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Constrained Control and Estimation of Homogeneous Reaction Systems Using Extent-Based Linear Parameter Varying Models

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ABSTRACT: In this paper, a model predictive control (MPC) strategy for nonlinear homogeneous reaction systems is proposed. The nonlinear system is first transformed to a linear parameter varying (LPV) system by means of a linear transformation known as extents decomposition. The resulting LPV system is further converted to a linear time invariant (LTI) system by means of a parametric state feedback and feedforward control laws. The use of this description results in linear MPC with a quadratic performance index and nonlinear state parameter constraints. However, based on the polytopic nature of the parameter of the LPV systems, the constraints are transformed to a set of intersected polyhedrons. The final result is a linear MPC problem with linear constraints that can be easily converted and solved as a quadratic programming problem. Finally, the performance of the control strategy is illustrated in simulation and compared with a controller based on a constant-parameter LTI model.

1. INTRODUCTION

The main characteristics of the process industry is the large-scale conversion of mass and energy for the production of materials with specific value and use. In particular, reaction systems are fundamental for such objectives, because it is generally at the reaction step where products can be crafted to meet the desired quality characteristics. Therefore, monitoring and controlling reaction systems is key for a safe, sustainable, and satisfactory production of materials.1−3 Designing control strategies for systems given by LPV representations is not an easy task, especially if the system is subject to constraints. Some of the MPC approaches proposed for LPV systems have been described in the work done by Lu and Arkun11 and Casavola et al.12 We can also find multi-parametric approaches described as explicit MPC for LPV systems,13 tube-based model predictive control (TMPC),14,15 MPC for quasi-LPV systems (QMPC)16,17 and model learning MPC.18 Although MPC methods for LPV systems proposed in the literature are well-defined mathematically, the real-time implementations are difficult, because of their complexity and high computational load. Therefore, there is a need for model-based strategies that are computationally efficient and easy to commission and maintain.

It is well-known that reaction systems are driven by transport and thermodynamic phenomena. Mass and energy conservation laws are used to build models that allow for a precise description of the process dynamics at the expense of increasing model complexity.
complexity, making them impractical for online model-based operation. Despite the aforementioned complexity, these reaction system models exhibit a specific structure of sum of effects that can be exploited to obtain a suitable representation for control and estimation. In this sense, the concept of extents transformations was introduced by Asbjørnsen to address reaction variant and invariant dynamics in batch reaction system. The former approach was extended by Amrhein et al. to reaction systems with inlets and outlets and multiphase systems (Bhatt et al., Marquez-Ruiz et al.). The extent transformation is a subspace decomposition approach by means of a linear map that decouples relevant variables for control (inputs, outputs, and disturbances), while maintaining the physical meaning of the variables. The extent-based representation of the process presents many advantages, such as model reduction, identification of reaction systems from measured data, parametric sensitivity analysis, model-based control, etc. One of the key features of the extent transformation is that it allows the development of an LPV representation with a diagonal state matrix. 

In this paper, the aforementioned LPV representation is used to propose a new MPC strategy for nonlinear homogeneous reaction systems. Given the time-varying nature of the parameter in the LPV formulation, parametric state-feedback and feed-forward laws are designed. These parametric control laws are exploited to convert the original LPV system into a linear time invariant (LTI) system. In addition, the state feedback and feed-forward laws require full state information. Therefore, observers are also developed to estimate unmeasured states and disturbances. The effect of these control laws allows to recast the original nonlinear MPC problem as a linear MPC with a quadratic performance index and nonlinear state-parameter constraints. The latter are then transformed to a set of intersected polyhedrons based on the assumption that the parameter varies within a polytope. The procedure simplifies the original problem, resulting in a linear MPC with linear constraints. The linear MPC is finally solved as a quadratic programming problem.

The paper is organized as follows: In section 2, mechanistic model of a homogeneous reaction system based on mass and energy conservation laws is discussed. This is followed by the introduction of extent of reaction and inlets and the LPV representation. In section 3, we describe the control strategy for extent-based LPV systems. In section 4, observability analysis, as well as state and reaction rate estimation, are performed, exploiting the LPV structure. In section 5, the proposed control strategy is applied to a case study of a CSTR with an equilibrium reaction. Finally, section 6 presents the conclusion of this work.

2. LPV REPRESENTATION OF HOMOGENEOUS REACTION SYSTEMS

Consider a homogeneous reaction system with \( S \) species, \( R \) independent reactions, \( p \) independent inlet flows, and one outlet flow (shown in Figure 1).

The mass and energy balance equations for this system are given by

\[
\begin{align*}
\dot{n}(t) & = -\theta(t)I_{n+1} n(t) + W_n 0 u_n(t) + N^T Vr(t), \\
n(0) & = n_0 \\
T(t) & = \alpha(t) \gamma(t) Q_n(t) + \beta(t) \overline{r}(t) \\
T(0) & = T_0
\end{align*}
\]

where \( n(t) \in \mathbb{R}^S \) is the number of moles, \( T(t) \in \mathbb{R} \) the temperature, and \( V \) the reaction mixture volume. \( r \in \mathbb{R}^S \) is the reaction rate vector, \( u_{in} \in \mathbb{R}^p \) and \( u_{out} \in \mathbb{R} \) are the inlet and outlet mass flows, respectively; \( m \) is the reacting mixture mass, \( N \in \mathbb{R}^{S \times S} \) the stoichiometric coefficient matrix, \( W_n \in \mathbb{R}^{S \times p} \) the inlet composition matrix (defined as \( W_n = M_w^{-1} w_{in} \)), \( M_w \in \mathbb{R}^{S \times S} \) the diagonal molecular weight matrix, and \( W_{out} \in \mathbb{R}^{S \times p} \) the matrix of weight fraction. Finally, the terms \( \theta(t), \alpha(t), \beta(t), \) and \( \gamma(t) \) are defined as

