# Control of Homogeneous Reaction Systems using Extent-Based LPV Models \*

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## Abstract:

This paper proposes the use of the extent decomposition on homogeneous reaction systems for control purposes. The decomposition results in a Linear Parameter-Varying (LPV) representation, upon which parametric feedback and feedforward strategies are developed. In the first part of the paper, three different ways to obtain the Extent-Based LPV (ELPV) representation of the system are proposed. The representation is advantageous since the physical meaning of all the variables are kept, and it has a Jordan type of structure which is used to establish controllability conditions. In the second part, general parametric feedback and feedforward control laws are proposed for the ELPV system. The nonlinear state-parameter dependence is first considered in the feedback term. This fact allows converting the original ELPV system into a Linear Time Invariant (LTI) system, which is used to design optimal control laws for reference tracking. Finally, the performance of the control strategy for the ELPV system is illustrated in simulation and compared with a controller based on a constant-parameter LTI model (ELTI).

*Keywords:* Linear Parameter Varying (LPV) Systems, Extent-based models, Homogeneous Reaction Systems.

## 1. INTRODUCTION

The use of rigorous models for online model-based applications, such as control and monitoring, is an ongoing research area in process control. This is not surprising as rigorous models contain valuable information to predict states and anticipate disturbances. On the other hand, most industrial processes are driven by chemical kinetics, thermodynamics and transport phenomena, which are described by nonlinear differential algebraic equations. Despite the computational resources, these kinds of models are in general inconvenient for online modelbased applications, because the implementation of nonlinear strategies in the process industry remains a big challenge. Therefore, a good alternative is to find different representations of rigorous models using state transformation such as projection methods, state space decomposition, or the inclusion of empirical linear models (grey-box modeling). These methods have been reviewed by Marquardt (2002). Nevertheless, this type of approaches presents several disadvantages. Perhaps one of the most relevant is the loss of physical interpretation of the transformed variables. This issue becomes very important when imposing constraints on the control design, and during process monitoring. An attractive alternative is the concept of extent decomposition (Srinivasan et al., 1998), which arises as a useful tool to deal with this problem. The extent approach is derived from the work on reaction variant-invariant decomposition of reaction systems for process analysis (Asbjørnsen, 1972; Fjeld et al., 1974) and allows for the calculation of the contribution of every phenomenon in the process independently. For example, the mole balance equation of a Continuous Stirred Tank Reactor (CSTR) can be decomposed into its phenomenological contributions (reaction, inlet flow, and outlet flow) (Srinivasan et al., 1998; Amrhein et al., 2010). This separation by phenomena is a subspace separation using a linear transformation that allows the decoupling of relevant variables for control (inputs, outputs, and disturbances) while maintaining the physical meaning of the variables. This approach presents many advantages, such as model reduction, identification of reaction systems from measured data, parametric sensitivity analysis among others. The extent decomposition is used in this paper to propose a general framework to control homogeneous reaction systems.

Moreover, from the control perspective, the extent decomposition allows for the development of a Linear Parameter-Varying (LPV) representation with a diagonal state matrix. The LPV systems describe a family of linear systems parametrized by a vector of parameters (Tóth, 2010). Nonetheless, the identification of the LPV system is not an easy task, and it is possibly the most challenging aspect of this kind of systems, see for example (Bamieh and Giarre, 2002; Balas et al., 2003; Bruzelius et al., 2004; Tóth et al., 2010; Bachnas et al., 2014). In this paper, the LPV representation mentioned above for homogeneous reaction system based on extents is proposed. This approach helps to reduce the identification procedure due to two main reasons: the derivation of the model is natural, resulting directly from First Principle Models (FPM), and the second one is the physical meaning of the LPV system variables and parameters.

Normally, LPV systems are controlled by gain-scheduling approaches (Apkarian and Gahinet, 1995; Apkarian et al., 1995; Apkarian and Adams, 1998). However, in this paper, the particular structure of the LVP system matrices and the physical interpretation of its parameters are used to propose parametric state feedback and feedforward laws. The final result is an

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LTI representation of the closed-loop system, which is used to design optimal control laws for reference tracking.

The paper is organized as follows: In section 2 the extent of reaction and inlets are introduced and based on the extent concept, the LPV representation for a homogeneous reaction system is presented. In section 3 the control strategy for extentbased LPV systems is proposed. Here, the diagonal form of the LPV systems is exploited to propose parametric feedback and feedforward laws. In section 4 the control strategy for Extent-Based LPV systems (ELPV) is illustrated in the simulation results and compared with a controller based on a constantparameter LTI model (ELTI). Finally, in section 5 the conclusions are presented.

