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IHMPC and POD to the control of a non-isothermal tubular reactor

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Abstract: This paper presents the result of applying POD (Proper Orthogonal Decomposition) and IHMPC (Infinite Horizon Model Predictive Control) to the control of a non-isothermal tubular reactor. This paper is based on a previous work of O.M. Agudelo, J.J. Espinosa, B. De Moor *Control of a Tubular Chemical Reactor by means of POD and Predictive Control Techniques*, in Proceedings of the European Control Conference 2007 (ECC 2007), pp. 1046-1053, Kos, Greece, 2007 ,where a finite horizon model predictive control and POD techniques are applied a non-isothermal tubular reactor. In this paper the control objective is to keep the operation of the reactor at a desired operating condition in spite of the disturbances in the feed flow. POD and Galerkins method are used to derive the low order linear model that captures the dominant dynamics of the PDEs, which are subsequently used for controller design. Two IHMPC formulations are constructed on the basis of the low order linear model and are demonstrated, through simulation, to achieve the control objectives.

Keywords: Infinite Horizont Model Predictive Control (IHMPC), Proper Orthogonal Decomposition (POD), Non-Isothermal Tubular Reactor.

1. INTRODUCTION

The dynamics of tubular reactors are typically described by nonlinear PDEs (Partial Differential Equations) which are derived from mass and energy balance principles. The control of such systems can be addressed by transforming the PDEs and the boundary conditions into a set of ODEs (Ordinary Differential Equations), which would make possible the application of the control theory developed for lumped parameter systems. However, the design of the controllers would be very difficult or practically impossible due to the high order models obtained by approximating the PDEs.

Proper orthogonal decomposition (POD) is a powerful method for data analysis aimed at obtaining low-dimensional approximate descriptions of a high-dimensional process. The POD provides a basis for the modal decomposition of an ensemble of functions, such as data obtained in the course of experiments or numerical simulations. The most striking feature of the POD is its optimality: it provides the most eficient way of capturing the dominant components of an infinite-dimensional process with only a finite number of modes, and often surprisingly few modes. In general POD is a methodology that first identifies the most energetic modes in a time-dependent system, and subsequently provides a means of obtaining a low-dimensional description of the system's dynamics where the low-dimensional system is obtained directly from the Galerkin projection of the governing equations on the empirical basis set (the POD modes).

This paper presents the result of applying POD and IHMPC to the control of a non-isothermal tubular re-

actor. The control goal is to keep the operation of the reactor at a desired operating condition in spite of the disturbances in the feeding flow. Two IHMPC formulations are constructed on the basis of the low order linear model and are demonstrated, through simulation, to achieve the control objectives.

This paper is organized as follows: Section II presents a description of the process and the optimization algorithm for obtaining the optimal operating profile. Section III shows the derivation of the reduced order model by means of POD. In Section IV we show theory and design of two extended IHMPC.

2. NON-ISOTHERMAL TUBULAR REACTOR

The system to be controlled is a non-isothermal tubular reactor where a single, first order, irreversible, exothermic reaction takes place (A→B). The reactor is surrounded by 3 cooling/heating jackets as it is shown in Figure 1. The temperatures of the jackets fluids (T_{j1}, T_{j2} and T_{j3}) can be manipulated independently in order to control the concentration and temperature profiles in the reactor. It is assumed that the reacting mixture flows as a plug through the reactor body in the axial direction. In this dynamics only three phenomena are taken into account, namely, convection , reaction and heat transfer (between the reactor and its jackets). In this study we are not considering the diffusion/dispersion phenomena and we are neglecting the effects of the reactor wall. Under the previous assumptions, the mathematical model of the tubular chemical reactor consists of the following coupled nonlinear PDEs:
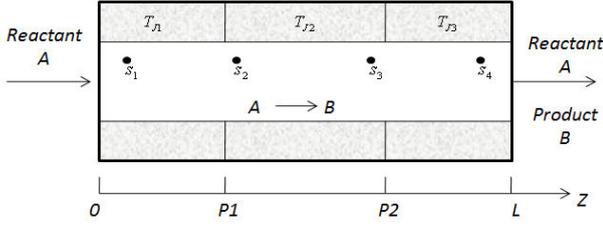
Fig. 1. Tubular Chemical Reactor with 3 cooling/heating jackets.