\[
\begin{align*}
\theta(t) & = \frac{u_{out}}{m(t)} \\
\alpha(t) & = \frac{C_{P_{in}} T_{in}}{m(t) C_{P_{in}}} \\
\beta(t) & = \frac{\Delta H_f^\circ N^T}{m(t) C_{P_{in}}} \\
\gamma(t) & = \frac{1}{m(t) C_{P_{in}}}
\end{align*}
\]

where \( \Delta H_f^\circ \in \mathbb{R}^{S \times S} \) is the vector of standard enthalpy of formation. If we assume no or small variations in the parameters, the reaction rate represented in the vector \( r \) is the main nonlinearity in eq 1. The reaction rate \( r \) is usually modeled using the mass-action principle and the Arrhenius equation. This particular parametrization of the reaction rate can be exploited for analysis, as well as for controller and observer design purposes. In the following, for ease of notation, we drop the explicit dependence of \( n, T, \) and \( \theta \) on time.

Assumption 1. In this work, the time-varying parameters \( \alpha, \beta, \) and \( \gamma \) are assumed to be constant. Note that it can be done by assuming a local controller that keeps the total mass in the process constant \((m(t) = m)\) or inside a bounded set \( m \in \mathbb{M} \).

2.1. Decoupling Disturbances: Extent of Reaction and Inlet Flow. The change observed in the number of moles of each species in a chemical reaction is proportional to their reaction coefficients \( \nu_r \). This proportionality is exactly the same for all the species present in the reaction, which allows for the study of the reaction as a unique global dynamic effect. A way to quantify this feature is introducing a variable to measure the evolution of a reaction as a whole, called the extent of reaction \( x_r \). This new variable \( x_r \) characterizes the extent or degree of completion achieved by a particular reaction (Smith et al.). In the specific case where the variations in the number of moles is only due to a chemical reaction, the moles space can be partitioned in two subspace: the reaction variant subspace and the reaction invariant subspace, with the reaction variant subspace dynamics being solely described by the extent of reaction. The space partition can be performed finding a suitable invertible linear map, such that the initial conditions in the mole

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Image 1. Homogeneous reaction system.
space \( n_0 \) are mapped exactly to 0 in the reaction space. Furthermore, if the process contains other physical contributions, e.g., one or several inlet streams, the moles space is now affected by two independent dynamics, i.e., reaction and inlet flows. This situation corresponds to the general case of continuous stirred-tank reactors, and the extent of reaction cannot be directly computed as done previously. To give a solution to this problem, the extents of reaction are complemented with the extent of inlet flow (Amrhein et al.\textsuperscript{29}). Generally, it can be shown that it is possible to find a linear transformation \( T : \mathbb{R}^5 \to \mathbb{R}^{5+p+1} \) such that the system given by the model described by eq \( 1 \) can be expressed in terms of new decoupled states with zero initial conditions in the reaction and inlet spaces. This new representation is as follows:

\[
\begin{bmatrix}
  x_r \\
  x_{in} \\
  \lambda \\
  T
\end{bmatrix} = \begin{bmatrix}
  -\beta R & 0 & 0 & 0 & 0 \\
  0 & -\beta p & 0 & 0 & 0 \\
  0 & 0 & -\theta & 0 & 0 \\
  0 & 0 & 0 & 0 & T
\end{bmatrix} \begin{bmatrix}
  x_r \\
  x_{in} \\
  \lambda \\
  T
\end{bmatrix} + \begin{bmatrix}
  0 \\
  0 \\
  0 \\
  \gamma
\end{bmatrix} \begin{bmatrix}
  u_{in} \\
  \nu_r \\
  \theta
\end{bmatrix}
\]

where \( x_r \in \mathbb{R}^5 \) is the extent of reaction, \( x_{in} \in \mathbb{R}^p \) the extent of inlet flow, and \( \lambda \in \mathbb{R} \) the discounting factor for the initial conditions. Also, the number of moles can be calculated using the extents from the following equation:

\[
n = N^T x_r + W_{in} x_{in} + n_0 d
\]

**Remark 1.** The linear transformation \( T : \mathbb{R}^5 \to \mathbb{R}^{5+p+1} \) can be written as

\[
\begin{bmatrix}
  x_r \\
  x_{in} \\
  \lambda \\
\end{bmatrix} = \begin{bmatrix}
  T_1^T \\
  T_2^T \\
  T_3^T
\end{bmatrix} \begin{bmatrix}
  n
\end{bmatrix}
\]

where \( T_1 \), \( T_2 \), \( T_3 \) are the transformation matrices of the reaction space, \( T_2 \) of the inlet space, and \( T_3 \) of the reaction and inlet flow invariant space, all with discounted initial conditions \( n_0 \). The calculation of the matrices \( T_i, i = 1, 2, 3 \) can be done by means of a singular value decomposition of \( N^T \) and \( W_{in} \). Details about this procedure can be found in the works of Srivivasan et al.\textsuperscript{28} and Amrhein et al.\textsuperscript{29} Also, the aforementioned transformation requires the following conditions:

