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ON-LINE NEIGHBOURING-EXTREMAL CONTROLLER DESIGN FOR SETPOINT-TRANSITION IN PRESENCE OF UNCERTAINTY

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Abstract: In this paper we present an approach suitable for optimal constrained control of processes subject to uncertainties. The controller follows from a nominal solution of dynamic optimisation of a theoretical model which needs not to be very accurate. The nominal optimal control trajectory is identified as a sequence of arcs and boundaries. Real output measurements are used to cancel model mismatch and to augment nominal inputs on-line using state-feedback law. Neighbouring-extremal controller is designed to follow the nominal output trajectory in interior arcs using necessary conditions for optimality (NCO). Methodology will be implemented for setpoint-transition of van de Vusse reactor type. Finally, the performance of neighbouring-extremal controller will be benchmarked using several perturbation scenarios.

Keywords: NCO-tracking, dynamic optimisation problem, neighbouring-extremal, necessary conditions for optimality

1. INTRODUCTION

Batch and semi-batch plants are widely used in the industry and studied in academia for their non-linear behavior especially when consecutive and side reactions are presented. For these processes, the mathematical model is known with limited accuracy and controller design has to deal with variations. In the presence of model mismatches and uncertainties there are demands on advanced process control schemes.

In the last decade, approaches which deals with limited model accuracy and with highly non-linear behavior have been addressed. The presence of uncertainty can be solved using multiple approaches: Linear-Quadratic-Gaussian control (Zhou et al., 1995), NCO-tracking (Srinivasan and Bonvin, 2007; Srinivasan et al., 2003; Srinivasan and Bonvin, 2004; François et al., 2007), robust H_∞ loop-shaping (McFarlane and Glover, 1989; Zhou et al., 1995), adaptive control (Åström and Wittenmark, 1983 1989), robust control (Bakošová and Puna, 2007; Bakošová et al., 2008), or whole process re-optimisation: NMPC (Garcia et al., 1989; Allgöwer and Zheng, 2000; Abel and Marquardt, 1998). Most of these methods incorporate direct output measurements or reconstruct them with observers. There is a difference in the controller design and the implementation: if design is performed on-the-fly or can be done off-line; or if main controller implementation is simple and can by applied on commonly used hardware in the industry. Next limitation for controllers which perform on-line is sampling rate, especially for NMPC where whole optimisation process must be repeated, or for LQG and for adaptive control where controller parameters are also updated at each sampling period.

In this work, we apply NCO-tracking approach. Nominal optimal solution is used to calculate state-feedback gain matrices for state variations around the nominal trajectory. The augmented action is determined at each sampling time by adjustment of the nominal input profile with the pre-computed gain and the actual difference between the measurements and the nominal output profiles. The implementation then consist of the storage of the nominal input, output profiles, and the gain matrices for state-feedback at sampling periods in which the controls will be updated. In addition, a short sampling time allows to control the processes with the fast dynamic behavior.

The proposed NCO-tracking controller is applied on setpoint-transition of van de Vusse reactor model (Klatt and Engell (1993)) in presence of parameter and initial state variations.

2. THEORETICAL BACKGROUND

2.1 *Optimal Control Problem*

We assume the following dynamic optimisation problem with simple bound constraints:

$$\min J = \Phi(\boldsymbol{x}(t_f)) + \int_0^{t_f} L(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\theta}) \mathrm{d}t \quad (1)$$

$s.t.$

$$\dot{\boldsymbol{x}} = \boldsymbol{F}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{\theta}); \quad \boldsymbol{x}(0) = \boldsymbol{x}_0 \quad (2)$$

$$\boldsymbol{u}^L \leq \boldsymbol{u}(t) \leq \boldsymbol{u}^U \quad (3)$$

where t stands for the time variable, t_f the fixed time, $\boldsymbol{u}$ the control vector, $\boldsymbol{x}$ the state vector with initial state $\boldsymbol{x}_0$, $\boldsymbol{\theta}$ the vector of uncertain time-invariant parameters, $\boldsymbol{F}$ the system dynamics, J the scalar cost function to be minimised, Φ the terminal cost function, and L integral cost function. All functions in (1)–(3) are assumed to be continuous and continuously differentiable with respect to their arguments. Then, there exists an unique optimal control solution $\boldsymbol{u}^*(t)$ for given nominal parameter values $\bar{\boldsymbol{\theta}}$. This solution may consist of several arcs: boundary arcs (trajectories lie on the constraints) and interior arcs (trajectories within constraints).

