A Strategy for the Exact Solution of Multiparametric/Explicit Quadratically Constrained NMPC Problems *

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Abstract: Multiparametric programming has proven to be an efficient strategy to alleviate the computational burden of solving model predictive control problems online. Recently, it has been shown that through a second-order Taylor approximation to the Basic Sensitivity Theorem, the exact solution of multiparametric/explicit quadratically constrained nonlinear model predictive control problems is enabled. As a result, the state space is nonlinearly partitioned, and the optimal control actions are expressed as nonlinear functions of the states of the system. In this work, an algorithm for the complete exploration of the parameter space and the derivation of the parametric solution of the aforementioned problem is provided. The proposed strategy is utilized to implicitly explore the parameter space by identifying the unique and optimal active sets which describe the parametric solution. The applicability of the presented methodology is demonstrated on a regulation problem of a nonisothermal continuously-stirred tank reactor near an unstable steady-state.

Keywords: Model predictive and optimization-based control, Real time optimization and control, Nonlinear process control.

1. INTRODUCTION

Multiparmetric/explicit model predictive control (mpMPC or eMPC) is a control strategy, which aims to optimally control constrained systems. In contrast to traditional model predictive control (MPC), the online optimization problem is solved offline through multiparametric programming algorithms. The solution of the aforesaid problem results in the map of optimal partitions of the parameter space (critical regions), where the optimal control actions are expressed as a function of the parameters of the system. Hence, the solution of the MPC problem reduces from a repetitive solution of an optimization formulation at each sampling instant to a set of function evaluations. In this respect, mpMPC can be implemented for the control of various real-time optimization applications, such as embedded control systems (Dua and Pistikopoulos (1999)).

Since the last two decades and its first inception (Bemporad et al. (2002)), research efforts in the mpMPC literature have primarily focused on the optimal control problems which involve a quadratic performance index and linear constraints for continuous and hybrid systems. Such problems require the solution of a multiparametric Quadratic (mpQP) or Mixed-Integer Quadratic Programming (mp-MIQP) problem (Bemporad et al. (2002), Oberdieck and Pistikopoulos (2015)). However, nonlinearities which can

appear in the problem description, give rise to a nonlinear multiparametric program (mpNLP). In the cases where these expressions realize themselves as quadratic functions, a multiparametric Quadratically Constrained Quadratic Program (mpQCQP) needs to be solved. In a MPC framework, such terms could be ellipsoidal terminal sets, quadratic constraints on the inputs/states or quadratic functions which are used to approximate general nonlinear equations in the control formulation.

Contributions to address the solution of mpQCQPs have been based on algorithms to solve general mpNLPs. However, the solution of mpNLPs or mpMINLPs is very challenging and the exact solution of such classes of problems, without an *a posteriori* comparison of all feasible solutions, has not been provided. In particular, even though the initial contributions in mpNLP had been very influential (Fiacco (1976), Fiacco et al. (1983)), the majority of the subsequent efforts for the solution of these problems has been based on approximations of the original optimization formulation (Dua and Pistikopoulos (1999), Johansen (2004), Grancharova et al. (2007), Katz et al. (2020)) or partially require an online solution element (Fotiou et al. (2006)). Recently, solution methods have been presented (Charitopoulos and Dua (2016), Charitopoulos et al. (2019)), based on Gröbner Bases and the analysis of critical solutions.

In this work and based on our previous contribution (Diangelakis et al. (2018)), we focus on convex mpQCQPs and provide an algorithm for the exact solution of quadratically

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constrained nonlinear model predictive control (NMPC) problems and the derivation of the optimal map of solutions. We illustrate the applicability of the proposed approach on the optimal regulation of a nonisothermal continuously-stirred tank reactor (CSTR) around an unstable steady-state, taking into account economic criteria.