- \( T_1^T N^T = I_{R_r} \), \( T_1^T W_{in} = 0_{R_r \times p} \)
- \( T_2^T N^T = 0_{p \times R_r} \), \( T_2^T W_{in} = I_p \)
- \( T_3^T N^T = 0_{1 \times R_r} \), \( T_3^T W_{in} = 0_{1 \times p} \)
- \( \text{rank}(N^T W_{in}) = R_1 + p < S \)
- \( \text{rank}(N^T W_{in} n_0) = R_1 + p + 1 \leq S \)
- \( I_{R_r} - R_r - p T_3^T n_0 \neq 0 \)

Finally, it is important to mention that the inverse of \( T \), \( T^{-1} : \mathbb{R}^{5+p+1} \to \mathbb{R}^5 \) can be calculated as

\[
T^{-1} = \begin{bmatrix}
  N^T \\
  W_{in} \\
  n_0
\end{bmatrix}
\]

One of the advantages of the moles space decomposition is the preservation of the physical meaning of each of the generated subspaces. In this sense, the reaction space corresponds to that of variations in the number of moles due to the contribution of the chemical reaction, and the inlet space corresponds to such variations due to inlet streams present in the system. The structure of this representation can serve for system analysis. Since the model is perfectly decoupled, the uncontrollable states (initial conditions in the mole space) and disturbances (reaction rates) are obvious. Model-based techniques such as model reduction or state-disturbance decoupling are considerably simplified.

The existence of the linear map \( T \) can be viewed as an input/disturbance-to-state decoupling problem. Notice the first requirement is that \( \text{im}(N^T) \oplus \text{im}(W_{in}) \oplus \text{im}(n_0) \subseteq \mathbb{R}^5 \), which guarantees uniqueness of the decomposition, where \( \oplus \) is the direct sum. The second requirement is that \( \text{ker}(N) \cap \text{ker}(W_{in}^T) = N_r \), which guarantees the existence of trajectories in the moles space that are reaction and inlet invariant. The last requirement is that \( \text{im}(n_0) \subseteq N_r \), which implies that the initial conditions must lie in the reaction and inlet invariant subspace, providing independent information about the trajectories in the mole space. If these conditions are satisfied, then the reaction, inlet, and invariant subspaces can be generated performing an orthogonal decomposition of the moles space. Finally, note that eq \( 2 \) can be written as

\[
\dot{x} = A(\theta)x + Bu + Dd
\]

\[
y = Cx
\]

where \( x = [x_r^T, x_{in}^T, \lambda]^T, u = [u_{in}^T, Q_{in}]^T, \) and \( d = V_r \). The output \( y = [n^T, T]^T \) is given by

\[
\begin{bmatrix}
  n \\
  T
\end{bmatrix} = \begin{bmatrix}
  W_{in} & 0 & x_{in} \\
  0 & T & 0
\end{bmatrix} + \begin{bmatrix}
  N^T \\
  0
\end{bmatrix} \begin{bmatrix}
  x_r \\
  0 \\
  n_0
\end{bmatrix} \lambda
\]

For model-based control purposes, especially MPC, the plant states must be available at each time instant to perform prediction and optimal input computation. However, there are some unmeasured number of moles, which makes the development of an observer to estimate these unmeasured states necessary. Moreover, the reaction rate \( r \) affects the number of moles and the temperature in the reactor, making the estimation of the reaction rate also relevant for control. In order to simplify the dynamic nature of \( r \), the reaction will be interpreted as an artificial bounded external disturbance. This approach is actually valid under some mild assumptions that will be explained in section 4.

### 3. MPC OF HOMOGENEOUS REACTION SYSTEMS USING EXTENT-BASED LPV MODELS

We first analyze the system described in eq \( 2 \) before providing the details of the MPC formulation. Note that, in the model described by eq \( 2 \), the manipulated variables \( u_{in} \) and \( Q_{in} \) do not have any effect on the extents of reaction \( x_r \) and, therefore, the states \( x_r \) are uncontrollable modes. This fact is stated in the following theorem.

**Theorem 1.** Consider the homogeneous reaction system given by the set of equations described by eq \( 2 \), where the reaction rate \( r \) is assumed as a bounded disturbance \( r \in D, D \) being convex and compact. Then, if \( \theta \neq 0 \), the system described by eq \( 2 \) is uncontrollable, where the uncontrollable modes are stable if \( \theta > 0 \). In addition, the uncontrollable modes are separable and correspond to the extents of reaction \( x_r \) and the discount factor \( \lambda \).

The proof follows along the lines of the Hautus test of controllability\textsuperscript{26} and can be found in the work of Marquez-Ruiz.
et al.22 The proof can be easily particularized to the single-phase homogeneous reaction systems case. Separating the uncontrollable states \((x, \lambda)\), the system described by eq 2 can be written as

\[
\dot{x} = A_x(\theta)x + B_u u + D_d d \\
y = C_x x + C_u x_u
\]

(8)

with \(x = [x^T \theta^T]^T \in \mathbb{R}^{p+1}\) are the controllable states and \(x_u = [x^T_u \lambda^T]^T \in \mathbb{R}^{p+1}\) are the uncontrollable states. Matrices \(A_x, B_u, C_x,\) and \(D_d\) can be easily removed from eq 2, eliminating the uncontrollable states. Define \(x = x_u\) such that eq 8 can be written as eq 9,

\[
\dot{x} = A(\theta)x + B u + D d \\
y = C x + C_u x_u
\]

