions, results of both control techniques were checked to define the suitable number of degrees of freedom for each method. The two-phase MPCs with the control horizons of two and three samples provided almost the same results in the transitions, which is confirmed by Figure 8. Therefore, the two-phase MPC with the control horizon of two samples is selected for further evaluation. The MPCs with three and five Laguerre functions introduced in ref 11 achieved a similar quality of the production rate tracking, which is shown in Figure 9. However, the former controller was noticeably more aggressive in changing the operating conditions, which can be seen for example on the plot of the content of component A in the purge, which is a good indicator of the reactor state. Thus, the results of the later MPC with five Laguerre functions were used for the comparison.

The results of the selected controllers (the two-phase MPC with $N = 2$ and the Laguerre MPC with $N = 5$) are shown in Figure 10. The two-phase MPC followed the production rate set point slightly more tightly especially during the second transition. The product composition was tracked equally well by both of the controllers. Furthermore, the MPC with Laguerre functions changed the component A in the purge flow very rapidly, which required aggressive manipulations of the component A feed flow rate and the purge flow rate. In particular, higher purge flow rate peaks were obtained by the MPC with Laguerre functions leading to higher average running costs in the second transition period. In addition, the MPC using the Laguerre functions allowed a 20% deviation in the separator level, whereas the two-phase MPC kept the level variations within 10%. Both controllers achieved satisfactory accuracy in tracking all other set points. The average computation times and the average running costs are summarized in Table 4 for all considered controllers. In brief, in this case study the two-phase MPC slightly outperforms the MPC with Laguerre functions in control performance. The computation time of the two-phase MPC stays below 60% of that of its competitor. The MPC with blocking probably requires more degrees of freedom to achieve satisfactory feasibility and performance.

Next, the controller performance was tested by examining the evolution of the MPC objective during the second

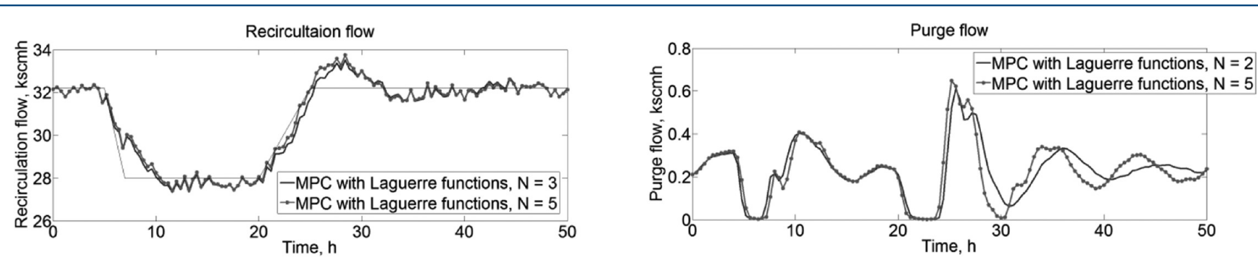

Figure 12. Comparison of the results of the MPCs using three and five Laguerre functions.