2.2 *Necessary Conditions for Optimality*

According to (Bryson and Ho, 1975), the Hamiltonian function H is defined as follows

$$H(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}, \boldsymbol{\lambda}, \boldsymbol{\mu}^L, \boldsymbol{\mu}^U) = L(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta}) + \quad (4)$$
$$+ \boldsymbol{F}(\boldsymbol{x}, \boldsymbol{u}, \boldsymbol{\theta})^T \boldsymbol{\lambda} + \boldsymbol{\mu}^{L^T}(\boldsymbol{u}^L - \boldsymbol{u}) + \boldsymbol{\mu}^{U^T}(\boldsymbol{u}^U - \boldsymbol{u})$$

where $\boldsymbol{\lambda}$ denotes adjoint vector function given by

$$\dot{\boldsymbol{\lambda}} = -\boldsymbol{H}_x = -\boldsymbol{F}_x^T \boldsymbol{\lambda} - \boldsymbol{L}_x; \ \boldsymbol{\lambda}(t_f) = \boldsymbol{\Phi}_x(t_f), \quad (5)$$

The vectors and matrices with subscript $_x$ denote partial derivatives of the corresponding variable with respect to state $\boldsymbol{x}$.

Lagrange multiplier vector functions are denoted by $\boldsymbol{\mu}^L$, $\boldsymbol{\mu}^U$ and satisfy following conditions

$$\boldsymbol{\mu}^{L^T}(\boldsymbol{u}^L - \boldsymbol{u}); \qquad \boldsymbol{\mu}^L \geq \boldsymbol{0} \quad (6)$$
$$\boldsymbol{\mu}^{U^T}(\boldsymbol{u}^U - \boldsymbol{u}); \qquad \boldsymbol{\mu}^U \geq \boldsymbol{0}. \quad (7)$$

Note that Lagrange multipliers are equal to zero $\boldsymbol{\mu}^L = \boldsymbol{\mu}^U = \boldsymbol{0}$ along an interior arc, while they are non-zero $\boldsymbol{\mu}_i^L \neq \boldsymbol{\mu}_i^U \neq \boldsymbol{0}$, $i \in \{1, ..., n_u\}$ along a boundary arc. The first and second order necessary conditions of optimality for the problem described by (1)–(3) are of the form

$$\boldsymbol{H}_u = \boldsymbol{L}_u + \boldsymbol{F}_u^T \lambda - \boldsymbol{\mu}^L + \boldsymbol{\mu}^U = \boldsymbol{0}; \quad \boldsymbol{H}_{uu} > \boldsymbol{0}, \quad (8)$$

where the positive definite matrix $\boldsymbol{H}_{uu}$ denotes the second partial derivative of H with respect to control $(\partial^2 H / \partial \boldsymbol{u}^2)$.

2.3 *Neighbouring-Extremal Control for Nonsingular Problems*

Even a small disturbance in the model parameters results in changes of the optimal control trajectory $\boldsymbol{u}^*(t)$, $0 \leq t \leq t_f$. Let us consider the first-order approximation for augmented optimal trajectory of a perturbed control

$$\boldsymbol{u}(t; \zeta) = \boldsymbol{u}^*(t) + \zeta \delta \boldsymbol{u}(t) + \boldsymbol{o}(\zeta), \quad (9)$$

and use theory of neighbouring extremal (Bryson and Ho, 1975) for computing the correction $\delta \boldsymbol{u}$ in a such manner that the first-order variation of necessary conditions for optimality heads to zero along the augmented control $\boldsymbol{u}^*(t) + \zeta \delta \boldsymbol{u}(t)$. The correction of $\delta \boldsymbol{u}$ is computed as the solution to the variational LQ minimum problem (Breakwell et al., 1963; Kelley et al., 1963)

$$\min \delta^2 J(\delta \boldsymbol{u}) = \frac{1}{2} \delta \boldsymbol{x}(t_f)^T \boldsymbol{\Phi}_{xx}^* \delta \boldsymbol{x}(t_f) +$$
$$+ \frac{1}{2} \int_0^{t_f} \begin{pmatrix} \delta \boldsymbol{x} \\ \delta \boldsymbol{u} \end{pmatrix}^T \begin{pmatrix} \boldsymbol{H}_{xx}^* & \boldsymbol{H}_{xu}^* \\ \boldsymbol{H}_{ux}^* & \boldsymbol{H}_{uu}^* \end{pmatrix} \begin{pmatrix} \delta \boldsymbol{x} \\ \delta \boldsymbol{u} \end{pmatrix} \mathrm{d}t \quad (10)$$

