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Simulation of NMPC for a Laboratory Adiabatic CSTR with an Exothermic Reaction

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***Abstract*— In this paper, we present nonlinear system identification and nonlinear model predictive control (NMPC) for a laboratory-scale adiabatic continuous stirred tank reactor (CSTR) with an exothermic reaction. We describe the equipment used in the process, and we present a process model based on first principles. We use a maximum likelihood estimation (MLE) approach based on the process model and the continuous-discrete extended Kalman filter (CD-EKF) to estimate four model parameters. The NMPC is based on the process model (with the estimated model parameters), the CD-EKF, and a nonlinear least-squares regulator with input (Tikhonov) and rate-of-movement regularization. We present simulations demonstrating that the NMPC (implemented in Python and C) can track any stable and unstable steady state for this system with multiple steady states in some operational regions.**

I. Introduction

In this paper, we discuss implementation of nonlinear model predictive control (NMPC) for an adiabatic continuous stirred tank reactor (CSTR) with a second order irreversible exothermic reaction. This reaction was described by [1], and it is a reaction of sodium thiosulfate and hydrogen peroxide in aqueous solutions. [2], [3] provide extensive analysis of the dynamics of this reaction using principles for nonlinear dynamical analysis of reaction systems comprehensively described by [4]–[6]. [7] provide an overview of the analysis, dynamics, and control of chemical reactors until the mid 1980s. The current understanding of modeling, dynamics, and simulation of adiabatic CSTRs with exothermic reactions was established in the 1950s to 1970s [8]–[10], while the control of such systems using NMPC algorithms appeared in the literature in 1990s to 2000s [11]–[25]. Most of these NMPC papers were based on simulation and did not contain experimental verification nor issues related to system identification. [26]–[28] discuss identification of models using normal forms and concepts from nonlinear analysis of differential equations. In the 2010s, papers related to economic model predictive control (EMPC) for CSTRs appeared [29]–[32]. They relied on the much earlier observation that for some reactions, the optimal mode of operation is not at a steady state but in an inherently dynamic mode [33]–[35]. Recently, [36] and [37] presented integrated systems for NMPC specification based on extended Kalman filters (EKFs) for state estimation [38]–[40].

We suggest an NMPC based on filtering and predictions with the continuous-discrete EKF (CD-EKF) for the exothermic second order irreversible reaction in an adiabatic laboratory CSTR [41]. The CD-EKF is also used as the predictor in a maximum likelihood (ML) based algorithm for system identification (i.e. parameter estimation) and as the predictor in the dynamic optimization of a certainty equivalent (CE) regulator in the NMPC. We use the estimated parameters in the mathematical model in the NMPC. In order to be able to track the unstable steady states, we implement the dynamic optimization using a simultaneous method. We implement the NMPC algorithm in Python (for rapid prototyping) and in C (for computational performance). While we have previously applied the NMPC based on the CD-EKF for an artificial pancreas for people with type 1 diabetes [42]–[44], the van der Pol oscillator [45], and isoenergetic-isochoric vapor-liquid equilibrium processes [46], the application of NMPC based on the CD-EKF to a CSTR is novel. Also the experimental verification of the capability of the NMPC to track any of the multiple steady states in the adiabatic CSTR with an exothermic reaction is new and opens the opportunity to investigate NMPC for inherently dynamical operation of such systems.

This paper is organized as follows. We describe the laboratory process and its control system in Section II. In Section III, we present the process model and we describe the NMPC algorithm (i.e. the CD-EKF and the nonlinear least-squares regulator) as well as the ML based parameter estimation. We present simulation results in Section IV, and conclusions are given in Section V.

II. Process description

Fig. 1 shows an overview of the laboratory CSTR and its control system [41]. The exothermic reaction,

$$\begin{aligned}\mathrm{Na_2S_2O_3(aq)} + 2\mathrm{H_2O_2(aq)} \rightarrow \\ \frac{1}{2}\mathrm{Na_2SO_4(aq)} + \frac{1}{2}\mathrm{Na_2S_3O_6(aq)} + 2\mathrm{H_2O(aq)},\end{aligned} \tag{1}$$

is conducted in a laboratory scale adiabatic CSTR with a volume of 105 mL. A low level control system based on a Siemens PLC controls the system. The high level NMPC communicates with the low level control system using OPC.