2. MULTIPARAMETRIC PROGRAMMING

2.1 Explicit Model Predictive Control

In the seminal contribution of (Bemporad et al. (2002)), it was shown that a MPC problem can be reformulated into a mpQP. Assume the following MPC problem as in (1)

$$\min_{u} J = x_{N}^{T} P x_{N} + \sum_{k=1}^{OH-1} x_{k}^{T} Q R x_{k} \sum_{k=0}^{CH-1} u_{k}^{T} R u_{k}$$
s.t. $x_{k+1} = A x_{k} + B u_{k} + C d_{k}$
 $y_{k} = D x_{k} + E u_{k}$ (1)
 $\frac{x}{2} \leq x_{k} \leq \overline{x}$
 $\frac{u}{2} \leq u_{k} \leq \overline{u}$
 $\frac{y}{2} \leq y_{k} \leq \overline{y}$
 $\frac{d}{2} \leq d_{k} \leq \overline{d}$

In formulation (1), $x \in \mathbb{R}^{n_x}$ is the vector of the states of the system, $u \in \mathbb{R}^{n_u}$ is the vector of control actions, $y \in \mathbb{R}^{n_y}$ is the vector of the outputs, $d \in \mathbb{R}^{n_d}$ is the vector of measured disturbances, QR and R are the weights of the controller, P is derived from the solution of the discrete Riccati equation, and OH and CH are the output and control horizons respectively. The matrices A, B, C, D, E define the linear discrete state-space model describing a given process, where the index k denotes the sampling instant. In a multiparametric programming setting, the aforementioned states, outputs and disturbances are treated as uncertain bounded parameters incorporated in (2)

$$\min_{u} f(u,\theta) = \frac{1}{2}u^{T}Qu + u^{T}H^{T}\theta + \theta^{T}Q_{\theta}\theta + c_{u}^{T}u + c_{\theta}^{T}\theta + c_{c}$$

s.t.
$$g_i(u, \theta) := A_i u \leq b_i + F_i \theta$$

 $u \in \mathbb{R}^{n_u}, \theta \in \Theta := \left\{ \theta \in \mathbb{R}^{(n_x + n_y + n_d)} | P_A \theta \leq P_b \right\}$
 $Q \succ 0$
 $i \in \mathbb{I}$
(2)

In problem (2), $Q \in \mathbb{R}^{n_u \times n_u}$, $H \in \mathbb{R}^{(n_x+n_y+n_d) \times n_u}$, $c_u \in \mathbb{R}^{n_u \times 1}$, $c_\theta \in \mathbb{R}^{(n_x+n_y+n_d) \times 1}$ and c_c a scalar. The index $i \in \mathbb{I}$ corresponds to the i^{th} inequality constraint, where for each constraint $g_i(x,\theta)$, we have $A_i \in \mathbb{R}^{1 \times n_u}$, $F_i \in \mathbb{R}^{1 \times (n_x+n_y+n_d)}$, and b_i is a scalar, while Θ , described by the matrices $P_A \in \mathbb{R}^{w \times (n_x+n_y+n_d)}$ and $P_b \in \mathbb{R}^{w \times 1}$, represents a polytopic convex subset of the parameter space in which the parameters θ vary.

Problem (2) can be efficiently solved using state-of-the-art software (Oberdieck et al. (2016), Herceg et al. (2013)). The optimal multiparametric solution of (2) returns a list of critical regions, where in each critical region the vector of the bounded uncertain parameters is related to the optimal continuous control law. Hence, the explicit offline solution of the MPC problem is given by Eq. (3)

$$u^* = K_i \theta^* + r_i, \ \theta^* \in CR^i = \{CR^i_A \theta \le CR^i_b\}$$
(3)

where u^* is the optimal control action at the parameter realization θ^* . The convex polytope CR^i defines the i^{th} critical region, and K_i and r_i characterize the optimal control action. Each critical region, CR^i , is associated with a unique set of active inequality constraints. The derivation of each critical region is achieved by (i) ensuring the inactive constraints of the problem remain inactive, and (ii) by guaranteeing that the optimal Lagrange multipliers at the optimal control action remain positive for the corresponding parameter space.