$s.t.$

$$\delta \dot{\boldsymbol{x}} = \boldsymbol{F}_x^* \delta \boldsymbol{x} + \boldsymbol{F}_u^* \delta \boldsymbol{u} + \boldsymbol{F}_\theta^* \delta \boldsymbol{\theta}; \quad (11)$$
$$\delta \boldsymbol{x}(0) = \delta \boldsymbol{x}_0 \quad (12)$$
$$\boldsymbol{u}^L - \boldsymbol{u}^*(t) \leq \delta \boldsymbol{u}(t) \leq \boldsymbol{u}^U - \boldsymbol{u}^*(t). \quad (13)$$

that corresponds to minimisation of the second-order variation of the cost functional subject to the linearised dynamics. A superscript * (e.g. $\boldsymbol{H}_{uu}^*$) means that the variable is evaluated upon nominal trajectories $\boldsymbol{u}^*(t), \boldsymbol{x}^*(t), \boldsymbol{\lambda}^*(t)$, for $0 \leq$

$t \le t_f$. A perturbed optimal control $\boldsymbol{u}(t;\zeta)$ exists in a neighbourhood of $\zeta = 0$, provided that the LQ problem (10)–(13) itself has an optimal solution (Pesh, 1990). The control variation $\delta\boldsymbol{u}$ satisfying the strengthened Legendre-Clebsch condition of positive definiteness $\boldsymbol{H}^*_{uu} > \boldsymbol{0}$ and for unconstrained problems $\boldsymbol{\mu}^L(t) = \boldsymbol{\mu}^U(t) = \boldsymbol{0}$ is then given by

$$\delta\boldsymbol{u}(t) = -(\boldsymbol{H}^*_{uu})^{-1}(\boldsymbol{H}^*_{ux}\delta\boldsymbol{x}(t) + \boldsymbol{F}^{*T}_u\delta\boldsymbol{\lambda}(t) + \boldsymbol{H}^*_{u\theta}\delta\boldsymbol{\theta}) \quad (14)$$

where $\delta\boldsymbol{x}(t)$ and $\delta\boldsymbol{\lambda}(t)$ satisfy the following two-point boundary-value problem (TPBVP)

$$\begin{pmatrix}\delta\dot{\boldsymbol{x}}(t)\\ \delta\dot{\boldsymbol{\lambda}}(t)\end{pmatrix} = (\boldsymbol{T}_x \ \boldsymbol{T}_\lambda)\begin{pmatrix}\delta\boldsymbol{x}(t)\\ \delta\boldsymbol{\lambda}(t)\end{pmatrix} + \boldsymbol{T}_\theta\delta\boldsymbol{\theta} \quad (15)$$

$$\delta\dot{\boldsymbol{x}}(0) = \delta\dot{\boldsymbol{x}}_0, \quad \delta\dot{\boldsymbol{\lambda}}(t_f) = \boldsymbol{\Phi}^*_{xx}\delta\boldsymbol{x}(t_f) \quad (16)$$

where

$$\boldsymbol{T}_x = \begin{pmatrix}\boldsymbol{F}^*_x - \boldsymbol{F}^*_u(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{H}^*_{ux}\\ -\boldsymbol{H}^*_{xx} + \boldsymbol{H}^*_{xu}(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{H}^*_{ux}\end{pmatrix} \quad (17)$$

$$\boldsymbol{T}_\lambda = \begin{pmatrix}-\boldsymbol{F}^*_u(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{F}^{*T}_u\\ -(\boldsymbol{F}^*_x - \boldsymbol{F}^*_u(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{H}^*_{ux})^T\end{pmatrix} \quad (18)$$

$$\boldsymbol{T}_\theta = \begin{pmatrix}\boldsymbol{F}^*_\theta - \boldsymbol{F}^*_u(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{H}^*_{u\theta}\\ -\boldsymbol{H}^*_{x\theta} + \boldsymbol{H}^*_{xu}(\boldsymbol{H}^*_{uu})^{-1}\boldsymbol{H}^*_{u\theta}\end{pmatrix} \quad (19)$$

Furthermore, a neighbouring-extremal state-feedback law can alternatively be designed via backward sweep method (Bryson and Ho, 1975), that assumes a linear relation between the state and adjoint variables and parameters $\delta\boldsymbol{\lambda}(t) = \boldsymbol{S}_x(t)\delta\boldsymbol{x}(t) + \boldsymbol{S}_\theta(t)\delta\boldsymbol{\theta}(t)$

$$\delta\boldsymbol{u} = -\boldsymbol{K}_x(t)\delta\boldsymbol{x}(t) - \boldsymbol{K}_\theta(t)\delta\boldsymbol{\theta}(t) \quad (20)$$

$$\boldsymbol{K}_x(t) = (\boldsymbol{H}^*_{uu})^{-1}(\boldsymbol{H}^*_{ux} + \boldsymbol{F}^{*T}_u\boldsymbol{S}_x(t)) \quad (21)$$