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Fig. 1. The laboratory adiabatic CSTR and its control system.

The reactor is a three-neck round bottom flask with an evacuated jacket for thermal insulation which is considered adiabatic. A magnetic stirrer inside the flask mixes the reaction solution. The reaction volume is constant due to overflow into a waste collection tank.

Three K-type thermocouples are inserted into the flask where they measure the temperature of each reactant being fed and the temperature of the reaction solution. The temperature of the reactants can be assumed identical and constant for the present experimental conditions.

A peristaltic pump capable of flow rates in the range 0 to 400 mL/min on each tube is used to pump the reactants into the reactor. These flow rates correspond to residence times in the range infinity to 7.9 seconds. The pump throughput versus RPM follows a linear relationship which is estimated prior to the experiment. The dynamics of the pump subject to changes in the rotational speed are negligible.

Reactants are stored in 25 L containers placed inside a freezer to ensure a stable feed temperature of approximately 0.5°C. The feed to the system consists of a 1.6 M aqueous $Na_2S_2O_3$ solution and a 2.4 M aqueous H_2O_2 solution. This implies that H_2O_2 is the limiting reactant. The $Na_2S_2O_3$ solution is prepared by dissolving $Na_2S_2O_3{\cdot}5H_2O$ in hot demineralized water with mixing to ensure complete dissolution. The concentrations of the cooled feed solutions are determined accurately by titrimetric analysis.

Finally, the PLC provides analog inputs and outputs for interacting with instruments as well as an OPC interface allowing computer control. Thus, the high level NMPC can obtain sensor measurements and effectuate new setpoints online. Additionally, the touch screen human-machine interface (HMI) gives convenient access to a mimic diagram of the process and trend curves during the experiment.

III. Numerical Methods

In this section, we describe the mathematical model and the numerical methods used for realization of the NMPC.

A. Process model

The chemical reaction (1) is represented as

$$A + 2B \rightarrow \frac{1}{2}C + \frac{1}{2}D + 2E. \tag{2}$$

It occurs at the reaction rate r and its enthalpy of reaction is ΔH_r. The reaction rate is

$$r = r(C_A, C_B, T) = k(T) C_A C_B, \tag{3}$$

where $k(T)$ is given by an Arrhenius expression:

$$k(T) = k_0 \exp\left(\frac{-E_a}{RT}\right). \tag{4}$$

The production rate of molecule A and B are given from the reaction rate, r, and the stoichiometry of (2):

$$R_A = R_A(C_A, C_B, T) = -r(C_A, C_B, T), \tag{5a}$$
$$R_B = R_B(C_A, C_B, T) = -2r(C_A, C_B, T). \tag{5b}$$

This implies that the mass balances for components A and B as well as the energy balance for the adiabatic CSTR may be represented by the system of ODEs

$$\dot{C}_A = \frac{F}{V}(C_{A,in} - C_A) + R_A(C_A, C_B, T), \tag{6a}$$
$$\dot{C}_B = \frac{F}{V}(C_{B,in} - C_B) + R_B(C_A, C_B, T), \tag{6b}$$
$$\dot{T} = \frac{F}{V}(T_{in} - T) + R_T(C_A, C_B, T), \tag{6c}$$

where

$$R_T(C_A, C_B, T) = \beta r(C_A, C_B, T), \tag{7}$$

and $\beta = -\Delta H_r/(\rho c_P)$. As the reactor is operated such that B is the limiting reactant, we define the extent of reaction, X, as

$$X = \frac{C_{B,in} - C_B}{C_{B,in}} = 1 - \frac{C_B}{C_{B,in}}. \tag{8}$$

Using this definition, the extent of reaction must be strictly between 0 and 1, i.e. $X \in (0, 1)$. We assume that the inlet temperature is uncertain, and we represent this uncertainty using a stochastic differential equation for the temperature:

$$dC_A = \left[\frac{F}{V}(C_{A,in} - C_A) + R_A(C_A, C_B, T)\right] dt, \tag{9a}$$
$$dC_B = \left[\frac{F}{V}(C_{B,in} - C_B) + R_B(C_A, C_B, T)\right] dt, \tag{9b}$$
$$dT = \left[\frac{F}{V}(T_{in} - T) + R_T(C_A, C_B, T)\right] dt + \frac{F}{V}\sigma_T d\omega. \tag{9c}$$

Table I lists nominal values of the parameters in the model.