Advantages of the explicit form of the controllers include the construction of the optimal partitions of the parameter space before the operation of a process has been initiated, the enhanced online computational performance due to the alleviation from the repetitive solution of optimization problems, and the ability to embed optimal control schemes in complex engineering applications, such us the integration of design, control and scheduling of process systems (Burnak et al. (2019), Tian et al. (2020)).

3. AN ALGORITHM FOR QUADRATICALLY CONSTRAINED NMPC

3.1 Basic Sensitivity Theorem: The Quadratic Case

We consider problems described by (4)

$$\min_{u} f(u,\theta) = \frac{1}{2} u^{T} Q u + u^{T} H^{T} \theta + \theta^{T} Q_{\theta} \theta + c_{u}^{T} u \\ + c_{\theta}^{T} \theta + c_{c}$$
s.t. $g_{i}(u,\theta) := u^{T} Q_{c,i} u + u^{T} H_{c,i}^{T} \theta + A_{c,i} u \\ \leq b_{c,i} + F_{c,i} \theta + \theta^{T} Q_{c,\theta,i} \theta$

$$u \in \mathbb{R}^{n_{u}}, \theta \in \Theta := \left\{ \theta \in \mathbb{R}^{(n_{x}+n_{y}+n_{d})} | P_{A} \theta \leq P_{b} \right\}$$
 $Q \succ 0, Q_{c,i} \succ 0$
 $i \in \mathbb{I}$

$$(4)$$

 $Q_{c,i} \in \mathbb{R}^{n_u \times n_u}, H_{c,i} \in \mathbb{R}^{(n_x+n_y+n_d) \times n_u}, A_{c,i} \in \mathbb{R}^{1 \times n_u}, F_{c,i} \in \mathbb{R}^{1 \times (n_x+n_y+n_d)}, Q_{c,\theta,i} \in \mathbb{R}^{(n_x+n_y+n_d) \times (n_x+n_y+n_d)}.$ Linear equality constraints are omitted from the problem formulation for brevity. Note that the matrices Q and $Q_{c,i}$ are positive definite. If the matrices $Q_{c,i}, H_{c,i}$, and $Q_{c,\theta,i}$ do not exist, problem (4) is equivalent to (2).

Assume that there exist Lagrange multipliers λ_i which correspond to p active constraints, and that the first-order KKT conditions hold (Floudas (1995))

$$\begin{aligned} \nabla_u L(u^*, \lambda^*, \theta^*) &:= \nabla_u f(u^*, \theta^*) + \sum_{i=1}^p \lambda_i^* \nabla_u g_i(u^*, \theta^*) = 0 \\ g(u^*, \theta^*) &\leq 0 \\ \lambda_i^* g_i(u^*, \theta^*) &= 0, \quad i = 1, \dots p \\ \lambda_i^* &\geq 0 \quad i = 1, \dots p \\ \forall i \in \mathbb{I} \end{aligned}$$

For the construction of the parametric solution of the problem described by (4), the vector F, which incorporates the equalities of the KKT conditions is defined

$$F(u,\lambda,\theta) = \begin{bmatrix} \nabla_u L(u,\lambda,\theta) \\ \lambda_i g_i(u,\theta) \end{bmatrix} = 0$$
(5)

where $L(u, \lambda, \theta)$ is the Lagrange function of problem (4) and λ_i is the corresponding Lagrange multiplier associated with active constraint $g_i(u, \theta)$, where $F \in \mathbb{R}^{(n_u+p) \times 1}$.