(9)

Equation 9 will be used in the next sections to formulate MPC controllers for the system given by the model described by eq 1. Given a system of the form described by eq 2, we consider the following problem:

\[
\min_{\{u_j\}_{j=0}^{N-1}} \|v_{k+N}\|^2_F + \sum_{j=0}^{N-1} \|k_{j+1}\|^2_W + \|u_{k+j}\|^2_R + \|\Delta u_{k+j}\|^2_S
\]

subject to

\[
x_{k+1} = A_x(\theta_{k+j})x_{k+j} + B_u u_{k+j} + D_d d_{k+j} \\
y_{k+j} = C_u x_{k+j} + C_{u,u} u_{k+j} \\
x_{k+j} \in X, \quad u_{k+j} \in U, \quad d_{k+j} \in D \\
x_{k+N} \in \Omega, \quad \theta_{k+j} \in \Theta
\]

(10)

where \(A_x, B_u, C_u, C_{u,u},\) and \(D_d\) are the discrete versions of the \(A, B, C, C_w,\) and \(D\) matrices in eq 9. These matrices can be found by the diagonal structure of the predicted states and the parameters \(\theta\). However, in this paper, we make use of the diagonal structure of the \(A\) matrix, and the physical interpretation of the parameter \(\theta\) to solve eq 10. To this end, the parametric state feedback and feedforward proposed by Marquez-Ruiz et al.23 for the extant LPV systems is used, and this is stated in the following theorem.

**Theorem 2.** Consider the homogeneous reaction system given by the set of equations described by eq 9, where the reaction rate \(r\) is assumed to be a measured or estimated disturbance. Then, if \(\gamma \neq 0\), there exist a parametric feedback gain \(K(\gamma) \in \mathbb{R}^{p+1 \times p+1}\), and a feedforward gain \(K_d \in \mathbb{R}^{p+1 \times k}\), such that \(u = K(\gamma)x + v + K_d d\), and the closed-loop representation of the system described by eq 9 has an equivalent LTI representation given by

\[
\dot{x} = \begin{bmatrix}
8I_p & 0 \\
0 & I_p
\end{bmatrix} x + \begin{bmatrix}
0 & I_p \\
\alpha & \gamma
\end{bmatrix} v \\
y = C x + C_u x_u
\]

(11)

where \(\theta\) are the constant desired poles of the closed-loop system, and \(v \in \mathbb{R}^p\) are the new input variable of the system. \(K(\theta)\) and \(K_d\) are given by

\[
K(\theta) = \begin{bmatrix}
(\theta - \gamma)I_p & 0 \\
\frac{\alpha}{\gamma} (\theta - \gamma) & \frac{1}{\gamma}
\end{bmatrix} \\
K_d = -B^T D = - \begin{bmatrix}
0 \\
\beta \gamma
\end{bmatrix}
\]

(12)

The proof of the Theorem 2 can be found in the work of Marquez-Ruiz et al.23

**Remark 2.** Note that, if \(\gamma \neq 0\), the rank(\(B\)) = \(p + 1\), then \(B^T = B^{-1}\) = \(K\), where \(\gamma\) is the Moore–Penrose pseudoinverse. This fact leads to the conclusion that the inverse of \(B\) can be always calculated analytically. Also, by the definition of \(\gamma = \frac{1}{m_{\text{haus}}^\text{mix}}\), the condition of \(\gamma \neq 0\) for homogeneous reaction systems is always satisfied if the product \(mC_{\text{mix}}\) is bounded.

Now, with the state representation described by eq 11 and the parametric feedback and feedforward controllers, we can write a discrete model of the system as follows:

\[
x_{k+1} = \tilde{A}_x x_k + \tilde{B} v_k \\
y_k = \tilde{C}_x x_k + \tilde{C}_u x_u
\]

where \(\tilde{A}, \tilde{B}, \tilde{C},\) and \(\tilde{C}_u\) are the discrete versions of \(A, B, C,\) and \(C_u\).

Having obtained an LTI system representation, we can formulate a linear MPC problem as follows:

\[
\min_{\{u_k\}_{k=0}^{N-1}} \|v_{k+N}\|^2_F + \sum_{j=0}^{N-1} \|k_{j+1}\|^2_W + \|u_{k+j}\|^2_R + \|\Delta u_{k+j}\|^2_S
\]

subject to

\[
x_{k+1} = \tilde{A}_x x_k + \tilde{B} v_k \\
y_k = \tilde{C}_x x_k + \tilde{C}_u x_u \\
u_k = K(\theta_k) x_k + v_k - K_d d_k
\]

(13)

where \(\tilde{A}, \tilde{B}, \tilde{C},\) and \(\tilde{C}_u\) are the discrete versions of \(A, B, C,\) and \(C_u\).