TABLE I

NOMINAL PARAMETER VALUES.

Parameter	Value	Unit	Parameter	Value	Unit
ρ	1.0	kg/L	V	0.105	L
c_P	4.186	kJ/(kg·K)	$C_{A,in}$	1.6/2	mol/L
k_0	exp(24.6)	L/(mol·s)	$C_{B,in}$	2.4/2	mol/L
E_a/R	8500	K	T_{in}	273.65	K
ΔH_r	-560	kJ/mol		= 0.5	°C

B. Mathematical model

We formulate the NMPC algorithm for stochastic continuous-discrete mathematical models in the form

$$d\boldsymbol{x}(t) = f(\boldsymbol{x}(t), u(t), p)dt + \sigma(\boldsymbol{x}(t), u(t), p)d\boldsymbol{\omega}(t), \quad (10a)$$

$$\boldsymbol{y}(t_k) = g(\boldsymbol{x}(t_k), p) + \boldsymbol{v}(t_k; p), \quad (10b)$$

$$\boldsymbol{z}(t) = h(\boldsymbol{x}(t), p), \quad (10c)$$

where $\boldsymbol{x}(t)$ are the state variables, $\boldsymbol{y}(t_k)$ are the measurements, and $\boldsymbol{z}(t)$ are the outputs. The stochastic model of the CSTR (9) is in the form (10a), and the temperature sensor, which is corrupted by measurement noise, is represented by (10b). The temperature is measured at discrete times, t_k, and the measurement noise is normally distributed, i.e. $\boldsymbol{v}(t_k; p) \sim N_{iid}(0, R_k)$ where $R_k = R_v(t_k, p)$. The output, $\boldsymbol{z}(t)$, is the temperature which we want to control. $\{\boldsymbol{\omega}(t)\}$ is a standard Wiener process, i.e. $d\boldsymbol{\omega}(t) \sim N_{iid}(0, Idt)$.

C. State estimation

We use the extended Kalman filter for the continuous-discrete system (10) for one-step prediction and filtering. At time t_k, it computes the filtered state estimate, $\hat{x}_{k|k}$, and its covariance, $P_{k|k}$, assuming that the filtered state-covariance pair, $(\hat{x}_{k-1|k-1}, P_{k-1|k-1})$, at the previous sampling time is available along with the current measurement, y_k, and the manipulated variable, $u(t) = u_{k-1}$, used in the previous interval, $t_{k-1} \le t < t_k$.

1) One-step prediction: The filtered mean-covariance pair, $(\hat{x}_{k-1|k-1}, P_{k-1|k-1})$, at time t_{k-1} is used as initial conditions,

$$\hat{x}_{k-1}(t_{k-1}) = \hat{x}_{k-1|k-1}, \quad (11a)$$

$$P_{k-1}(t_{k-1}) = P_{k-1|k-1}, \quad (11b)$$

for the system of ordinary differential equations (ODEs)

$$\frac{d}{dt}\hat{x}_{k-1}(t) = f(\hat{x}_{k-1}(t), u_{k-1}, p), \quad (12a)$$

$$\frac{d}{dt}P_{k-1}(t) = A_{k-1}(t)P_{k-1}(t) + P_{k-1}(t)A_{k-1}(t)' + \sigma_{k-1}(t)\sigma_{k-1}(t)'. \quad (12b)$$

The system of ODEs (12) are solved for $t_{k-1} \le t \le t_k$ with

$$A_{k-1}(t) = \frac{\partial f}{\partial x}(\hat{x}_{k-1}(t), u_{k-1}, p), \quad (13a)$$

$$\sigma_{k-1}(t) = \sigma(\hat{x}_{k-1}(t), u_{k-1}, p). \quad (13b)$$

The solution at time t_k is the one-step prediction

$$\hat{x}_{k|k-1} = \hat{x}_{k-1}(t_k), \quad (14a)$$

$$P_{k|k-1} = P_{k-1}(t_k). \quad (14b)$$

2) Filter: The filter uses the one-step prediction of the states, $\hat{x}_{k|k-1}$, and its covariance, $P_{k|k-1}$, as well as the measurement, y_k, to compute the filtered state, $\hat{x}_{k|k}$, and its covariance, $P_{k|k}$, at time t_k.