## 2. EXTENT-BASED LPV REPRESENTATION FOR A HOMOGENEOUS REACTION SYSTEM

The extent of reaction is a measure of the degree of completion of any reaction. In other words, they quantify the progress of a reaction while it consumes the reactants (Vandezande et al., 2013). The extent of reaction can be applied directly to a chemical reaction process where the evolution of moles in time is solely related to the reaction and the amount of reacting mixture. Under this circumstance, the system is uniquely driven by the chemical reaction. Hence, the dynamic space can be split into two subspaces, namely the reaction variant and reaction invariant. The reaction variants coincide with the extent of reaction if and only if the initial conditions of the former are strictly zero. Moreover, if the process contains an inlet stream, then the change of moles in time is affected by two independent dynamics, reaction and inlet flow. Under this situation, the reactor dynamics cannot be expressed in terms of the extent of reaction directly. To circumvent this situation, the concept of extent is broadened to the extents of reaction, and inlet flows (Amrhein et al., 2010).

### 2.1 Extent of Reaction and Inlet Flow

Consider the mole balance equation for a homogeneous reaction system with S species,  $R_I$  independent reactions, p independent inlet flows and one outlet flow, given by:

$$\dot{n}(t) = V(t)N^{\mathsf{T}}r(t) + W_{in}u_{in}(t) - \frac{u_{out}(t)}{m(t)}n(t) \quad n(0) = n_0 \quad (1)$$

where  $n \in \mathbb{R}^{S}$  is the number of moles, *V* is the reaction mixture volume;  $r \in \mathbb{R}^{R_I}$  is the reaction rate vector;  $u_{in} \in \mathbb{R}^p$  and  $u_{out} \in$ volume;  $F \in \mathbb{R}^{n}$  is the reaction rate vector;  $u_{in} \in \mathbb{R}^{r}$  and  $u_{out} \in \mathbb{R}^{1}$  are the inlet and outlet mass flows; *m* is the reacting mixture mass;  $N \in \mathbb{R}^{R_{l} \times S}$  is the stoichiometric coefficient matrix and  $W_{in} \in \mathbb{R}^{S \times p}$  is the inlet composition matrix defined as  $W_{in} = M_{w}^{-1}w_{in}$ ;  $M_{w} \in \mathbb{R}^{S \times S}$  is the diagonal molecular weight matrix and  $w_{in} \in \mathbb{R}^{S \times p}$  the matrix of weight fraction. Equation (1) is nonlinear due to the reaction rate represented in the vector r(t). One could find a linear transformation  $\mathscr{T}$  such that the system can be expressed in terms of new states that each of them only evolves with respect to the reaction and the inlet flow as follows:

$$\begin{bmatrix} x_r \\ x_{in} \\ x_{inv} \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{T}_1^{\mathsf{T}} \\ \mathcal{T}_2^{\mathsf{T}} \\ \mathcal{T}_3^{\mathsf{T}} \end{bmatrix}}_{\mathcal{T}} (n - \lambda n_0) \Longrightarrow \begin{bmatrix} x_r \\ x_{in} \\ \lambda \end{bmatrix} = \underbrace{\begin{bmatrix} \mathcal{T}_1^{\mathsf{T}} \\ \mathcal{T}_2^{\mathsf{T}} \\ \mathcal{T}_2^{\mathsf{T}} \\ \mathcal{T}_2^{\mathsf{T}} \end{bmatrix}}_{\mathcal{T}_e} n \quad (2)$$

where  $x_r \in \mathbb{R}^{R_I}$  is the extent of reaction,  $x_{in} \in \mathbb{R}^p$  is the extent of inlet flow,  $x_{inv} \in \mathbb{R}^{S-R_I-p}$  is the extent of reaction and inlet flow

invariants. In addition,  $\lambda \in [0,1]$  is the initial conditions discounting factor, and following the definition given by Amrhein et al. (2010),  $\lambda$  can be defined in terms of the  $x_{inv}$  as,

$$\lambda = \frac{\mathbf{1}_{S-R-p}^{\mathsf{T}} \mathbf{x}_{inv}}{\mathbf{1}_{S-R-p}^{\mathsf{T}} \mathscr{T}_{3}^{\mathsf{T}} \mathbf{n}_{0}} + 1$$

The relationship between with  $\mathscr{T}$  and  $\mathscr{T}_{\ell}$  is given by (Amrhein et al., 2010),

$$\begin{aligned} \mathcal{T}_{1_e}^{\mathsf{T}} &= \mathcal{T}_1^{\mathsf{T}} (I_S - n_0 \mathcal{T}_{3_e}^{\mathsf{T}}) \\ \mathcal{T}_{2_e}^{\mathsf{T}} &= \mathcal{T}_2^{\mathsf{T}} (I_S - n_0 \mathcal{T}_{3_e}^{\mathsf{T}}) \\ \mathcal{T}_{3_e}^{\mathsf{T}} &= \frac{\mathbf{1}_{S-R-p}^{\mathsf{T}} \mathcal{T}_3^{\mathsf{T}}}{\mathbf{1}_{S-R-p}^{\mathsf{T}} \mathcal{T}_3^{\mathsf{T}} n_0} \end{aligned}$$

where  $\mathcal{T}_{l_{e}}$  is the transformation matrix of the reaction space,  $\mathscr{T}_{2_e}$  is the transformation matrix of the inlet space, and  $\hat{\mathscr{T}}_{3_e}$  is the transformation matrix of the reaction and inlet flow invariant space, all with discounted initial conditions  $n_0$ .