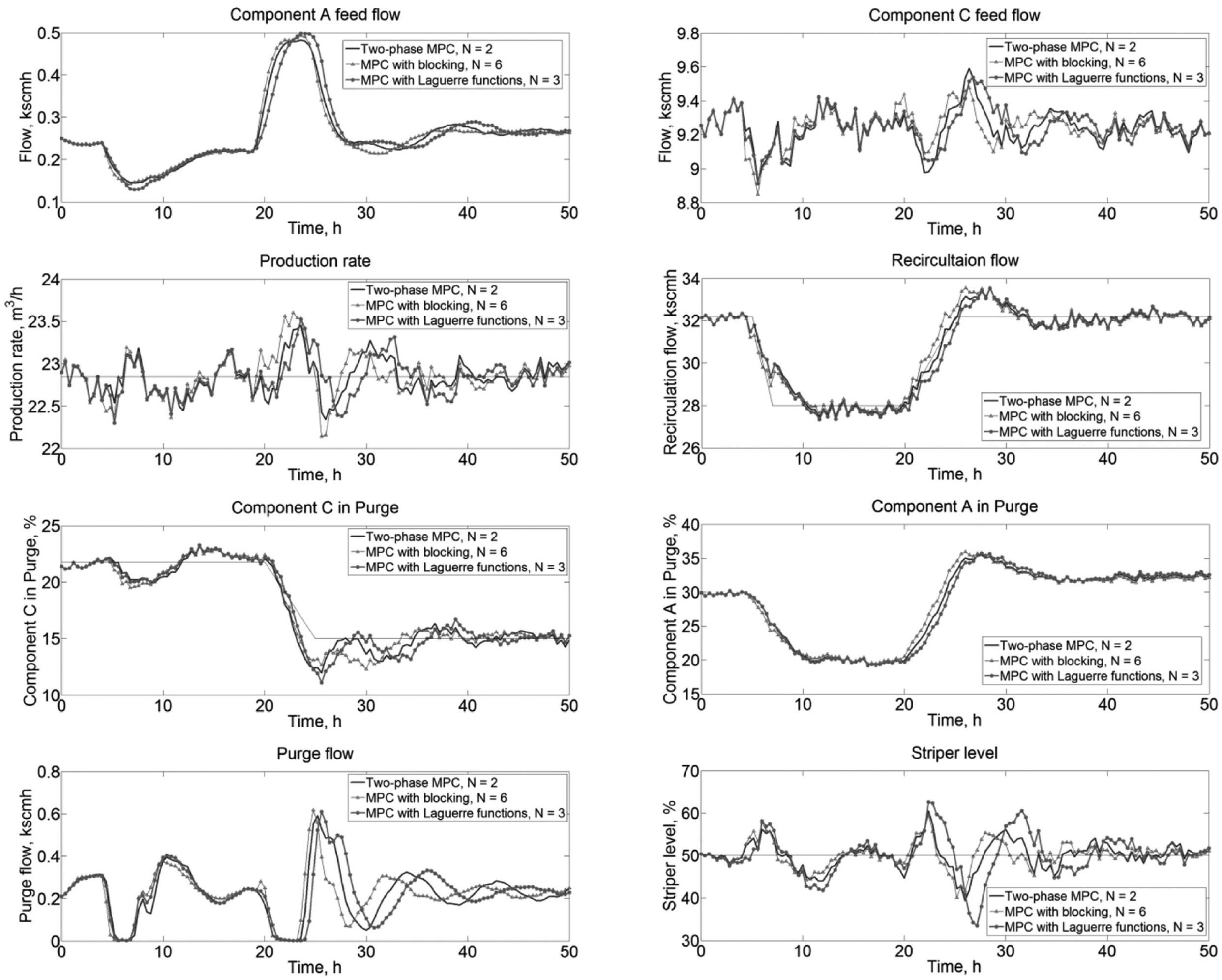

Figure 13. Case study 2: Simulation results for three MPCs.

Table 5. Average Computation Time and the Running Cost of the MPCs in Case Study 2

MPC name	no. of decision variables	av calculation time, s		av running costs	
		transition 1	transition 2	transition 1	transition 2
MPC with blocking, $N = 6$	48	0.116	0.111	142.9	117.9
Laguerre MPC, $N = 3$	24	0.175	0.188	143.8	122.2
Laguerre MPC, $N = 5$	40	0.256	0.253	140.6	120.2
two-phase MPC, $N = 2$	32	0.131	0.126	139.1	119.5
two-phase MPC, $N = 3$	40	0.153	0.150	139.4	119.6

transition period, which is shown in Figure 11. During the transition, the two-phase MPC produced a smooth and decreasing curve, confirming that the transition went well. The objective of the MPC with Laguerre functions has a peak at about 23 h of simulation time, indicating that the controller had some difficulties in finding a good solution.

4.2. Results of the Recirculation Rate and Component C in the Purge Variation Tests. The second scenario contains two transitions. During the first transition, the recirculation set point was linearly switched from the nominal value, which is 32.2 kscmh, to 28 kscmh between 5 and 7 h of simulation time. In the second transition period, taking place from 20 to 25 h of simulation time, the recirculation rate was driven back to its nominal value, and the concentration of component C in the purge was simultaneously changed from 21.6 to 15%. In other words, this scenario aims to check the ability of the controllers to change the reactor content composition and the operating conditions while the production rate and the product specification stay constant.