The filtered state, $\hat{x}_{k|k}$, is computed by

$$\hat{y}_{k|k-1} = g(\hat{x}_{k|k-1}, p), \quad C_k = \frac{\partial g}{\partial x}(\hat{x}_{k|k-1}, p), \quad (15a)$$

$$e_k = y_k - \hat{y}_{k|k-1}, \quad R_{e,k} = R_k + C_k P_{k|k-1} C_k', \quad (15b)$$

$$\hat{x}_{k|k} = \hat{x}_{k|k-1} + K_k e_k, \quad K_k = P_{k|k-1} C_k' R_{e,k}^{-1}, \quad (15c)$$

where $R_k = R_k(p)$. The corresponding covariance, $P_{k|k}$, is obtained from the expression

$$P_{k|k} = (I - K_k C_k)P_{k|k-1}(I - K_k C_k)' + K_k R_k K_k'. \quad (16)$$

The Joseph-stabilized form (16) is preferred to the classical form,

$$P_{k|k} = P_{k|k-1} - K_k R_{e,k} K_k', \quad (17)$$

because it guarantees that the filtered covariance is symmetric and positive semi-definite [47].

D. Regulation

The regulator in the NMPC is based on certainty equivalence and a weighted least-squares objective with regularization on the inputs and the rate-of-movement of the inputs. We express the regulator as the optimal control problem

$$\min_{x,u} \ \phi_k = \phi_{z,k} + \phi_{u,k} + \phi_{\Delta u,k}, \quad (18a)$$

$$s.t. \quad x(t_k) = \hat{x}_{k|k}, \quad (18b)$$

$$\frac{d}{dt}x(t) = f(x(t), u(t), p), \quad t_k \le t \le t_k + T_p, \quad (18c)$$

$$z(t) = h(x(t), p), \quad t_k \le t \le t_k + T_p, \quad (18d)$$

$$u(t) = u_{k+j|k}, \quad j \in \mathcal{N}, \quad t_{k+j} \le t < t_{k+1+j}, \quad (18e)$$

$$u_l \le u_{k+j|k} \le u_u, \quad j \in \mathcal{N}, \quad (18f)$$

$$\Delta u_l \le \Delta u_{k+j|k} \le \Delta u_u, \quad j \in \mathcal{N}, \quad (18g)$$

where the objective function terms are

$$\phi_{z,k} = \frac{1}{2}\int_{t_k}^{t_k+T_p} \|z(t) - \bar{z}(t)\|_{Q_z}^2 \, dt, \quad (19a)$$

$$\phi_{u,k} = \frac{1}{2}\int_{t_k}^{t_k+T_p} \|u(t) - \bar{u}(t)\|_{Q_u}^2 \, dt, \quad (19b)$$

$$\phi_{\Delta u,k} = \frac{1}{2}\sum_{j=0}^{N-1} \|\Delta u_{k+j}\|_{\bar{Q}_{\Delta u}}^2 . \quad (19c)$$

The prediction and control horizon, T_p, is defined as $T_p = NT_s$ where N is the discrete prediction and control horizon and T_s is the sampling time. Furthermore, $\mathcal{N} = \{0, 1, \ldots, N-1\}$, $t_{k+j} = t_k + jT_s$ for $j \in \mathcal{N}$, and $t_{k+j+1} = t_{k+j} + T_s$. In order for the tuning to be consistent in the limit $T_s \to 0$, the rate-of-movement penalty is computed as $\bar{Q}_{\Delta u} = Q_{\Delta u}/T_s$. The units of Q_z, Q_u, and $Q_{\Delta u}$ are chosen such that ϕ_k is dimensionless.