Assumption 1. In this work, it is assumed that  $1_{S-R-n}^{\mathsf{T}} \mathscr{T}_{3}^{\mathsf{T}} n_0 \neq 1$ 0. This condition is satisfied if and only if rank $([W_{in}^{T}, n_{0}]) = p + p$ 1 (Amrhein et al., 2010).

The nonlinear differential equation (1) for the mole balance is transformed to:  $( \star )$ 

$$\dot{x}_{r}(t) = -\frac{u_{out}(t)}{m(t)}x_{r}(t) + V(t)r(t), \quad x_{r}(0) = 0$$
  
$$\dot{x}_{in}(t) = -\frac{u_{out}(t)}{m(t)}x_{in}(t) + u_{in}(t), \quad x_{in}(0) = 0 \quad (3)$$
  
$$\dot{\lambda}(t) = -\frac{u_{out}(t)}{m(t)}\lambda(t), \qquad \lambda(0) = 1$$

Now, the moles can be calculated using the extents from the following equation:

$$n(t) = N^{\mathsf{T}} x_r(t) + W_{in} x_{in}(t) + n_0 \lambda(t)$$
(4)

The Figure 1 shows a scheme of the extents transformations.



Fig. 1. Decomposition of the space of numbers of moles into reaction space, inlet-flow space, and one-dimensional space describing the discounting of  $n_0$ 

The aforementioned transformation requires the following conditions:

•  $\mathscr{T}_{1_a}^{\mathsf{T}} N^{\mathsf{T}} = I_R, \ \mathscr{T}_{1_a}^{\mathsf{T}} W_{in} = \mathbf{0}_{R \times p}$ 

• 
$$\mathscr{T}_{2}^{\mathsf{T}}N^{\mathsf{T}} = 0_{p \times R}, \ \mathscr{T}_{2}^{\mathsf{T}}W_{in} = I_{p}$$

- $\mathcal{T}_{2_e}^{\mathsf{T}} \mathbb{N}^\mathsf{T} = 0_{1 \times R}, \ \mathcal{T}_{2_e}^\mathsf{T} \mathbb{W}_{in} = 0_{1 \times p}$   $\mathcal{T}_{3_e}^\mathsf{T} \mathbb{N}^\mathsf{T} = 0_{1 \times R}, \ \mathcal{T}_{3_e}^\mathsf{T} \mathbb{W}_{in} = 0_{1 \times p}$   $\operatorname{rank}([\mathbb{N}^\mathsf{T} \ \mathbb{W}_{in}]) = \mathbb{R}_I + p < S$   $\operatorname{rank}([\mathbb{N}^\mathsf{T} \ \mathbb{W}_{in} \ n_0]) = \mathbb{R}_I + p + 1.$

The calculation of the matrices  $\mathcal{T}_i$ ,  $\forall i = 1, 2, 3$  can be done by means of a singular value decomposition of  $N^{T}$  and  $W_{in}$ . Details about this procedure can be found in (Srinivasan et al., 1998) and (Amrhein et al., 2010). Notice the decoupling effect that the extent of reaction and inlet flow has on the system dynamics. Under this representation, the independent evolution of the reaction, the inlet flow, and outlet flow can be easily observed.

#### 2.2 Inclusion of Energy Balance

So far it has been shown how the extents of reaction and inlet are used in isothermal systems. Let us make the system description more realistic combining the extent representation equations (3) with the energy balance as follows:

$$\begin{aligned} \dot{x}_r &= -\theta x_r + V(t)r(t) \\ \dot{x}_{in} &= -\theta x_{in} + u_{in}(t) \\ \dot{\lambda} &= -\theta \lambda \\ \dot{T} &= -\theta T(t) + \alpha u_{in}(t) - \beta V(t)r(t) + \gamma Q_{in} \end{aligned} \tag{5}$$

where  $\theta = \frac{u_{out}(t)}{m(t)}$ ,  $\alpha = \frac{C_{p_{in}}T_{in}}{m(t)C_{p_{mix}}}$ ,  $\beta = \frac{\Delta H_f^{\ominus}N^{\intercal}}{m(t)C_{p_{mix}}}$ ,  $\gamma = \frac{1}{m(t)C_{p_{mix}}}$ ,  $C_{p_{in}}T_{in} = [C_{p_{in},1}T_{in,1}, \dots, C_{p_{in},p}T_{in,p}] \in \mathbb{R}^{1 \times p}$ ,  $\Delta H_f^{\ominus} \in \mathbb{R}^{1 \times S}$  is the vector of standard enthalpy of formation and  $T(0) = T_0$ .