Hence, we can use the diagonal structure of the \(A\) matrix, and the physical interpretation of the parameter \(\theta\) to solve eq 10. To this end, the parametric state feedback and feedforward proposed by Marquez-Ruiz et al.23 for the extant LPV systems is used, and this is stated in the following theorem.
where $\mathcal{V}$ is defined as
$$\mathcal{V} = \{ v_{k+1} | K(\theta_{k+1})x_{k+1} + v_{k+1} - K_d x_{k+1} \in \mathcal{U} \}$$

3.2. Constraint Satisfaction and Calculation of $\mathcal{V}$

We note that, with the parametric feedback and feedforward, the states constraints $A x_{k+1} \leq b$ are unaffected by the parameter $\theta$ and do not have to be addressed at the moment. However, the input constraints are dependent on the parameter $\theta$ and must be addressed. Constraint satisfaction means that
$$A_u u_{k+1} \leq b_u \quad \forall \theta_{k+1} \in \Theta$$

Replacing $u_{k+1} = K(\theta_{k+1})x_{k+1} + v_{k+1} - K_d x_{k+1}$ into eq 20 yields
$$A_u v + A_d K(\theta_{k+1}) x_{k+1} \leq b_u + A_d K_d x_{k+1} \quad \forall \theta_{k+1} \in \Theta$$

Now, due to $u_{out} \in \mathcal{U}_{out} = \{ u_{out} | u_{out} \leq u_{out, max} \}$, $m \in \mathcal{M} = \{ m | m_{min} \leq m \leq m_{max} \}$, and $\theta = u_{out}/m$, the set $\Theta$ is given by a polytope with four vertices. This fact is explained by Figure 2.

**Figure 2.** Polytope for $\theta$ generated by the boundaries of $u_{out}$ and $m$.

Therefore, the set $\Theta$ can be seen as a convex hull with vertices $\sigma_i$ and is represented by
$$\Theta = \left\{ \theta | \theta = \sum_{\mu_i=1}^{n_{\sigma}} \mu_i \sigma_i, \sum_{i=1}^{n_{\mu}} \mu_i = 1, \mu_i \geq 0 \right\}$$

with $n_{\mu} = 4$.

**Remark 3.** If the mass $m$ remains constant, the set $\Theta$ can be reduced to just two vertices. This is the case when a perfect mass controller is implemented and the outlet flow is given by $u_{out}(t) = \sum_{\mu_i=1}^{n_{\mu}} u_{\sigma_i}$.

Based on the work of Kvasnica et al., the polytopic nature of $\Theta$, the following lemma can be stated:

**Lemma 1.** Let $\mathcal{V}$ be a set defined as
$$\mathcal{V} = \{ v_{k+1} | K(\sigma_{i+1})x_{k+1} + v_{k+1} - K_d x_{k+1} \in \mathcal{U}, \forall i = 1, \ldots, n_{\sigma} \}$$

The set $\mathcal{V}$, given by
$$\mathcal{V} = \mathcal{V}_1 \cap \cdots \cap \mathcal{V}_{n_{\sigma}}$$

then is a polytope that satisfies eq 16.

The proof of the lemma can be seen in ref 27. Now, by stacking vectors with future states and control inputs, eq 23 can be written as
$$A_u \tilde{v} + A_d \tilde{R}(\sigma) \tilde{v} \leq B_u + A_d \tilde{R}_d x \quad \forall \theta_{k+1} \in \Theta$$

where $A_u = \text{diag}(A_u, \ldots, A_u)$, $B_u = [B_u^T, \ldots, B_u^T]^T$, $\tilde{R}_d = [K_d^T, \ldots, K_d^T]^T$, and $\tilde{R}(\sigma) = \text{diag}([K_d(\sigma), \ldots, K_d(\sigma)])$. Now, replacing $\tilde{x} = \Phi x + \Psi \tilde{v}$ in eq 25 yields
$$\left( A_u + A_d \tilde{R}(\sigma) \Psi \right) \tilde{v} \leq \left( B_u + A_d \tilde{R}_d x - A_d \tilde{R}(\sigma) \Phi x \right)$$

denotes the difference between the actual and the previous value of the control action. Hence, $\Delta$ is a bidiagonal matrix whose elements are $-I_{n_{\mu}}$ and $I_{n_{\mu}}$. 
Finally, eq 26 can be written as $A_{x} x = b_{y}, x$ with $A_{x} = \mathcal{A}_{u} \Lambda \mathcal{A}_{x} \mathcal{K}^{-1}(\sigma \Psi)$ and $b_{y} = \mathcal{B}_{u} \Lambda \mathcal{A}_{x} \mathcal{K}^{-1}(\sigma \Psi)$, where $\mathcal{A}_{x} \Lambda \mathcal{A}_{x} \mathcal{K}^{-1}(\sigma \Psi)$ is a polytope. Moreover, this model is implemented. The sequential strategy consists of an asymptotic formulation of the AO is then given by Table 1.

4. STATE AND DISTURBANCE ESTIMATION

In order to perform the estimation of the number of moles and the disturbance signal $r$, a sequential state and disturbance estimation strategy based on the work of Marquez-Ruiz et al. is implemented. The sequential strategy consists of an asymptotic observer (AO), to estimate the number of moles, and a parametric reaction rate estimator (RRE), to determine the reaction rate $r$. A schematic of the sequential strategy is shown in Figure 4.

![Sequential state and reaction rate estimation strategy](image)

Figure 4. Sequential state and reaction rate estimation strategy.