The solution to the optimal control problem is the parameters, $\{\hat{u}_{k+j|k}\}_{j=0}^{N-1}$, defining the optimal manipulated

input trajectory, $u(t)$, the corresponding state variables, $x(t)$, and the outputs, $z(t)$, for $t \in [t_k, t_k + T_p]$. It is only the manipulated inputs corresponding to the first control interval that are implemented:

$$u(t) = u_k = \hat{u}_{k|k}, \qquad t_k \le t < t_{k+1} = t_k + T_s. \tag{20}$$

E. Parameter estimation

The parameters, θ, for the NMPC may be estimated by solution of [13]

$$\min_{\theta} V(\theta) = V(\theta; \{u_k, y_k\}), \tag{21a}$$

$$s.t. \quad \theta_l \le \theta \le \theta_u. \tag{21b}$$

For the parameter estimation problems solved in this work, the bound constraints (21b) are not active at the solution. However, including bound constraints can avoid searching in regions of the parameter space where the solution is not expected to be. In ML estimation, the objective function, $V(\theta)$, is the negative log-likelihood function,

$$V_{ML}(\theta) = \frac{1}{2}(N_e + 1)n_y \ln(2\pi) + \frac{1}{2}\sum_{k=0}^{N_e}\left(\ln\left[\det R_{e,k}\right] + e_k' R_{e,k}^{-1} e_k\right). \tag{22}$$

Note that in the case $\sigma(\boldsymbol{x}(t), u(t), p) = 0$ and the initial state is known exactly, $P_{0|-1} = 0$, the estimation reduces to output-error estimation similar to least-squares or regularized least-squares estimation [13].

We compute the (approximate) covariance, the standard deviation, and the correlation of the solution to the parameter estimation problem (21) as [48]

$$\Sigma_\theta = H^{-1}(\theta^*), \tag{23a}$$

$$\sigma_{\theta_i} = \sqrt{(\Sigma_\theta)_{i,i}}, \tag{23b}$$

$$\Gamma_\theta = \mathrm{diag}(\sigma_\theta)^{-1}\Sigma_\theta\,\mathrm{diag}(\sigma_\theta)^{-1}, \tag{23c}$$

where $H(\theta^*)$ is the Hessian matrix of (22) and Γ_θ is the correlation matrix.

F. Numerical solution of the optimal control problem

As the NMPC must be able to operate the CSTR at stable as well as unstable operating points, the single-shooting optimization (control vector parametrization) algorithm cannot be applied. Instead, we must use either a multiple-shooting algorithm [49] or the simultaneous method [50]. In the closed-loop simulation presented in Section IV, we use simultaneous collocation.

IV. Simulation Results

In this section, we present 1) parameter estimation results based on an ML approach and 2) a closed-loop simulation of NMPC based on the estimated parameters. We implement the NMPC algorithm using Python and C. We estimate $p = [\beta; k_0; E_a/R; \sigma_T]$. Fig. 2 shows a nominal simulation (black dashed), a stochastic simulation (blue solid), and simulated noisy measurements of the temperature (red dots) based on the stochastic simulation. When generating these measurements, we choose the feed flow rate (also shown in Fig. 2) to cover the steady state feed flow rates corresponding to the temperature setpoints used in the NMPC (see Fig. 3 and 4). The covariance of the measurement noise is $R_v(t_k, p) = 1.0$. Table II shows the parameter values estimated from the noisy temperature measurements together with the corresponding standard deviations and the correlation matrix.

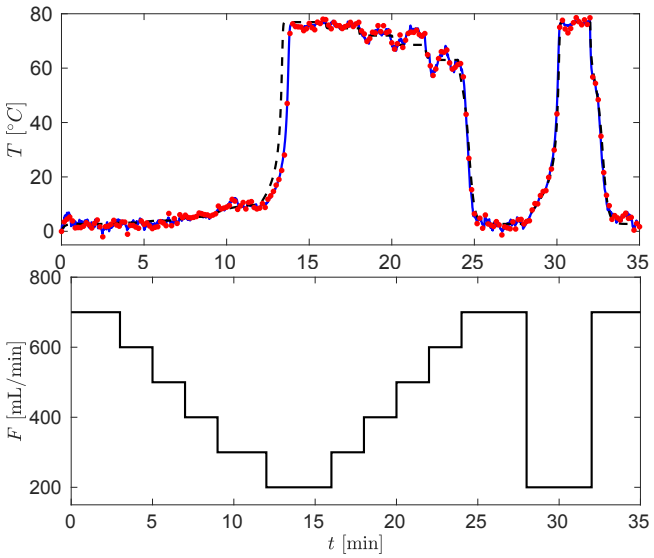

Fig. 2. Temperature measurements used in the parameter estimation.