$$\boldsymbol{K}_\theta(t) = (\boldsymbol{H}^*_{uu})^{-1}(\boldsymbol{H}^*_{u\theta} + \boldsymbol{F}^{*T}_u\boldsymbol{S}_\theta(t)) \quad (22)$$

$$\dot{\boldsymbol{S}}_x(t) = -\boldsymbol{H}^*_{xx} - \boldsymbol{S}_x(t)\boldsymbol{F}^*_x - \boldsymbol{F}^{*T}_x\boldsymbol{S}_x(t) + (-\boldsymbol{H}^*_{xu} + \boldsymbol{S}_x(t)\boldsymbol{F}^*_u)\boldsymbol{K}_x(t) \quad (23)$$

$$\boldsymbol{S}_x(t_f) = \boldsymbol{\Psi}^*_{\boldsymbol{xx}} \quad (24)$$

$$\dot{\boldsymbol{S}}_\theta(t) = -\boldsymbol{H}^*_{x\theta} - \boldsymbol{S}_\theta(t)\boldsymbol{F}^*_x - \boldsymbol{F}^{*T}_x\boldsymbol{S}_\theta(t) + (-\boldsymbol{H}^*_{xu} + \boldsymbol{S}_x(t)\boldsymbol{F}^*_u)\boldsymbol{K}_\theta(t) \quad (25)$$

$$\boldsymbol{S}_\theta(t_f) = \boldsymbol{0} \quad (26)$$

It is implicitly assumed for constrained control sequence that the uncertainty is sufficiently small for the perturbed optimal control to have the same sequence of constrained and unconstrained arcs as the nominal solution. Neighbouring-extremal is obtained similarly to unconstrained case: by solving either TPBVP or Riccati equation with possible discontinuities at junction times between constrained and unconstrained arcs. In practice, this assumption does not cause an apparent performance loss.

3. DESIGN EXAMPLE

3.1 *Plant model*

We consider a chemical reactor with side and follow-up reactions – van de Vusse scheme (van de Vusse, 1964), where desired cyclopentenol (B) is produced from cyclopentadiene (A) by acid-catalysed electrophilic addition of water in dilute solution. In addition, cyclopentanediol (C) is consecutive product of cyclopentenol (B) and addition of another water molecule, and dicyclopentadiene (D) is a side product of strong Diels-Alder reaction between the educt and the product.

The plant model presented in Klatt and Engell (1993) consists of material balances of the reactant (A) and the product (B) as well as energy balances of the plant and the cooling jacket as follows

$$\dot{c_A} = -k_1(T)c_A - k_2(T)c_A^2 + (c_{in} - c_A)u_1, \quad (27a)$$

$$\dot{c_B} = k_1(T)(c_A - c_B) - c_B u_1, \quad (27b)$$

$$\dot{T} = h_r(c_A, c_B, T) + \alpha(T_c - T) + (T_{in} - T)u_1, \quad (27c)$$

$$\dot{T}_c = \beta(T - T_c) + \gamma u_2 \quad (27d)$$

with reaction enthalpy given as

$$h_r(c_A, c_B, T) = -\sigma[k_1(T)(c_A\Delta H_{AB} + c_B\Delta H_{BC}) + k_2(T)c_A^2\Delta H_{AD}] \quad (28)$$

and kinetic rate constants are expressed as Arrhenius functions of temperature in °C.

$$k_i(T) = k_{i0}\mathrm{e}^{-\frac{\frac{E_i}{R}}{T+273.15}}, \quad i = 1, 2. \quad (29)$$

We define states variables as $\boldsymbol{x} = [c_A \ c_B \ T \ T_c]^T$. The model parameters are defined in Table 1.

The controlled inputs are input flow rate q normalised by the volume of the plant V_R and cooling system capacity $\dot{Q}$. Both inputs are constrained in the form of lower and upper bounds

$$u_1 = \frac{q}{V_R}, \quad 5\,\mathrm{h}^{-1} \le u_1 \le 35\,\mathrm{h}^{-1} \quad (30a)$$

$$u_2 = \dot{Q}, \quad -8500\,\mathrm{kJ.h}^{-1} \le u_1 \le 0\,\mathrm{kJ.h}^{-1} \quad (30b)$$

The product concentration and the plant temperature were chosen as controlled outputs

$$y_1 = c_B, \qquad y_2 = T. \quad (31)$$

The aim of the optimisation problem is to drive reactor's operational conditions from the original steady-state to another operational point. The particular numeric values of states and inputs at the operational points are summarised in Table 1. The transition is performed with several scenarios, whereby the desired stationary point is always reached without violating input constraints. Thus, the performance index is defined as LQ integral