Assumption 2. In this work, the parameters  $\alpha$ ,  $\beta$  and  $\gamma$  are considered constant. For that a local controller for the total mass is assumed such that m(t) = m.

### 2.3 Extent-based LPV representations

There are three ways to get an LPV representation for the set of equations (5). The first one is based on a time scale separation of the dynamics of the system, the second is using a change of variable to eliminate the reaction rate from the equations, and the third one is assuming the reaction rate directly as a disturbance. In the following, every method is explained.

**Remark** 1. The initial condition discounting factor  $\lambda$  does not depend on the manipulated variables of the system  $u_{in}$  and  $Q_{in}$ , therefore, and for control purposes, the differential equation of  $\lambda$  can be removed from the state space representation of the system in (5).

**1.Time scale separation:** In this case, the dynamics of  $x_r$  is much faster than  $x_{in}$  and T, therefore  $\dot{x}_r \approx 0$  compared to  $\dot{x}_{in}$  and  $\dot{T}$ . Therefore, rearranging (5), we obtain the following LPV system,

$$\begin{bmatrix} \dot{x}_{in} \\ \dot{T} \end{bmatrix} = \begin{bmatrix} -\theta I_p & 0 \\ 0 & -\theta \end{bmatrix} \begin{bmatrix} x_{in} \\ T \end{bmatrix} + \begin{bmatrix} I_p & 0 \\ \alpha & \gamma \end{bmatrix} \begin{bmatrix} u_{in} \\ Q_{in} \end{bmatrix} + \begin{bmatrix} 0 \\ \beta \theta \end{bmatrix} x_r$$

$$\begin{bmatrix} n \\ T \end{bmatrix} = \begin{bmatrix} W_{in} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{in} \\ T \end{bmatrix} + \begin{bmatrix} N^{\mathsf{T}} \\ 0 \end{bmatrix} x_r + \begin{bmatrix} n_0 \\ 0 \end{bmatrix} \lambda$$
(6)

where  $I_p \in \mathbb{R}^{p \times p}$  is the identity matrix. Finally, system (6) can be seen as:

$$\dot{x} = A(\theta)x + Bu + D(\theta)d$$
  

$$y = Cx + C_d d + C_\lambda \lambda$$
(7)

with  $x \in \mathbb{R}^{p+1}$ ,  $u \in \mathbb{R}^{p+1}$ ,  $y \in \mathbb{R}^{S+1}$ ,  $\theta \in \mathbb{R}^1$  and  $d \in \mathbb{R}^{R_l}$ , where  $C = \begin{bmatrix} W_{in} & 0 \\ 0 & 1 \end{bmatrix}$ ,  $C_d = \begin{bmatrix} N & 0 \end{bmatrix}^{\mathsf{T}}$  and  $C_{\lambda} = \begin{bmatrix} n_0^{\mathsf{T}} & 0 \end{bmatrix}^{\mathsf{T}}$ .

**2.***Change of variable:* When  $\dot{x}_r$  cannot be neglected in the model, the nonlinear reaction rate r(t) plays an important role in the plant's behavior. Thus we want to find a transformation

such that  $x_r$  can be expressed linearly in terms of a new variable. Let us define a change of variable z as:

$$z = \beta x_r + T = \mathscr{Z} \begin{bmatrix} x_r \\ T \end{bmatrix}$$
(8)

where  $\mathscr{Z} = [\beta \ 1]$ . Then, taking derivatives of both sides of equation (8) with respect to time, and only considering time-varying the states  $x_r$  and T, we obtain,

$$\dot{z} = -\theta z + \alpha u_{in} + \gamma Q_{in}$$

Assumption 3. During the differentiation of z, the mass m and heat capacity of the mixture  $C_{P_{mix}}$  are assumed constant, i.e. the term  $m(t)C_{P_{mix}}$  does not vary significantly during the operation.

Stacking the dynamics in a vector  $x_{in}$ , and z, we obtain the following model,

$$\begin{bmatrix} \dot{x}_{in} \\ \dot{z} \end{bmatrix} = \begin{bmatrix} -\theta I_p & 0 \\ 0 & -\theta \end{bmatrix} \begin{bmatrix} x_{in} \\ z \end{bmatrix} + \begin{bmatrix} I_p & 0 \\ \alpha & \gamma \end{bmatrix} \begin{bmatrix} u_{in} \\ Q_{in} \end{bmatrix}$$
$$\begin{bmatrix} n \\ T \end{bmatrix} = \begin{bmatrix} W_{in} & n_0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} x_{in} \\ \lambda \end{bmatrix} + \begin{bmatrix} N^{\mathsf{T}} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_r \\ T \end{bmatrix}$$
(9)

**Remark** 2. Using equation (8), we can find an expression for  $[x_r \ T]^{\mathsf{T}}$  in terms of *z*. However,  $\mathscr{Z}$  cannot be set to 1 by means of its pseudo-inverse.  $\mathscr{Z}$  is full row-rank, thus it has a right pseudo-inverse, i.e.  $\mathscr{Z} \mathscr{Z}^{\dagger} = 1$  ( $\dagger$  represents the Moore-Penrose psedoinverse). Therefore, we need to solve an underdetermined equation to obtain an approximate value of *z*.