We use the parameter estimates in the NMPC whereas the true system is represented by a stochastic simulation based on the nominal parameter values. The closed-loop simulation time interval is 20 min, and we use $T_s = 1$ s, $N = 180$, $Q_z = 10^4$ min^{-1}°C^{-2}, $Q_u = 0$ min mL^{-2}, $Q_{\Delta u} = 0.01$ min^3 mL^{-2}, $u_l = 0$ mL/min, $u_u = 800$ mL/min, $\Delta u_l = -800$ mL/min, and $\Delta u_u = 800$ mL/min. Fig. 3 shows the steady states of the deterministic model (6) together with seven selected steady states which constitute the setpoints, $\bar{T}(t)$, used in the NMPC (see Fig. 4).

Fig. 5 shows the closed-loop simulation of NMPC of the exothermic reaction in the adiabatic CSTR. The red circles denote temperature measurements. For both C_A, C_B, and T, the filtered estimates (blue solid) almost completely coincide with the true values (black solid), i.e. they are accurately estimated by the CD-EKF. The NMPC algorithm successfully tracks both the stable and the unstable steady state setpoints. It is more difficult for the NMPC to track steady states where the flow rate is high because this increases the size of the process noise term in (9c). Fig. 6 shows the computation time per control interval of the NMPC computations, and the worst-case computation time is 0.1 s.

V. Conclusions

In this paper, we present an NMPC algorithm for temperature tracking in a laboratory-scale adiabatic CSTR with an exothermic reaction. The NMPC algorithm is based on the CD-EKF, a simultaneous collocation method, and parameter

TABLE II

ML PARAMETER ESTIMATES.

Param.	Nom.	Estim.	Std. dev.	Correlation		
β	133.78	131.66	0.68			
$\log(k_0)$	24.6	24.43	0.43	-0.50		
E_a/R	8500.0	8448.5	74.458	-0.41	0.34	
σ_T	5.0	3.66	0.045	-0.098	0.35	-0.75

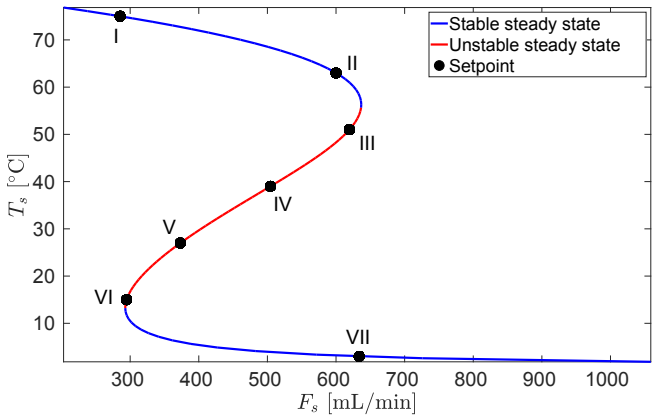

Fig. 3. Steady states (based on the nominal parameter values).

estimates obtained using an ML based algorithm. We describe a continuous-discrete stochastic model of the CSTR, which is used in the algorithms, and we demonstrate, using a closed-loop simulation, that the NMPC algorithm is able to track both stable and unstable steady states. Finally, we present simulation results which demonstrate that it is possible to estimate model parameters and to implement NMPC (based on the estimated parameters) for the laboratory-scale adiabatic CSTR.