Based on the conditions and principles of the Basic Sensitivity Theorem (Diangelakis et al. (2018)), a once continuously differentiable vector function $\eta = [u(\theta)^T, \lambda(\theta)^T]^T$ exists, satisfying the second-order sufficient conditions for a local minimum along with the associated Lagrange multipliers $\lambda(\theta)$. Namely, without loss of generality the vector F can be written as

$$F = \begin{bmatrix} \begin{bmatrix} Q + \sum_{i=1}^{p} \lambda_i Q_{c,i} \end{bmatrix} u + \begin{bmatrix} H^T + \sum_{i=1}^{p} H_{c,i}^T \end{bmatrix} \theta + c_u + \sum_{i=1}^{p} \lambda_i A_{c,i} \end{bmatrix} \\ u^T Q_{c,i} u + u^T H_{c,i}^T \theta + A_{c,i} u - b_{c,i} - F_{c,i} \theta - \theta^T Q_{c,\theta,i} \theta \end{bmatrix} = 0$$
$$\lambda_i > 0 \quad \forall i$$

Concatenating the vectors η and θ we define the vector $\alpha = [\eta^T | \theta^T]^T$. Assuming a given feasible parameter realization θ^* and a corresponding optimal solution described by u^* and λ^* , and if $\nabla_{\theta}\eta(\theta^*)$ and $\nabla_{\theta\theta}\eta(\theta^*)$ exist, a second-order Taylor expansion of the vector F around $\alpha^* = [\eta^{*T} | \theta^{*T}]^T$ is expressed as

$$F \approx \left[\frac{1}{2}(a-a^*)^T \nabla_{aa} F(a^*) + \nabla_a F(a^*)\right](a-a^*) = 0 \quad (6)$$

Hence, for problems which are described with a convex quadratic objective function, convex quadratic and/or linear constraints the exact solution for convex mpQCQps is enabled and be obtained through the solution of the system of quadratic equations described by (6).

3.2 Exploration of the Parameter Space

Strategies for the exploration of the parameter space in multiparametric programming problems can be identified in geometrical, combinatorial, and combinations of the aforementioned approaches. Geometrical algorithms are based on the fact that given an initial critical region, the neighborhood around each facet is explored to identify adjacent critical regions, until the full parameter space is explored. On the other hand, combinatorial algorithms aim to implicitly explore the parameter space by enumerating all possible active sets which can yield an optimal solution for a feasible parameter realization. In this work, the complete exploration of the parameter space is achieved by utilizing an active set-based approach, inspired by (Gupta et al. (2011)). The proposed approach employs a strategy for the identification of optimal active-sets. To avoid the exhaustive enumeration of active sets a pruning criterion is employed. A candidate active set can be infeasible, feasible or optimal. If the active set results to an optimal solution, the active set will yield a critical region.

Let $\mathbb V$ refer to the set of the indices of the inequality constraints in $\mathbb I$

$$\mathbb{V} = \{1, \dots, r\} \tag{7}$$

We define the set $\mathbb{AS},$ which includes all candidate active sets

$$\mathbb{AS}(\mathbb{V}) = \{\{\mathbb{A}_1 = \{\}, \mathbb{A}_2 = \{1\}, ..., \mathbb{A}_{r+2} = \{1, 2\}, ..., \mathbb{A}_{2^r} = \{1, 2, ..., r\}\}$$
(8)

We highlight that for a deterministic QCQP with n optimization variables and r inequality constraints, where r > n, the number of strongly active constraints at the optimal solution can be up to n. The number of optimal active sets, represented by the set \mathbb{AS}' , where $\mathbb{AS}' \subset \mathbb{AS}$, is

$$\mathbb{AS}'(\mathbb{V}) = \left\{ \mathbb{A}_1 = \{\}, \mathbb{A}_2 = \{1\}, ..., \mathbb{A}_{\binom{r}{n}} = \{1, 2, ..., n\} \right\}$$
(9)

where \mathbb{AS} is the set of all possible candidate active sets.