Finally, system (9) can be seen as:

$$\dot{x} = A(\theta)x + Bu$$
  

$$y = C_z x + C_\lambda \lambda$$
(10)

with  $x \in \mathbb{R}^{p+1}$ ,  $u \in \mathbb{R}^{p+1}$  and  $y \in \mathbb{R}^{S+1}$ . Where  $C_{\lambda} = [n_0^{\mathsf{T}} \ 0]^{\mathsf{T}}$ ,  $C_z = \begin{bmatrix} [W_{in}^{\mathsf{T}} \ 0]^{\mathsf{T}} | C_N \mathscr{Z}^{\dagger} \end{bmatrix}$ , and  $C_N = \begin{bmatrix} N^{\mathsf{T}} \ 0 \\ 0 \ 1 \end{bmatrix}$ .

**3.***Reaction rate as a disturbance:* In this case the reaction rate r(t) is assumed as a disturbance such that the system (5) can be written as:

$$\begin{bmatrix} \dot{x}_r \\ \dot{x}_{in} \\ \dot{T} \end{bmatrix} = \begin{bmatrix} -\theta I_{R_I} & 0 & 0 \\ 0 & -\theta I_p & 0 \\ 0 & 0 & -\theta \end{bmatrix} \begin{bmatrix} x_r \\ x_{in} \\ T \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ I_p & 0 \\ \alpha & \gamma \end{bmatrix} \begin{bmatrix} u_{in} \\ Q_{in} \end{bmatrix} + \begin{bmatrix} I_{R_I} \\ 0 \\ \beta \end{bmatrix} Vr$$
$$\begin{bmatrix} n \\ T \end{bmatrix} = \begin{bmatrix} W_{in} & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{in} \\ T \end{bmatrix} + \begin{bmatrix} N^{\mathsf{T}} \\ 0 \end{bmatrix} x_r + \begin{bmatrix} n_0 \\ 0 \end{bmatrix} \lambda$$
(11)

Note again that the manipulated variables  $u_{in}$  and  $Q_{in}$  do not have any effect on the extents of reaction  $x_r$ , 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 (11), where the reaction rate r is assumed as a bounded disturbance  $r \in \mathbb{D}$ , with  $\mathbb{D}$  convex and compact. Then, if  $\theta \neq 0$ , the system (11) 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  $x_r$ .

The proof follows along the lines of the Hautus test of controllability (Hautus, 1970). However, the proof is omitted due to the space limitations. Finally, separating the uncontrollable states  $(x_r)$ , the system (11) can be seen as:

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

$$y = Cx + C_u x_u$$
(12)

with  $x \in \mathbb{R}^{p+1}$ ,  $u \in \mathbb{R}^{p+1}$ ,  $y \in \mathbb{R}^{S+1}$  and  $d \in \mathbb{R}^{R_I}$ , where  $C_u = \begin{bmatrix} N^{\mathsf{T}} & n_0 \\ 0 & 0 \end{bmatrix}$  and  $x_u = [x_r \ \lambda]^{\mathsf{T}}$  are the uncontrollable states.

**Remark** 3. The LPV representation (7), (10) and (12) are equivalent representations if feedforward controllers are included to eliminate the disturbances  $x_r$  and r in (6) and (11). Therefore, in the rest of this work, we will be working with the LPV representation (12).

Assumption 4. In this work, it is assumed that the number of moles *n* and the temperature *T* can be measured, therefore, the extent of reaction  $x_r$ , the discounting factor  $\lambda$ , the uncontrollable states  $x_u$ , and the reaction rate *r* can be estimated directly from *n* and  $\mathcal{T}_e$ .