Before the comparison of the control techniques, the simulation results were evaluated to define the suitable number of the degrees of freedom. The two-phase MPCs with the control horizon of two and three samples provided almost undistinguishable results, and the controller with the control horizon of two samples is selected for further evaluation. The MPCs with three and five orthogonal functions achieved similar quality of the set points tracking. In particular, the recirculation flow rate dynamics is shown in Figure 12. However, the former controller produced a lower peak in the purge rate during the second transition and smoother trajectories at the end of the simulation period. Thus, the results of the former MPC with three Laguerre functions are considered in more detail.

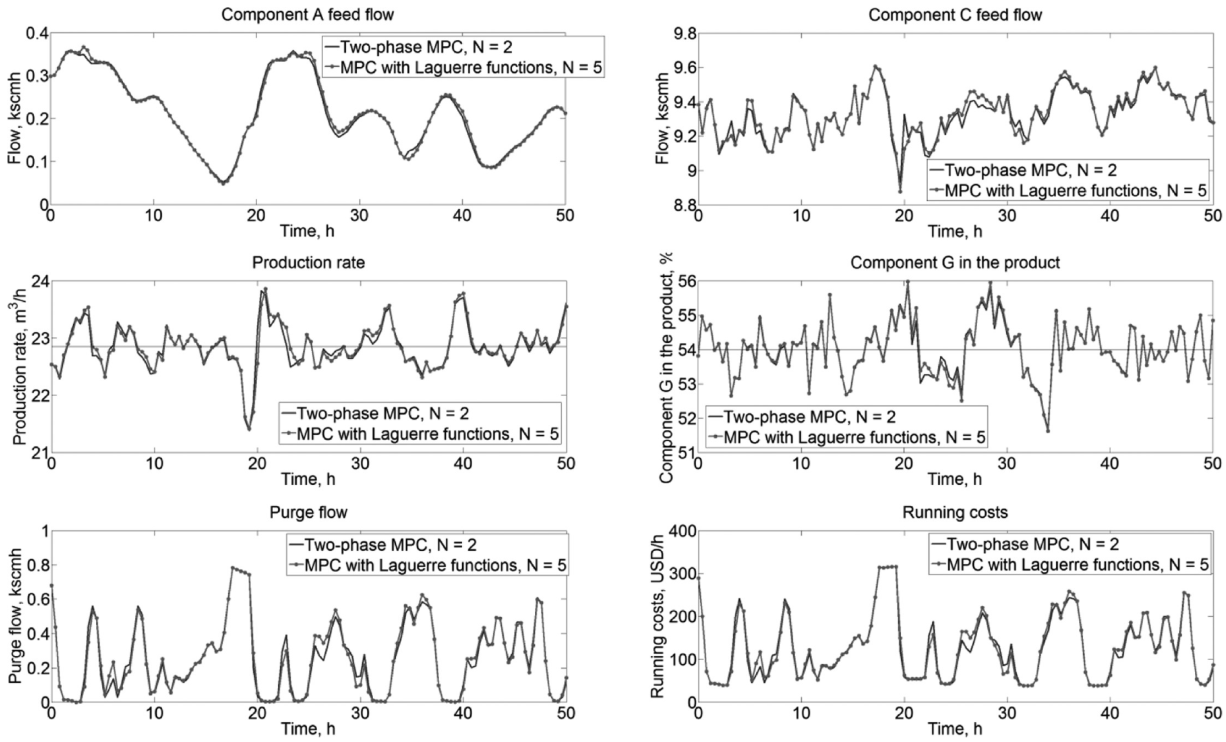

Figure 14. Case study 3: Simulation results for the two-phase MPC (N = 2) and MPC with five Laguerre functions.