Firstly we solve the following feasibility problem for every candidate active set:

$$\min_{\substack{u,\theta\\u,\theta}} 0 \\
\text{s.t.} \quad g_i(u,\theta) = 0, \forall i \in \mathbb{A}_k \\
g_j(u,\theta) \le 0, \forall j \ne i \\
\theta \in \Theta := \{\theta \in \mathbb{R}^m \mid P_A \theta \le P_b\} \\
u \in \mathbb{R}^{n_u}, \mathbb{A}_k \subset \mathbb{AS}'$$
(10)

The solution of problem (10) determines whether there is a pair of the vectors x, θ , which yields a solution and hence render the given active set to be feasible. The remaining active sets which do not lead to a feasible solution are discarded from consideration because if they cannot be feasible, they cannot be optimal. A schematic diagram of our active set approach is illustrated in Figure 1.

Proposition 1. Let \mathbb{A}_1 and \mathbb{A}_2 be two candidate active sets for the solution of (10). If $\mathbb{A}_1 \subset \mathbb{A}_2$ and \mathbb{A}_1 leads to an infeasible solution, then \mathbb{A}_2 will also lead to an infeasible solution.

Proposition 1 follows from the fact that if a given active set leads to an infeasible solution and since $\mathbb{A}_1 \subset \mathbb{A}_2$, the active set \mathbb{A}_2 will make the problem even more constrained, and hence remain infeasible. For problem (10) a feasible solution suffices for a given active set to be considered since it indicates that there is feasible parameter space that might lead to an optimal parametric solution.

After the completion of this step, a candidate active set combination could be either feasible and/or optimal. Therefore, problem (11) is formulated for the remaining active sets, to determine whether a given active set will provide a globally optimal solution and the corresponding critical region



Fig. 1. A schematic diagram which represents the active set approach used for the solution of problem (10).

$$\max_{\substack{t,x,\theta,\lambda,s}} t$$
s.t.
$$\nabla_x L(x,\theta,\lambda) = 0$$

$$g_i(x,\theta) = 0, \qquad \forall i \in \mathbb{A}_k$$

$$g_j(x,\theta) + s_j = 0, \qquad \forall j \neq i$$

$$t \leq \lambda_i \qquad \forall i \in \mathbb{A}_k \qquad (11)$$

$$t \leq s_j \qquad \forall j \neq i$$

$$\theta \in \Theta := \{\theta \in \mathbb{R}^m \mid P_A \theta \leq P_b\}$$

$$\lambda_i \geq 0, s_j \geq 0, t \geq 0$$

$$x \in \mathbb{R}^n, \theta \in \mathbb{R}^m, \mathbb{A}_k \subset \mathbb{AS}'$$

In problem (11), t is a scalar, which assists in the identification of degenerate active sets. The solution of this problem can be (i) Feasible with t > 0. The given active set is optimal along with the corresponding unique critical region, (ii) Feasible with with t = 0. The mpQCQP is degenerate due to failure of the strict complementary slackenss (SCS) or the linear independence constraint qualification (LICQ), (iii) Infeasible. There is not a parameter vector $\theta \in \Theta$ for which the given candidate active set can yield an optimal solution, and the active set is discarded. As soon as all optimal active sets have been identified, the second-order approach to the Basic Sensitivity Approach is applied to construct the optimal multiparametric solution.

The resulting system of quadratic equations is solved using SageMath, where the theory of Gröbner Bases and the Buchberger algorithm Buchberger and Winkler (1998) is utilized to construct the optimal multiparametric solution and the corresponding critical regions.

3.3 Degeneracy

Primal degeneracy occurs as a consequence of the presence of weakly active constraints in the critical region. In the current approach, primal degeneracy can occur if $\lambda_i = 0$ or $s_j = 0$. If a Lagrange multiplier is zero for the currently considered active set, the corresponding constraint is not part of the optimal active set. That optimal active set would have already been discovered in a parent node of that active set in a previous step of the proposed algorithm. On the other hand if a slack variable $s_j = 0$, which leads to the corresponding $g_j(x^*, \theta^*) = 0$, that j^{th} constraint must be included in the optimal active set combination. However, this active set combination will be discovered later in a child subsequent node of the currently considered active set. Hence, these cases are not kept as optimal active sets since they would have already been checked in a previous step of the algorithm or will be discovered in a future step of the algorithm. Dual degeneracy cannot occur in the class of problems considered in this work since the matrices Q and $Q_{c,i}$ are positive definite. An overview of the overall algorithm is shown in Table 1.