This scheme works under the following assumptions:

**Assumption 3.** The temperature $T$ and the number of moles of $S_{m}$ components $n_{m} \in \mathbb{R}^{n}$ can be measured, where $S_{m} < S$. This implies that the mole numbers of $S - S_{m}$ components $(n_{um})$ are not measured; mathematically, the number of moles $n$ can be written as

$$n = \begin{bmatrix} n_{um} \\ n_{m} \end{bmatrix} = \begin{bmatrix} n_{um}^{T} \\ n_{m}^{T} \end{bmatrix} \begin{bmatrix} x_{u} \\ W_{um} \end{bmatrix} + \begin{bmatrix} n_{0,um} \\ n_{0,m} \end{bmatrix} \lambda,$$

where $n_{um} \in \mathbb{R}^{R \times (S - S_{m})}$, $n_{m} \in \mathbb{R}^{R \times S_{m}}$, $W_{um} \in \mathbb{R}^{R \times (S - S_{m})}$, $W_{um}^{T} \in \mathbb{R}^{R \times S_{um}}$, $n_{0,um} \in \mathbb{R}^{R \times S_{um}}$, $n_{0,m} \in \mathbb{R}^{R \times S_{m}}$, and $n_{0,m}^{T} \in \mathbb{R}^{R \times S_{m}}$.

Therefore, the estimation of $n_{um} \in \mathbb{R}^{R \times S_{um}}$ is necessary to reconstruct the extent of reaction $x_{u}$, the discounting factor $\lambda$, the uncontrolled states $x_{u}$, and the reaction rate $r$, based on the knowledge of $n$ and $T$. Finally, the conditions for the estimation of $n_{um}$ are given in the next theorem.

**Theorem 3.** Consider the homogeneous reaction system given by the set of eq 2, where the reaction rate $r$ is assumed as a bounded disturbance. If $\text{rank} \begin{bmatrix} n_{um} \\ W_{um} \end{bmatrix} = R_{S}$, then $n_{um}$ is necessary to reconstruct the extent of reaction $x_{u}$, the discounting factor $\lambda$, the uncontrolled states $x_{u}$, and the reaction rate $r$. Therefore, the estimation of $n_{um}$ in combination with $n_{um}^{T}$ is possible.

Then, the resulting overall dynamics become

$$\dot{\hat{x}}_{u} = A_{u} \hat{x}_{u} + B_{u} \dot{r},$$

where $\hat{x}_{u}$ is dependent on $q_{e} \in \mathcal{K}(\beta)$, and $\hat{x}_{u} \in \mathbb{R}^{R + r}$. Moreover, this model is now suitable to develop the AO, and it does not contain the nonlinearities arising from the reaction rate $r$. The mathematical formulation of the AO is then given by Table 1.

<table>
<thead>
<tr>
<th>Table 1. Asymptotic Observer (AO) Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>model</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>$x_{u} = A_{u}(\beta) \hat{x}<em>{u} + B</em>{u}$</td>
</tr>
<tr>
<td>$y = C_{x} \hat{x}<em>{u} + C</em>{y} \dot{r}$</td>
</tr>
<tr>
<td>$\dot{\hat{r}} = m_{y} \hat{x}<em>{u} + m</em>{r} \dot{r}$</td>
</tr>
</tbody>
</table>

The advantage of using this representation is that no direct information on the reaction rate $r$ is necessary in the observer design. The estimation of $\hat{x}_{u}$ is dependent on $q_{e} \in \mathcal{K}(\beta)$. The latter variable is a function of the measured number of moles $n_{u}$. The computation of $q_{e}$ is explained through the following lemma.

**Lemma 2.** Consider the asymptotic observer given in Table 1, where $\hat{x}_{u} = \beta \hat{z}$, and $q_{e}$, with rank($\beta)$ = 1, and $q_{e} \neq 0$. Then, the state vector $\hat{y}_{e}$ can be written as

$$q_{e} = \begin{bmatrix} n_{um}^{T} \\ \lambda \end{bmatrix} \begin{bmatrix} n_{um} - W_{um} x_{u} - n_{0,um} \lambda \\ W_{um} x_{u} + n_{0,um} \end{bmatrix} \beta,$$

Notice that, to guarantee the existence of the left pseudoinverse of $n_{um}^{T}$, $\text{rank}(n_{um}) = R_{S}$. As a consequence, $S_{m} \geq R_{S}$, i.e., the number of measured species must be larger or equal to the number of independent reactions.

Moreover, the asymptotic estimator is stable and convergent if $\theta > 0$. This condition corresponds to the detectability condition from the model described by eq 2.
Asymptotic observers have been extensively studied in the literature (see, for example, the works of Bhatt [30] and Dochain et al. [31]). The design presented here is similar in structure to those described in the literature, but it uses temperature measurements rather than enthalpy measurement, exploiting the transformation variable $Z$ to reconstruct the states. Generally, this facilitates implementation, since enthalpy measurement is not available during plant operation.

4.2. Reaction Rate Estimator (Disturbance Estimation). Recall that the reaction rate is considered to be a disturbance signal given by $d = V_r$. In order to simplify the modeling of the reaction rate, it is assumed that $r \in \mathbb{D}$, with $\mathbb{D}$ being a convex and compact set. This implies that the reaction dynamics are asymptotically stable. Therefore, the representation in eq (2) is written as

$$
\begin{align*}
\dot{x} &= \begin{bmatrix} A(\theta) & D \\ 0 & R(\theta) \end{bmatrix} x + \begin{bmatrix} B \\ 0 \end{bmatrix} u \\
\dot{y} &= C_m x + \begin{bmatrix} \xi_m \end{bmatrix}
\end{align*}
$$

(30)

where $R(\theta) = -Q_{\mu}/Q_r$. Based on eq (30), the reaction rate estimator has the form described by Table 2.