Table 1. Parameters for plant model and the main stationary setpoints

$\alpha = 30.8285$ [h^{-1}]
$\beta = 86.688$ [h^{-1}]
$\gamma = 0.1$ [K.kJ^{-1}]
$\sigma = 3.556 \times 10^{-4}$ [m^3.K.kJ^{-1}]
$k_{10} = 1.287 \pm 20\% \times 10^12$ [h^{-1}]
$\frac{E_1}{R} = 9758.3$
$k_{20} = 9.043 \pm 20\% \times 10^6$ [m^3.mol^{-1}.h^{-1}]
$\frac{E_2}{R} = 8560$
$\Delta H_{AB} = 4.2$ [kJ.mol^{-1}]
$\Delta H_{BC} = -11$ [kJ.mol^{-1}]
$\Delta H_{AD} = -41.85$ [kJ.mol^{-1}]
$c_{in} = 5100 \pm 20\%$ [mol.m^{-3}]
$T_{in} = 104.9$ [K]
$c_{A,sp_1} = 3517.5$ [mol.m^{-3}]
$c_{B,sp_1} = 740$ [mol.m^{-3}]
$T_{sp_1} = 87$ [K]
$T_{c,sp_1} = 79.8$ [K]
$u_{1,sp_1} = 8.256$ [h^{-1}]
$u_{2,sp_1} = -6239$ [kJ.h^{-1}]
$c_{A,sp_2} = 2985$ [mol.m^{-3}]
$c_{B,sp_2} = 960$ [mol.m^{-3}]
$T_{sp_2} = 106$ [K]
$T_{c,sp_2} = 100.7$ [K]
$u_{1,sp_2} = 18.037$ [h^{-1}]
$u_{2,sp_2} = -4556$ [kJ.h^{-1}]

functional where the normalised tracking error variations between original and new stationary point are driven to zero in a finite time tf = 20min. The cost function then reads

$$\min_u J_0 = \int_0^{t_f} (\hat{\boldsymbol{y}}^T \boldsymbol{Q}_I \hat{\boldsymbol{y}} + \hat{\boldsymbol{u}}^T \boldsymbol{R}_I \hat{\boldsymbol{u}}) \mathrm{d}t \tag{32}$$

where

$$\hat{\boldsymbol{y}} = \begin{bmatrix} \dfrac{c_B - c_{B,sp_2}}{c_{B,sp_2}} & \dfrac{T - T_{sp_2}}{T_{sp_2}} \end{bmatrix}^T \tag{33}$$

$$\hat{\boldsymbol{u}} = \begin{bmatrix} \dfrac{u_1 - u_{1,sp_2}}{u_{1,sp_2}} & \dfrac{u_2 - u_{2,sp_2}}{u_{2,sp_2}} \end{bmatrix}^T \tag{34}$$

and matrices $\boldsymbol{Q}_I$ and $\boldsymbol{R}_I$ are positive-definite and symmetric weight matrices

$$\boldsymbol{Q}_I = \begin{bmatrix} q_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & q_n \end{bmatrix}, \quad \boldsymbol{R}_I = \begin{bmatrix} r_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & r_n \end{bmatrix} \tag{35}$$

3.2 *Open-loop Optimal Control*

To find the optimal sequence of arcs, a numerical solution of dynamic optimisation problem (27)–(32) was obtained. We employed our in-house dynamic optimisation package based on CVP approach and implemented in MATLAB environment: SUNDIALS toolbox for the forward and backward numerical integration of differential equations and MATLAB version of SNOPT for NLP solution. For this particular case study, we parametrise both control inputs piecewise on 40 stages of equal width (30 s).

The optimal control profiles of more aggressive control scenario is depicted in the third and fourth graph in Figure 1 (dash-dotted line). We can see that u_1 starts on upper bound and u_2 on lower bound and then they are followed by an interior arc. Similarly, the optimal control profiles of less aggressive control scenario are depicted in the third and fourth image in Figure 3. Observe, that upper bound of u_1 and lower bound for u_2 are shorter and the interior arcs are longer compared to more aggressive scenario. Along the interior arcs the following necessary conditions (see (8)) must hold for u_1 and u_2

$$H_{u_1} = 2\left(\frac{u_1 - u_{1,sp_2}}{u_{1,sp_2}^2}\right) r_1 + \lambda_{c_A}(c_{in} - c_A) - \lambda_{c_B} c_B + \lambda_T (T_{in} - T) = 0 \tag{36}$$

$$H_{u_2} = 2\left(\frac{u_2 - u_{2,sp_2}}{u_{2,sp_2}^2}\right) r_2 + \lambda_{T_c}\gamma = 0 \tag{37}$$