Table 1. Algorithmic strategy for the exact solution of mpQCQPs.

Step 1: Reformulate the NMPC to the form of problem (4). Step 2: For a given active set, solve problem (10). If the problem is feasible, the active set is kept. Otherwise, the active set is discarded along with all active sets which include it. Step 3: Formulate and solve (11) for all remaining active sets. If t > 0 the active set is optimal, while if t = 0 or the problem is infeasible, the considered active set is discarded. Step 4: If the active set includes quadratic constraints use (6) and analytically solve the system of quadratic equations to obtain the optimal parametric solution. Step 5: Substitute the parametric expressions on the inactive inequality constraints and Lagrange multipliers to define the optimal solution and the critical regions.

4. OPERATION OF A NONISOTHERMAL CSTR

4.1 Process Description

Consider the operation of an ideal nonisothermal CSTR, adopted by Kazantzis and Kravaris (2000). The irreversible reaction that is occurring in the reactor is

$$2Na_2S_2O_3 + 4H_2O_2 \rightarrow Na_2S_3O_6 + Na_2SO_4 + 4H_2O$$
 (12)

For the given reaction and by denoting $Na_2S_2O_3$ and H_2O_2 as components A and B respectively, the rate of consumption of $Na_2S_2O_3$ is given by the kinetic law

$$-r_A = k_o exp(-\frac{E}{RT})c_A c_B \tag{13}$$

where k_o is the pre-exponential factor, E the activation energy, R the gas constant, T the reactor temperature, and c_A and c_B , the concentrations of species A and B. By assuming constant mixture density and reactor volume, and that stoichiometry at the feed stream is present at all times (i.e. $c_B(t) = 2c_A(t)$), the dynamic model of the CSTR is given by the following ordinary nonlinear differential equations

$$\frac{dc_A}{dt} = \frac{F}{V}(c_{A,in} - c_A) - 2k_o exp(-\frac{E}{RT})c_A^2$$
$$\frac{dT}{dt} = \frac{F}{V}(T_{in} - T) - 2\frac{(\Delta H)_R}{\rho c_p}k_o exp(-\frac{E}{RT})c_A^2 \qquad (14)$$
$$-\frac{U_A}{V\rho c_n}(T - T_j)$$

In addition, considering a nominal value of the manipulated action, which is the dilution rate, $\frac{F}{V} = 0.2s^{-1}$, the resulting steady-states are presented in Table 2.

Table 2. The steady-states of system (14).

	ss_1	ss_2	ss_3
c_{As}	0.987	0.667	0.0755
T_s	271.664	308.499	376.270

The eigenvalues for these steady-states of the given system are depicted in Figure 2



Fig. 2. Eigenvalues for the steady-states of (14) for a value of the dilution rate of $\frac{F}{V} = 0.2s^{-1}$.

From the values of the steady-states of the system and through a local stability analysis, it is observed that the first and third steady-states are stable while the middle steady-state is unstable. The first steady-state results in a low yield and hence it is not a desired operating point for the CSTR. Apart from that, it has been experimentally identified that near the third steady-state undesirable side reactions occur (Vejtasa and Schmitz (1970)). The middle steady-state provides satisfactory yield results, while avoiding the impact of additional reactions to the process. The control objective is to regulate the operation of the CSTR around the aforementioned steady-state, by manipulating the dilution rate.