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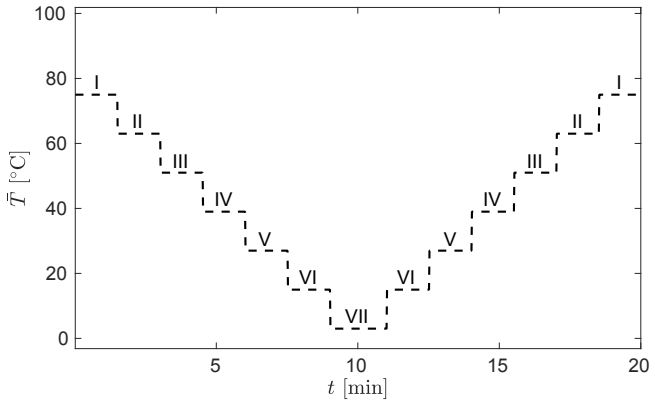

Fig. 4. Temperature target trajectory with operating points at both stable and unstable steady states.

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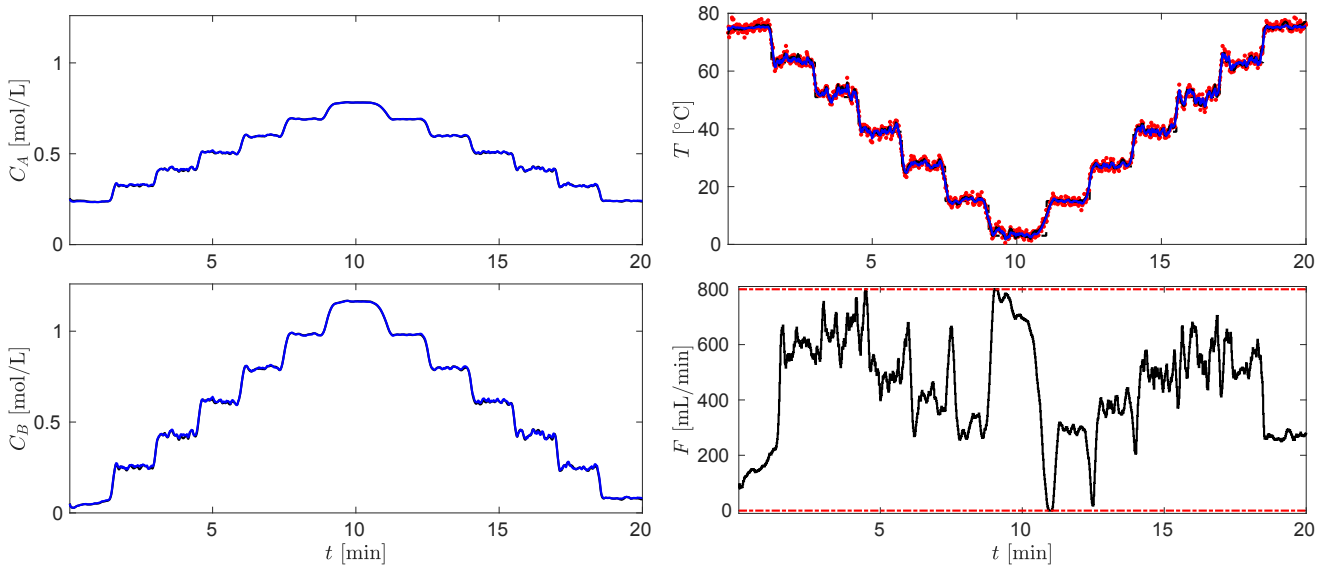

Fig. 5. Closed-loop simulation of NMPC of the adiabatic CSTR with an exothermic reaction.

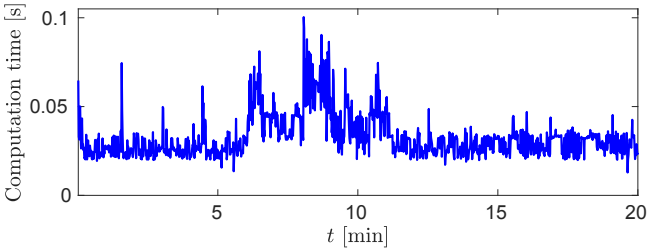

Fig. 6. CPU time per control interval for the NMPC computations (using the C implementation on an Ubuntu 16.04 LTS 64-bit workstation with eight Intel Core i7 3.60 GHz processors and 15.6 GB RAM).

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