These equations give expressions for optimal control trajectories

$$u_1^* = \frac{\frac{2}{u_{1,sp_2} r_1} - \lambda_{c_A}(c_{in} - c_A)}{\frac{2r_1}{u_{1,sp_2}^2}} + \frac{\lambda_{c_B} c_B - \lambda_T (T_{in} - T)}{\frac{2r_1}{u_{1,sp_2}^2}} \tag{38}$$

$$u_2^* = \frac{\frac{2}{u_{2,sp_2} r_2} - \lambda_{T_c}\gamma}{\frac{2r_2}{u_{2,sp_2}^2}} \tag{39}$$

Note that optimal control trajectories u_1^* and u_2^* of the nominal problem are computed iteratively because adjoints become unstable during forward integration. The procedure is as follows. Dynamic process (27)–(29) is integrated forward, the controls are explicitly given from (38)–(39). The unknown adjoint variables $\boldsymbol{\lambda}^*$ are taken from the nominal solution and then they are approximated during forward integration. Subsequently, in next iteration step $\boldsymbol{\lambda}$ are corrected during backward integration. At final stage, $\boldsymbol{\lambda}_{t_f}$ at final time must be equal to $\boldsymbol{\lambda}(t_f)$ given by the optimal problem.

3.3 *Neighbouring-extremal Feedback Control*

The standard approach of real-time optimisation consists of process model update using available measurements and followed by numerical reoptimisation that provides input to the plant. Instead of reoptimisation, the so called NCO-tracking approach is used in this work. The main idea is based on the fact that optimality requires meeting necessary conditions for optimality. NCO-tracking secures optimal operation via feedback without solving dynamic optimisation problem in real-time. The objective of NCO-tracking is to find zero gradients and to meet active constraints in presence of uncertainty that can be model mismatch or process disturbances. This will be handled on-line via neighbouring-extremal controller.

3.3.1. *NE controller design* In the section 3.2 we did analysis of the optimal control profiles of more and less aggressive scenario and we found a sequence of boundary and interior arcs that apply to the open-loop solution of the problem (1)–(3). Both inputs consist of a boundary arc followed by an interior arc, in more aggressive scenario and of the one interior arc, in less aggressive scenario. The optimal inputs (u_1^* and u_2^*) along the interior arcs, are given by (38)–(39). The switching times, between particular boundary arcs and interior arcs are taken from nominal solution. We assume that they are fixed and they are perturbated minimally. Only the interior arcs are updated in presence of uncertainty.

The NE controller can be designed in two different ways (i) by solving TPBVP described by (15), (ii) by solving matrix Riccati equation (20). From both we get the gain matrices $\boldsymbol{K}_x$ and $\boldsymbol{K}_\theta$ that determine optimal control response. This drives the perturbed system towards original optimal output trajectory.

3.3.2. *Performance of NE controller* To assess the performance of proposed NE controller two scenarios are studied: more and less aggressive control.

Performance will be demonstrated with parameter uncertainty of inlet concentration c_{in}, vector of initial conditions $\boldsymbol{x}_0$, and kinetic rate constants k_{10}, k_{20} that may vary in range of $\pm 20\%$. The weight coefficients are $r_1 = r_2 = 1$ and state penalisation is $q_1 = q_2 = 500$ for more aggressive and $q_1 = q_2 = 200$ for less aggressive scenario, respectively.

The corresponding control and response for various coefficient disturbances can be found in Figures 1–2 for more aggressive, and in Figures 3–4 for less aggressive scenario. Note that open-loop nominal controller is clearly unable to deal with presence of uncertainties, the desired setpoint is not reached in any case. In contrary, proposed NCO-tracking controller recovers influence of uncertainty and the reactor ends up at desired setpoint independent on controller aggressiveness. Same behavior can be observed in other simulations with various combinations of uncertainty, where the following cases were simulated:

C1 : $\Delta c_{in} = 20\%, \Delta k_{10} = -20\%, \Delta k_{20} = 10\%, \Delta x_0 = -20\%$

C2 : $\Delta c_{in} = -10\%, \Delta k_{10} = -20\%, \Delta k_{20} = 10\%$

C3 : $\Delta c_{in} = 10\%, \Delta k_{10} = -10\%, \Delta k_{20} = -20\%$

C4 : $\Delta c_{in} = -20\%, \Delta x_0 = 10\%$

In these cases, optimality loss is fully recovered while the input constraints remain satisfied and performance follow closely copy the original one.