### Table 2. Reaction Rate Estimator (RRE) Structure

<table>
<thead>
<tr>
<th>model</th>
<th>disturbance estimator</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_i = A_i(\theta)x_i + B_iu$</td>
<td>$\dot{x}_i = A_i(\theta)x_i + B_iu + L(\theta)(y - \hat{y})$</td>
</tr>
<tr>
<td>$y_m = y = C_m x_i$</td>
<td>$\hat{y} = C_m \hat{x}_i$</td>
</tr>
</tbody>
</table>

This estimator takes the state information from the estimates provided by the AO. Because of the sequential strategy implemented here, the convergence of the RRE must be faster than that of the AO. This can be ensured tuning the observer gain $L(\theta)$. However, the selection of $L(\theta)$ is restricted by the structure of the matrix $C_m$, which is displayed in the following theorem.

**Theorem 4.** Consider the model given in Table 2, and assume that $\theta$ is measured. If the matrix $C_m$ is full-column rank, then there exists a parametric observer gain that is defined as $L(\theta) = \{L_{i1}^T(\theta) \: L_{i2}^T(\theta)\}^T$ with $L_1 = (\mu - \theta)C_m$ and $L_2 = (\mu - \theta)D^T C_m^T$, where $\mu$ is the desired pole location, such that $|\mu| > |\theta|$.

The proof of Theorem 4 can be found in Appendix B.

5. CASE STUDY

Let us consider a nonisothermal continuously stirred tank reactor (CSTR) where a reversible reaction $A + B \rightleftharpoons C + D$ occurs. The system has four species $n_A$, $n_B$, $n_C$, and $n_D$ ($S = 4$), one independent reaction ($R_1 = 1$), and two constant and independent inlets $n_{in,1}$ and $n_{in,2}$ ($p = 2$) of $A$ and $B$. The reaction rates obey the mass-action principle and the Arrhenius law, and are given by the expressions

$$
r = k_jC_A C_B - k_j C_C C_D
$$

$$
k_{j,r} = k_{j,0} \exp \left( -\frac{E_{j,r}}{RT} \right)
$$

where $k_{j,0}$ is the pre-exponential factor in the Arrhenius law, and $E_{j,r}$ is the activation energy of the reaction. In this example, the numerical values of the parameters are given in Table 3.

The matrices $N$ and $W_{in}$ are given by

### Table 3. Parameters of the Case Study

<table>
<thead>
<tr>
<th>parameter</th>
<th>values and units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{j,r}$</td>
<td>$6.06 \times 10^5$ m$^3$ kmol$^{-1}$ h$^{-1}$</td>
</tr>
<tr>
<td>$k_{i,j}$</td>
<td>$9.84 \times 10^5$ m$^3$ kmol$^{-1}$ h$^{-1}$</td>
</tr>
<tr>
<td>$E_{j,r}$</td>
<td>$63800$ kJ kmol$^{-1}$</td>
</tr>
<tr>
<td>$E_j$</td>
<td>$71710$ kJ kmol$^{-1}$</td>
</tr>
<tr>
<td>$R$</td>
<td>$8.314$ kJ kmol$^{-1}$ K$^{-1}$</td>
</tr>
</tbody>
</table>

The initial conditions are $n_0 = [0.5, 1, 0.5, 0]^T$ kmol, and $T_0 = 373$ K. The states, outputs, and inputs of the system are defined as $x = [n_A n_B n_C n_D T]^T$, $y = [n_{in,1} n_{in,2}]^T$ and $u = [u_{in,1} u_{in,2} Q]^T$. In this example, the boundaries for the outlet flow and mass are given by $\bar{u}_{out} = \{1 \leq u_{out} \leq 20\}$ and $M = \{50 \leq m \leq 105\}$; therefore, the vertices $\sigma_i$ of the polytope are $\{0.02, 0.0095, 0.4, 0.1905\}$. In order to test the control strategy, the desired poles $\theta$ are selected be equal to $-1$, and set point changes in $n_A$ and $n_B$ are done at $200$ h, and at $400$ h for $T$. Figures 5, 6, 7, and 8 show the simulation results for outputs $y$, inputs $u$, and the parameter $\theta$ of the MPC (eq (14)) (called MPC-LPV) and the same controller assuming $\theta$ constant in the model used by the controller (called MPC-LTI). Clearly, the performance of the MPC-LPV is better than MPC-LTI. The main reason for that is the MPC-LTI controller is not taking variations in $\theta$ into account. This leads to having a mismatch between the LTI model and the nonlinear model. Therefore, the MPC-LTI controller is taking decisions that affect $\theta$ drastically (see Figure 8).

It is important to highlight that the constant $\theta$ for MPC-LPV is not the same as that for MPC formulations that use models obtained by linearization or by system identification around an operating point. The modeling approach used here considers $r$ to be a disturbance. Therefore, in this paper, we have compared the MPC-LPV procedure with another technique with the same considerations, i.e., considering $r$ to be a disturbance (MPC-LTI).
6. CONCLUSION

This paper proposes a model predictive control (MPC) strategy that is able to take into account parametric variations that affect the plant dynamics. The approach exploits the extent representation, given its decoupled dynamics. This representation allows for the detection of uncontrollable modes, and even time-scale separation in the process dynamics. To deal with parameter variation inherent to the extent-based LPV representation, state-feedback and feed-forward laws are developed to remove the effect of the time-varying dynamics the process. The state and disturbance information necessary to compute the control laws are estimated by means of observers. The parametric control laws allow for the design of a linear MPC with quadratic cost at the expense of introducing nonlinear state and parameter constraints. The MPC design is further simplified by limiting the parameter to a polytopic set that can be represented by intersections of multiple polyhedrons. This very simple but key step helps to formulate a linear MPC problem with linear constraints, and finally it is solved using quadratic programming.