4.2 Explicit Nonlinear Model Predictive Control

The Jacobian linearization of system (14) at ss_2 is considered, and the following deviation variables to shift the origin to the desired steady-state are defined

$$x = \begin{bmatrix} c_A - c_{As} \\ T - T_s \end{bmatrix}$$

$$u = \frac{F}{V} - \frac{F}{V}|_s$$
(15)

Consequently, the linearized dynamic model is discretized with a time step $\tau = 0.2s$, assuming zero-order hold, and the resulting state-space model is shown below

$$x_{k+1} = \begin{bmatrix} 0.9194 & -0.0013\\ 5.8554 & 1.1394 \end{bmatrix} x_k + \begin{bmatrix} 0.0685\\ -6.9670 \end{bmatrix} u_k$$
(16)

The states of the system, treated as uncertain parameters, are considered to be the measured outputs from the reactor. Based on the developed model the following NMPC problem is formulated, which aims to drive the system to the shifted origin from a given initial state vector

where $QR = \begin{bmatrix} 0.01 & 0 \\ 0 & 0.01 \end{bmatrix}$, R = 10, N = 2 and P is

the terminal weight matrix derived via the discrete-time Riccati equation. The lower and upper bound on the states are $-0.667 \frac{mol}{L}$ and -308.499K, and $1.667 \frac{mol}{L}$ and 100K respectively, while the bounds on the manipulated action are $-0.2s^{-1}$ and $0.8s^{-1}$. Additionally, we include a quadratic constraint in the problem formulation which incorporates a cost, with arbitrary parameters a = 33.4and $\beta = 10.6$, associated with the operation of the CSTR. Namely, it is assumed that the cost of operation of the reactor is a function of the reactant which needs to be purchased, as well as of a separation cost described by the product of the reactant flowrate and the concentration of A. The determination of the upper bound of the constraint is achieved by calculating the half of the maximum value of the aforementioned cost. Hence, it is required that the operation of the CSTR must not exceed the given maximum cost. Apart from that, a polytopic terminal set constraint is included in the problem formulation to impose the states to exist in that region at the end of the prediction horizon.

The resulting problem is reformulated by propagating the states into an mpQCQP. The problem is solved using the proposed algorithm. We assume that the initial concentration of A and the temperature of the reactor are 0.417 mol/L and 15K respectively. The full parametric solution is obtained in 31s using MATLAB and GAMS, and by using a global optimization algorithm (Tawarmalani and Sahinidis (2005), Misener and Floudas (2014)) to solve the deterministic optimization problems. The systems of quadratic equations are solved using SageMath. As a result, by solving the problem using the proposed approach, 326 candidate active sets are identified and the optimal map of parametric solutions includes 23 critical regions. The closed-loop response of the system is depicted in Figure 3. The solution of the NMPC was compared to the same problem, which did not include the quadratic constraint in the problem formulation. The resulting solution of the NMPC achieved a 5.2% reduction in the cost of operation of the reactor compared to the linear MPC.

5. CONCLUSION

In this work we presented an algorithmic strategy for the exact solution of multiparametric quadratically constrained quadratic programming problems. The identification of all critical regions of the parameter space is founded on an active set-based approach, which implicitly



Fig. 3. Concentration of A, temperature and dilution rate in deviation form through closed-loop simulation.

explores the parameter space. Based on that a secondorder approach to the Basic Sensitivity Theorem can be applied to construct the corresponding critical regions and the optimal multiparametric solution. The proposed approach was successfully applied in the regulation of a nonisothermal CSTR reactor near an unstable steadystate with economic considerations. Our current research efforts seek to expand to other classes of quadratically constrained optimal control problems.