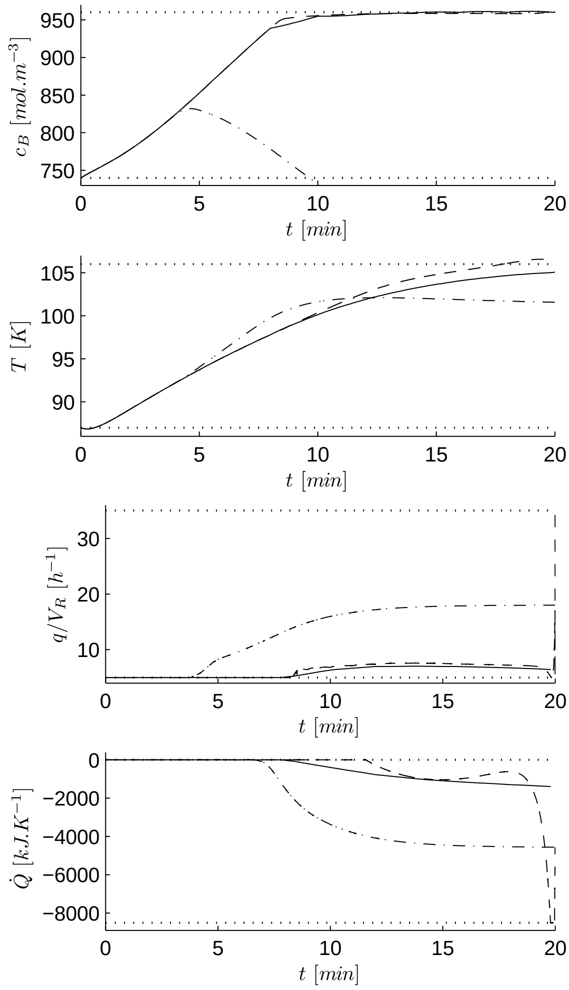

Fig. 1. More aggressive control with the perturbation scenario: $\Delta c_{in} = -20\%, \Delta k_{10} = -20\%, \Delta k_{20} = -20\%$. Dashed line: NCO tracking inputs; Solid line: optimal inputs to the perturbed problem; Dash-dotted line: open-loop nominal inputs

4. CONCLUDING REMARKS

Design of controller which tracks necessary conditions for optimality was presented and applied to the van de Vusse reactor model (Klatt and Engell, 1993) with uncertainties which may occur under realistic conditions. The dynamic optimisation problem was transformed to the control problem through nominal input decomposition into sequence of boundary and interior arcs.

Neighboring-extremal controller was introduced to track the necessary conditions for optimality

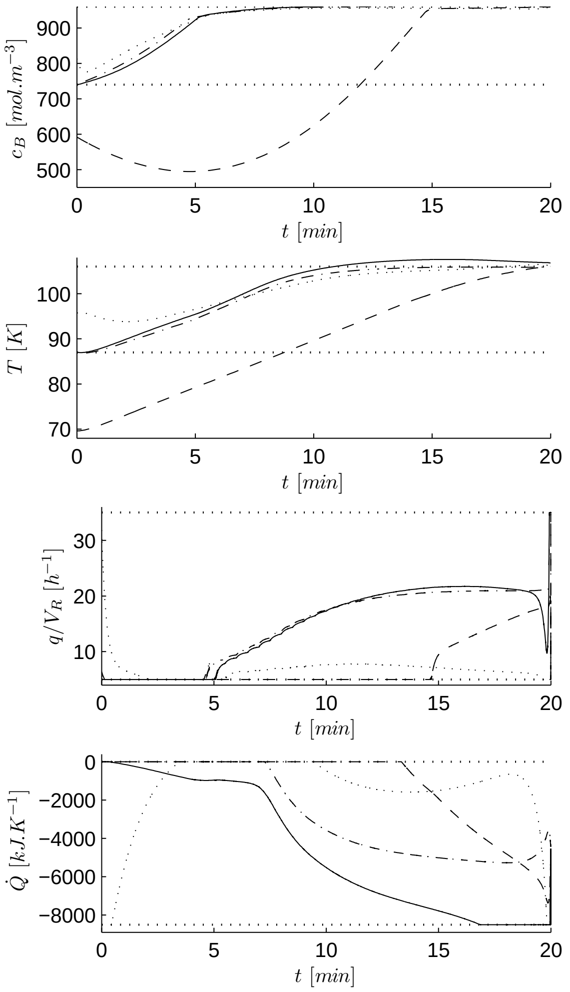

Fig. 2. Performance of NCO tracking with more aggressive control. Dashed line: C1, solid line: C2, dash-dotted line: C3, dotted line: C4.

along interior arcs. The nominal optimal control as well as state-feedback law were calculated offline for all variations of states and parameters and for a small neighbourhood around nominal trajectories. The simulation results shown in Figures 1–4 confirmed attractivity of proposed solution whereas desired setpoint was reached and inputs were within limits for both more and less aggressive control criterion. Opimality loss was successfully recovered in presence of parameter uncertainties. The approach is well-suited especially for the real-time optimisation with short sampling times.