The development of the MPC-LPV controller is tested and compared against an MPC-LTI controller in a nonisothermal CSTR where a single equilibrium reaction is performed. The idea is to demonstrate how the MPC-LPV outperforms the traditional MPC-LTI because of the incorporation of the varying parameter in the control loop. This example shows how this small piece of information is crucial to designing reliable control systems for reaction systems.

This approach is appealing because it provides a way of embedding dynamic information in the model-based control design, while accounting for different scenarios in the reaction system. Furthermore, the contribution of this work is the complexity reduction of the control strategy by means of LPV models, compared to more-traditional MPC implementation. The development takes advantage of sound properties of physical reaction system: the decoupled dynamic spaces, the boundedness of the reaction rate, and the general polytopic nature of the parameter set.

APPENDIX A

Proof of Theorem 3: Observability

Let \( C_m = \left[ \begin{array}{c} N_m^T \ W_{u,m} \ n_{0,m} \ 0 \end{array} \right] \in \mathbb{R}^{(S_m+1) \times (R_i+p+2)} \), and let \( A \in \mathbb{R}^{R_i+p+2} \) be the diagonal state matrix.

Let \( \text{rank}(C_m) = R_i + p + 2 \), and assume that the pair \((A,C_m)\) is not observable. Because of the lack of observability, by the Popov–Belevich–Hautus (PBH) theorem, there exists a vector \( v \neq 0 \) such that

\[
A v = -\theta v, \quad C_m v = 0
\]

However, since \( C_m \) is full-column rank, it follows that \( \text{rank}(C_m) = R_i + p + 2 \Leftrightarrow \ker(C_m) = \emptyset \). Hence, only \( v = 0 \) is contained in the kernel of \( C_m \). This contradicts the PBH theorem and the assumption of unobservability of the pair \((A,C_m)\).
APPENDIX B

Proof of Theorem 4: L(θ)

Using Theorem 3, the system is observable provided that rank(Cm) = R1 + p + 2, i.e., Cm is full-column rank. Let us define the error dynamics as \( \hat{x}_t = x_t - \hat{x}_t \); therefore,

\[
\dot{\hat{x}}_t = (A - LC)x_t
\]

The error dynamics converge asymptotically and arbitrarily fast by placing the poles of A using L. The state error matrix A - LC can be made equal to a matrix whose eigenvalues are at desired values. Let A = A1Cm and M and M1 be matrices whose eigenvalues are the observer desired pole locations. Hence, for some L1 and L2, the closed-loop matrix can be made equal to

\[
\begin{pmatrix}
A & D \\
-L_2 C_m & R
\end{pmatrix} = \begin{pmatrix}
M_1 & D \\
-(M_2 - R)D M_1 & R
\end{pmatrix}
\]

Performing block LDU decomposition on the left-hand side matrix, we get

\[
\begin{pmatrix}
I & \hat{A}D \\
-L_2 C_m A^{-1} & 0
\end{pmatrix} = \begin{pmatrix}
M_1 & D \\
-(M_2 - R)D M_1 & R
\end{pmatrix}
\]

Multiplying both sides with the inverse of the block upper triangular matrix on the right-hand side gives us

\[
\begin{pmatrix}
A & 0 \\
-L_2 C_m & R + L_2 C_m A^{-1}D
\end{pmatrix} = \begin{pmatrix}
M_1 & D \\
-(M_2 - R)D M_1 & R
\end{pmatrix}
\]

\[
\begin{pmatrix}
M_0 & 0 \\
-L_2 C_m & R + L_2 C_m A^{-1}D
\end{pmatrix} = \begin{pmatrix}
M_1 & D \\
-(M_2 - R)D M_1 & R
\end{pmatrix}
\]

The matrix on the right-hand side of the equation can be made block triangular if we choose L1 = (A - M1)Cm†. Replacing L1 in A = A - L1Cm it follows that A = A - (A - M1)Cm† = M1, and -M1A⁻¹D + D = -M1M1⁻¹D + D = 0. Thus, eq B-2 results in

\[
\begin{pmatrix}
M_0 & 0 \\
-L_2 C_m & R + L_2 C_m M_0 D
\end{pmatrix} = \begin{pmatrix}
M_1 & D \\
-(M_2 - R)D M_1 & R
\end{pmatrix}
\]

Furthermore, notice that L2 = (M2 - R)D M1 Cm† ensures that -L2 Cm = -(M2 - R)D M1 Cm and that R + L2 Cm A⁻¹D = R + (M2 - R)D M1 Cm A⁻¹D = M2. Finally, the closed-loop observer dynamics in eq B-3 are given by

\[
\begin{pmatrix}
M_0 & 0 \\
-(M_2 - R)D M_1 & M_2
\end{pmatrix}
\]

Note that the matrix is block diagonal, which implies that

\[
\text{eig} \left( \begin{pmatrix}
M_0 & 0 \\
-(M_2 - R)D M_1 & M_2
\end{pmatrix} \right) = \text{eig}(M_0) \cup \text{eig}(M_2)
\]

In particular, let us establish M1 = -μ1Cm and M2 = -μ2Cm. Since A = -θCm and R = -θR, it is desired that |μ| > θ. Hence, the observer is given by L1 = (μ - θ)Cm and L2 = (μ - θ)D Cm.

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Notes
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