### 3. CONTROL OF EXTENT-BASED LPV SYSTEMS

#### 3.1 Parametric State Feedback and Feedforward laws

In this section, a parametric state feedback policy is proposed to eliminate the parameter dependency of the *A* matrix. The LPV system (12) is converted into a diagonal, controllable LTI system that can be used to formulate a control strategy for the system (1). Also, a feedforward law is proposed to reject the disturbance *d*. The elimination of the parameter  $\theta$  of the *A* matrix is stated in the following theorem:

**Theorem** 2. Consider the homogeneous reaction system given by the set of equations (12), where the reaction rate *r* is assumed as a measured disturbance. Then, if  $\gamma \neq 0$ , there exist a parametric feedback gain  $K(\theta) \in \mathbb{R}^{p+1 \times p+1}$ , and a feedforward gain  $K_d \in \mathbb{R}^{p+1 \times R_I}$  such that  $u = K(\theta)x + v + K_d d$ , and the closed loop representation of the system (12) has an equivalent LTI representation given by,

$$\dot{x} = \begin{bmatrix} \vartheta I_p & 0 \\ 0 & \vartheta \end{bmatrix} x + \begin{bmatrix} I_p & 0 \\ \alpha & \gamma \end{bmatrix} v$$

$$y = Cx + C_u x_u$$
(13)

where  $\vartheta$  are the constant desired poles of the closed loop system, and  $v \in \mathbb{R}^p$  are the new inputs of the system.

**Proof.** Let  $K(\theta) \in \mathbb{R}^{p+1 \times p+1}$  and  $K_d \in \mathbb{R}^{p+1 \times R_I}$  be the parametric feedback and feedforward gains, then, the input vector *u* of the system can be written as,

$$u = \underbrace{K(\theta)x + v}_{\text{Feedback}} \underbrace{+K_d d}_{\text{Feedback}}$$
(14)

Replacing (14) in (12), we can write the LPV model (12) as,

$$\dot{x} = (A(\theta) + BK(\theta))x + Bv + (BK_d + D)d \tag{15}$$

Now, to eliminate the parameter dependency of the A matrix and the disturbance d from the equation (15) the following conditions must be accomplished:

$$A(\theta) + BK(\theta) = \begin{bmatrix} \vartheta I_p & 0 \\ 0 & \vartheta \end{bmatrix}$$
$$BK_d + D = 0$$

Defining the matrix  $A_{cl} = A(\theta) + K(\theta)B$ , then,

$$K(\theta) = B^{\dagger} (A_{cl} - A(\theta))$$
  
 $K_d = -B^{\dagger} D$ 

Now, if  $\gamma \neq 0$  the rank(B) = p + 1, then  $B^{\dagger} = B^{-1} = K$ . This fact leads to the conclusion that the inverse of *B* can be always calculated analytically. Finally the matrices  $K(\theta)$  and  $K_d$  are given by,

$$K(\theta) = \begin{bmatrix} (\theta - \vartheta)I_p & 0\\ \frac{\alpha}{\gamma}(\vartheta - \theta) & \frac{\theta - \vartheta}{\gamma} \end{bmatrix} = (\theta - \vartheta) \underbrace{\begin{bmatrix} I_p & 0\\ -\frac{\alpha}{\gamma} & \frac{1}{\gamma} \end{bmatrix}}_{K}$$
(16)  
$$K_d = -B^{\dagger}D = -\begin{bmatrix} 0\\ \frac{\beta}{\gamma} \end{bmatrix}$$

**Remark** 4. By the definition of  $\gamma = \frac{1}{m(t)C_{p_{mix}}}$ , the condition of  $\gamma \neq 0$  for homogeneous reaction system is always satisfied if the product  $m(t)C_{p_{mix}}$  is bounded.

**Remark** 5. Note that the matrix closed loop matrix  $A_{cl}$  is constant and does not depend of  $\theta$ , therefore, it is possible design linear controllers based on the system (13) for the new input *v*.

**Remark** 6.  $K(\theta)$  can be seen as the inverse of the transfer function of the system (12),  $K(\theta) = G^{-1}(\theta) = B^{-1}(\vartheta I_{p+1} - A(\theta))$ . This fact can be used in the context of the LPV systems to design optimal feedback and feedforward controllers.

## 3.2 Optimal Control law for Tracking

The next step to control the system (1) is to design a control strategy for tracking. Therefore, it is necessary to include an integral action into the controller, and this can be done by means of v as follows,

$$v = K_v \int_0^t \left( y_{ref} - y \right) d\tau$$

where  $K_{\nu} \in \mathbb{R}^{p+1 \times p+1}$  is the integral gain of the controller. Now, to calculate  $K_{\nu}$ , let define the following additional state for (13),

$$\dot{x}_e = y_{ref} - y = y_{ref} - Cx - C_u x_u$$
 (17)

Then, combining (13) with (17) we get the following augmented system,

$$\underbrace{\begin{bmatrix} \dot{x}\\ \dot{x}_e \end{bmatrix}}_{\dot{x}} = \underbrace{\begin{bmatrix} A_{cl} & 0\\ -C & 0 \end{bmatrix}}_{\tilde{A}} \underbrace{\begin{bmatrix} x\\ x_e \end{bmatrix}}_{\tilde{x}} + \underbrace{\begin{bmatrix} B\\ 0 \end{bmatrix}}_{\tilde{B}} v + \begin{bmatrix} 0 & 0\\ I & -C_u \end{bmatrix} \begin{bmatrix} y_{ref}\\ x_u \end{bmatrix}$$
(18)