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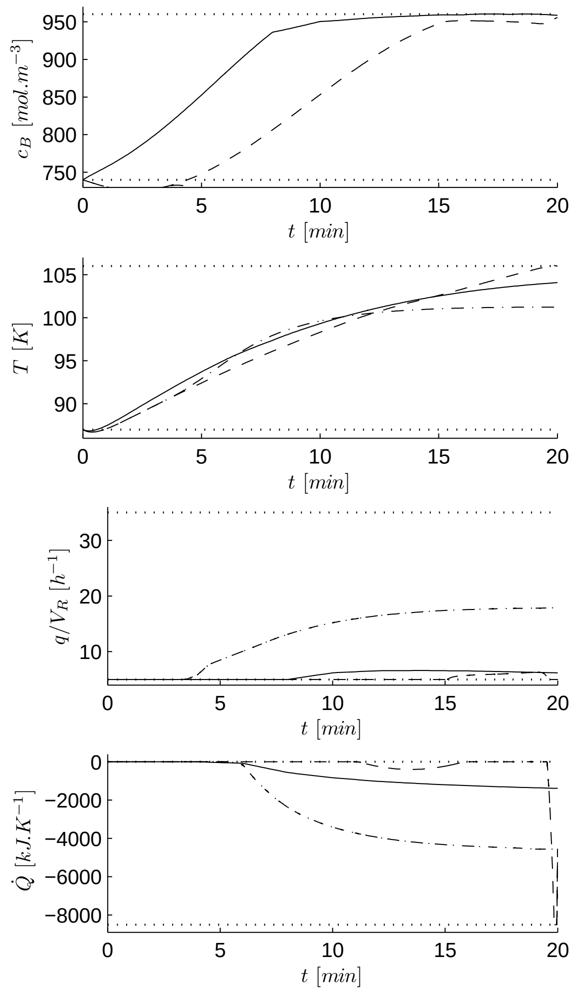

Fig. 3. Less aggressive control with the perturbation scenario: $\Delta c_{in} = -20\%, \Delta k_{10} = -20\%, \Delta k_{20} = -20\%$. Dashed line: NCO tracking inputs; Solid line: optimal inputs to the perturbed problem; Dash-dotted line: open-loop nominal inputs

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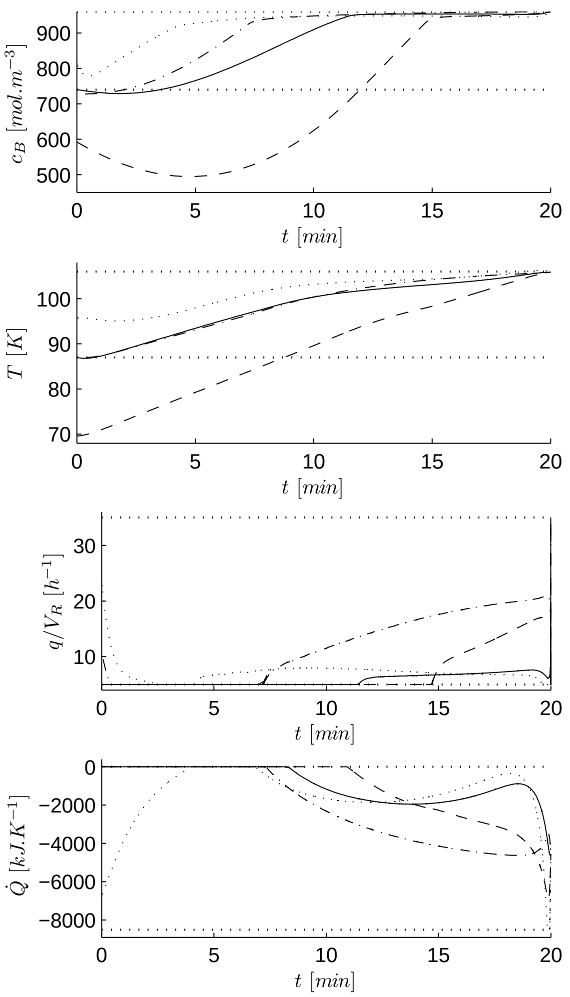

Fig. 4. Performance of NCO tracking with more aggressive control. Dashed line: C1, solid line: C2, dash-dotted line: C3, dotted line: C4.

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