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REFERENCES

- Bemporad, A., Morari, M., Dua, V., and Pistikopoulos, E.N. (2002). The explicit linear quadratic regulator for constrained systems. *Automatica*, 38(1), 3–20.
- Buchberger, B. and Winkler, F. (1998). Gröbner bases and applications, volume 17. Cambridge University Press Cambridge.
- Burnak, B., Diangelakis, N.A., Katz, J., and Pistikopoulos, E.N. (2019). Integrated process design, scheduling, and control using multiparametric programming. *Computers* & Chemical Engineering, 125, 164–184.
- Charitopoulos, V.M. and Dua, V. (2016). Explicit model predictive control of hybrid systems and multiparametric mixed integer polynomial programming. AIChE Journal, 62(9), 3441–3460.
- Charitopoulos, V.M., Papageorgiou, L.G., and Dua, V. (2019). Closed-loop integration of planning, scheduling and multi-parametric nonlinear control. *Computers & Chemical Engineering*, 122, 172–192.
- Diangelakis, N.A., Pappas, I.S., and Pistikopoulos, E.N. (2018). On multiparametric/explicit nmpc for quadrat-

ically constrained problems. *IFAC-PapersOnLine*, 51(20), 400–405.

- Dua, V. and Pistikopoulos, E.N. (1999). Algorithms for the solution of multiparametric mixed-integer nonlinear optimization problems. *Industrial & engineering chemistry research*, 38(10), 3976–3987.
- Fiacco, A.V. (1976). Sensitivity analysis for nonlinear programming using penalty methods. *Mathematical* programming, 10(1), 287–311.
- Fiacco, A.V. et al. (1983). Introduction to sensitivity and stability analysis in nonlinear programming, volume 90075. Academic press New York.
- Floudas, C.A. (1995). Nonlinear and mixed-integer optimization: fundamentals and applications. Oxford University Press.
- Fotiou, I.A., Rostalski, P., Parrilo, P.A., and Morari, M. (2006). Parametric optimization and optimal control using algebraic geometry methods. *International Journal* of Control, 79(11), 1340–1358.
- Grancharova, A., Johansen, T.A., and Tøndel, P. (2007). Computational aspects of approximate explicit nonlinear model predictive control. In Assessment and Future Directions of Nonlinear Model Predictive Control, 181– 192. Springer.
- Gupta, A., Bhartiya, S., and Nataraj, P. (2011). A novel approach to multiparametric quadratic programming. *Automatica*, 47(9), 2112–2117.
- Herceg, M., Kvasnica, M., Jones, C.N., and Morari, M. (2013). Multi-parametric toolbox 3.0. In 2013 European control conference (ECC), 502–510. IEEE.
- Johansen, T.A. (2004). Approximate explicit receding horizon control of constrained nonlinear systems. Automatica, 40(2), 293–300.
- Katz, J., Pappas, I., Avraamidou, S., and Pistikopoulos, E.N. (2020). Integrating deep learning models and multiparametric programming. *Computers & Chemical Engineering*, 106801.
- Kazantzis, N. and Kravaris, C. (2000). Synthesis of state feedback regulators for nonlinear processes. *Chemical Engineering Science*, 55(17), 3437–3449.
- Misener, R. and Floudas, C.A. (2014). Antigone: algorithms for continuous/integer global optimization of nonlinear equations. *Journal of Global Optimization*, 59(2-3), 503–526.
- Oberdieck, R., Diangelakis, N.A., Papathanasiou, M.M., Nascu, I., and Pistikopoulos, E.N. (2016). Popparametric optimization toolbox. *Industrial & Engineering Chemistry Research*, 55(33), 8979–8991.
- Oberdieck, R. and Pistikopoulos, E.N. (2015). Explicit hybrid model-predictive control: The exact solution. *Automatica*, 58, 152–159.
- Tawarmalani, M. and Sahinidis, N.V. (2005). A polyhedral branch-and-cut approach to global optimization. *Mathematical Programming*, 103(2), 225–249.
- Tian, Y., Pappas, I., Burnak, B., Katz, J., and Pistikopoulos, E.N. (2020). A systematic framework for the synthesis of operable process intensification systems-reactive separation systems. *Computers & Chemical Engineering*, 134, 106675.
- Vejtasa, S.A. and Schmitz, R. (1970). An experimental study of steady state multiplicity and stability in an adiabatic stirred reactor. *AIChE Journal*, 16(3), 410– 419.