To find  $K_{\nu}$ , the following optimization problem must be solved,

$$\min_{\nu} \int_{0}^{T} (x_{e}^{\mathsf{T}} Q_{e} x_{e} + \nu^{\mathsf{T}} R_{e} \nu) dt$$
subject to:  $\dot{x} = \tilde{A} \tilde{x} + \tilde{B} \nu$ 
(19)

Finally the solution of the optimization problem (19) is given by  $v = -R_e^{-1}B^{\mathsf{T}}Px_e = K_v x_e$ , where *P* is the solution of the algebraic Riccati equation  $P\tilde{A} + \tilde{A}^{\mathsf{T}}P - PBR^{-1}B^{\mathsf{T}}P + Q_e = 0$ . The final control strategy for the LPV system (12) can be seen in the Figure 2.

#### 4. EXAMPLE

Let us consider a non-isothermal CSTR where a reversible reaction  $A + B \subseteq C + D$  takes place. The system has four



Fig. 2. Control strategy for extent-based LPV homogeneous reaction systems.

species  $n_A$ ,  $n_B$ ,  $n_C$  and  $n_D$  (S = 4), one independent reaction ( $R_I = 1$ ), and two constant and independent inlets  $u_{in,1}$  and  $u_{in,2}$  (p = 2) of A and B. The reaction rates obey the mass-action principle and the Arrhenius law, and are given by  $r = k_f C_A C_B - k_r C_C C_D$ , where  $k_{f,r} = k_{o_{f,r}} exp\left(\frac{-E_{a_{f,r}}}{RT}\right)$  is the preexponential factor in the Arrhenius law, and  $E_a$  is the activation energy of the reaction. In this example, the numerical values of the parameters are given in the Table 1.

Table 1. Parameters of the case study

Parameter	Values and units
k <sub>of</sub>	$6.06 \times 10^5 \text{ m}^3 \text{kmol}^{-1} \text{h}^{-1}$
$k_{o_r}$	$9.84 \times 10^6 \text{ m}^3 \text{kmol}^{-1} \text{h}^{-1}$
$E_{a_f}$	63800 kJkmol <sup>-1</sup>
$E_{a_r}$	71710 kJkmol <sup>-1</sup>
R	8.314 kJkmol <sup>-1</sup> K <sup>-1</sup>

The matrices *N* and *W*<sub>in</sub> are given by:

$$N = \begin{bmatrix} -1 & -1 & 1 & 1 \end{bmatrix}, W_{in} = \begin{bmatrix} 0.01665 & 0 & 0 & 0 \\ 0 & 0.03121 & 0 & 0 \end{bmatrix}^{\mathsf{T}}$$

The initial conditions are  $n_0 = [0.5, 1, 0.5, 0]^{\mathsf{T}}$  kmol, and  $T_0 = 373$  K. The states, outputs and inputs of the system are defined as:  $x = [n_A, n_B, n_C, n_D, T]^{\mathsf{T}}$ ,  $y = [n_A, n_B, T]^{\mathsf{T}}$  and  $u = [u_{in,1}, u_{in,2}, Q_{in}]^{\mathsf{T}}$ . In this example, physical boundaries for the outlet flow and mass are stated, and given by  $\mathbb{U}_{out} = \{1 \le u_{out} \le 10\}$  and  $\mathbb{M} = \{95 \le m \le 105\}$ , therefore, the parameter  $\theta$  is always bounded.

The Figure 3 shows the comparison between the nonlinear model and the LPV representations of the process. In the Figure 3, the notation  $n_{x_r}$  refers to the time scale separation model,  $n_z$  the model with change of variables z, and  $n_r$  the model with the reaction rate as a disturbance. In the Figure 3, it is possible to observe that the three models are a good approximation of the nonlinear model in the number of moles. Nevertheless, for the temperature, the model based on time scale separation does not have a good response at the beginning of the simulation. However, the steady-state value and the shape of the curve are the same. Therefore, it is possible to conclude that the LPV models based on extents are a good representation of the nonlinear homogeneous reactor systems and can be used to design the ELPV.

In order to test the control strategy, the desired poles  $\vartheta$  are selected be equal to -1, and set point changes in  $n_A$  and T are done at 150 h and for  $n_B$  at 300 h. In addition, the parameter  $\theta = u_{out}(t)/m(t)$  is changed with a PI controller for the mass of the reactor, as follows:



Fig. 3. Open loop comparison of the LPV systems with the nonlinear model.

$$u_{out}(s) = \left(K_p + \frac{K_i}{s}\right) \left(m_{ref} - m(s)\right)$$

where  $m_{ref} = 99.105$  kg. The Figures 4, 5 and 6 show the simulation results for outputs *y*, inputs *u*, and the parameter  $\theta$  of the ELPV and ELTI. The performance of the ELPV is better than ELTI. The main reason for that is because the ELTI controller is not informed about the change in  $\theta$ , this leads to having a big mismatch between the LTI model and the nonlinear model. Therefore, the ELTI controller is taking decisions that affect the performance of the PI controller drastically (see Figure 6). Naturally, the results presented here are the consequence of the best tuning that we have found for the controllers.