The results of the selected controllers (the two-phase MPC with N = 2, the MPC with blocking, and the Laguerre MPC with N = 3) are shown in Figure 13. All controllers managed to prevent deviations in the production rate and component G in the product. Because of the objective weights selection, the recirculation rate and component C in the purge were not controlled tightly. However, these set points were tracked rather well by all controllers considered. It can be seen from the plots that the controllers delivered equally smooth trajectories of the A and C feed rates, and the purge rate peaks were similar in all cases. In brief, all three controllers handled the second scenario successfully, except that the MPC with Laguerre functions allowed bigger variations in the stripper level. The average computation times and the average running costs are summarized in Table 5 for all considered controllers.

4.3. Results of the Simulations with Disturbances. In the third scenario, the controllers were evaluated in the presence of random variations of the composition of the A and C feed stream. Namely, the content of components A, B, and C is varied, disturbing the stoichiometric ratio of the reactants and affecting the accumulation of the inert component B in the process. Therefore, the purge flow rate must be frequently set to a high level to remove an excess of the components from the reactor. In addition, the disturbance has a strong effect on the levels of the separator and the striper, which can also result in a process shutdown if an improper process control is applied. Thus, the aforementioned process outputs were studied in this scenario to evaluate the feasibility of the controllers. Since the disturbance itself provided enough excitation to test the plant control, all set points are kept constant as it is done in other works, such as Ricker and Lee.[25]

The MPC with blocking and the MPC using three Laguerre functions failed to find a feasible optimization solution at about 20 h of simulation time. Since the two-phase MPC with the control horizons of two and three samples provided almost identical results, the former controller is selected for the comparison. The two-phase MPC with the horizon of two samples and the MPC using five Laguerre functions provided very close results, which is demonstrated by Figure 14. In brief, both controllers achieved a stable production rate (the tracking error is almost always below 1 m^3/h) and product composition (the error is almost always within 2%) and avoided the operating conditions leading to a shutdown. The two-phase controller achieves slightly lower production cost of \$126.6/min and twice as fast average computation time (0.145 s) compared with its competitor (\$127.5/min and 0.280 s, respectively).

5. CONCLUSIONS

The paper presents a comparative study of three MPCs utilizing different parsimonious parametrizations of the control moves. The Tennessee Eastman challenge problem (TECP) was in particular selected for the comparative study because of its dynamics, including very fast and very slow responses, which results in requirement of long control and prediction horizons. A MPC based control strategy of the Tennessee Eastman process was developed using a model identified from process data. The squared A and C feed rates were included to the model inputs which resulted in much better model accuracy in a wide range of process operations. Furthermore, to achieve better state estimation and thereby more accurate model prediction, the separator temperature and content of components A and D in the purge flow were incorporated into the process model as states.

The simulation results demonstrated that the MPC optimization may need to adjust the distant future control moves of some of its manipulated variables to find a feasible solution. This in particular happens if some manipulated variables, having a short effect on a constrained controller output, must be adjusted to compensate for some long-term effects of other inputs on the same output variable. In the proposed control strategy, the MPC with blocking cannot probably achieve satisfactory performance using just 4 or 5 dof for each input, which is sufficient for the two-phase MPC and MPC using Laguerre functions. Both the two-phase MPC and MPC using Laguerre functions provided an adequate performance and good feasibility by using only 5 dof for each input. However, in the second transition of the first case study, the MPC using Laguerre functions faced some problems in finding a good solution, which in particular resulted in worse tracking of the production rate set point and slightly higher running costs compared with the two-phase MPC during the transition. This is also confirmed by a period of increasing of the MPC objective value during the first part of the transition. In all case studies, the two-phase MPC did not perform worse compared to the MPC using Laguerre functions.

The paper proposed an estimation of the maximum and minimum of the future control trajectory for the two-phase MPC. In the result, the number of constraints representing the lower and upper bounds on a manipulated variable reduced from twice the second-phase length to only 6, and a considerable computational savings was achieved. In particular, in all case studies the computation time of the two-phase MPC is below 60% of those of the MPC using Laguerre functions, whereas both controllers use 5 dof for each manipulated variable.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

Text giving the matrixes defining the linear model used for MPC implementation. This material is available free of charge via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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