Fig. 4. Closed-loop trajectories of the outputs  $n_A$ ,  $n_B$  and T of the ELPV (—) and ELTI (- - -) based controllers.



Fig. 5. Closed-loop trajectories of the inputs  $u_{in,1}$ ,  $u_{in,2}$  and Q of the ELPV (—) and ELTI (- - -) based controllers



Fig. 6. Evolution of the scheduling parameter  $\theta$  of the ELPV and ELTI based controllers.

## 5. CONCLUSION

In this paper, the extent decomposition approach is used to transform the general model of homogeneous reaction systems into an LPV system. To this end, we have investigated three options. An important feature of the ELPV system is its diagonal state matrix, which is used to guarantee the controllability and propose general parametric state feedback and feedforward laws. These control laws allow converting the original ELPV system into an LTI system. General conditions of existence for the parametric state feedback and feedforward have been established and analyzed. For the LTI system, optimal control laws for reference tracking have been designed. Finally, the control strategy for the ELPV system was illustrated in simulation and compared with a controller based on constant-parameter LTI model (ELTI). In this simulation, the ELPV based controller showed a better performance than the ELTI under the varying parameter  $\theta$ .

#### REFERENCES

- Amrhein, M., Bhatt, N., Srinivasan, B., and Bonvin, D. (2010). Extents of reaction and flow for homogeneous reaction systems with inlet and outlet streams. *AIChE Journal*, 56(11), 2873–2886.
- Apkarian, P. and Adams, R.J. (1998). Advanced gainscheduling techniques for uncertain systems. *IEEE transactions on control systems technology*, 6(1), 21–32.
- Apkarian, P. and Gahinet, P. (1995). A convex characterization of gain-scheduled  $H_{\infty}$  controllers. *IEEE Transactions on Automatic Control*, 40(5), 853–864.
- Apkarian, P., Gahinet, P., and Becker, G. (1995). Self-scheduled  $H_{\infty}$  control of linear parameter-varying systems: a design example. *Automatica*, 31(9), 1251–1261.
- Asbjørnsen, O.A. (1972). Reaction invariants in the control of continuous chemical reactors. *Chemical Engineering Science*, 27(4), 709–717.
- Bachnas, A., Tóth, R., Ludlage, J., and Mesbah, A. (2014). A review on data-driven linear parameter-varying modeling approaches: A high-purity distillation column case study. *Journal of Process Control*, 24(4), 272–285.
- Balas, G., Bokor, J., and Szabó, Z. (2003). Invariant subspaces for lpv systems and their applications. *IEEE Transactions on Automatic Control*, 48(11), 2065–2069.
- Bamieh, B. and Giarre, L. (2002). Identification of linear parameter varying models. *International journal of robust* and nonlinear control, 12(9), 841–853.
- Bruzelius, F., Pettersson, S., and Breitholtz, C. (2004). Linear parameter-varying descriptions of nonlinear systems. In *American Control Conference, 2004. Proceedings of the* 2004, volume 2, 1374–1379. IEEE.
- Fjeld, M., Asbjørnsen, O., and Åström, K.J. (1974). Reaction invariants and their importance in the analysis of eigenvectors, state observability and controllability of the continuous stirred tank reactor. *Chemical Engineering Science*, 29(9), 1917–1926.
- Hautus, M. (1970). Stabilization controllability and observability of linear autonomous systems. *Indagationes Mathematicae* (*Proceedings*), 73(Supplement C), 448 – 455.
- Marquardt, W. (2002). Nonlinear model reduction for optimization based control of transient chemical processes. In AIChE Symposium Series, 12–42. New York; American Institute of Chemical Engineers; 1998.
- Srinivasan, B., Amrhein, M., and Bonvin, D. (1998). Reaction and flow variants/invariants in chemical reaction systems with inlet and outlet streams. *AIChE Journal*, 44(8), 1858– 1867.
- Tóth, R. (2010). *Discretization of LPV Systems*, 143–169. Springer Berlin Heidelberg, Berlin, Heidelberg.
- Tóth, R., Van den Hof, P., Ludlage, J., and Heuberger, P. (2010). Identification of nonlinear process models in an lpv framework. *IFAC Proceedings Volumes*, 43(5), 877–882.
- Vandezande, J.E., Vander Griend, D.A., and DeKock, R.L. (2013). Reaction extrema: Extent of reaction in general chemistry. *Journal of Chemical Education*, 90(9), 1177– 1179.