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial z} - k_0 C e^{-\frac{E}{RT}}.$$

$$\frac{\partial T}{\partial t} = -v\frac{\partial T}{\partial z} - G_r C e^{-\frac{E}{RT}} + H_r(T_w - T) \qquad (1)$$

$$G_r = -\frac{\Delta H k_0}{\rho C_p}, H_r = -\frac{4h}{2r_s \rho C_p}$$

with the following boundary conditions:

$$C = C_{in} \text{ at z} = 0 \text{ and } T = T_{in} \text{ at z} = 0.$$

Here $C(z,t)$ is the reactant concentration in $[mol/l]$, $T(z,t)$ is the reactant temperature in $[K]$ and $T_w(z,t)$ is the reactor wall temperature in $[K]$ defined as follows (see Figure 1),

$$T_w = \begin{cases} T_{j1}, & 0 \leq z < Z_a \\ T_{j2}, & Z_a \leq z < Z_b \\ T_{j3}, & Z_b \leq z < L \end{cases} \qquad (2)$$

The parameters are presented in table 1.

Table 1. Values of the reactor parameters

Parameter	value
v	$0.1\ m \cdot s^{-1}$
L	$1\ m$
k_0	$10^6\ s^{-1}$
E	$11250\ cal \cdot mol^{-1}$
R	$1.986\ cal \cdot mol^{-1} \cdot K^{-1}$
C_{in}	$0.02\ mol \cdot l^{-1}$
T_{in}	$340\ K$
G_r	$4.25 \cdot 10^9 l\ K \cdot mol^{-1} \cdot s^{-1}$
H_r	$0.2\ s^{-1}$

The temperature of the jacket sections T_{j1}, T_{j2} and T_{j3} must be between $280\ K$ and $400\ K$ (input constraints), in addition, the temperature inside the reactor must be smaller than $400\ K$ (state constraint) in order to avoid the formation of side products. The kind of disturbances that affect the reactor are the variations in the temperature and concentration of the feed flow. In this system, only the temperature of the feed flow is measured directly. In addition, the reactor has a temperature sensor at the output and 4 temperature sensors (s_1, s_2, s_3 and s_4) distributed in its interior as it is shown in figure 1.

2.1 Operating point

The desired operating profiles (steady-state concentration and temperature profiles) of the reactor are derived by means of an optimization algorithm, which minimizes a cost function subject to the steady-state equations of the reactor described by (1), and the input and state constraints defined previously. The steady-state model of the reactor is given by the following Ordinary Differential Equations (ODEs):

$$\frac{dC}{dz} = -\frac{k_0}{v}C e^{-\frac{E}{RT}}$$

$$\frac{dT}{dz} = \frac{G_r}{v}C e^{-\frac{E}{RT}} + \frac{H_r}{v}(T_w - T) \qquad (3)$$

with $T = T_{in}$ at $z = 0$ and $C = C_{in}$ at $z = 0$, and the discrete version of (3) can be found by replacing the spatial derivatives by forward difference approximations as follows:

$$\overline{C}_{i+1} = \overline{C}_i - \frac{k_0 \Delta z}{v}\overline{C}_i e^{-\frac{E}{RT_f\overline{T}_i}}$$

$$\overline{T}_{i+1} = \overline{T}_i\left(1 - \frac{H_r\Delta z}{v}\right) + \left(\frac{G_r\Delta z C_f}{vT_f}\right)\overline{C}_i e^{-\frac{E}{RT_f\overline{T}_i}}$$

$$+ \left(\frac{H_r\Delta z}{v}\right)\overline{T}_{w,i} \qquad (4)$$

$$\overline{T}_0 = \frac{T_{in}}{T_f},\ \ C_0 = \frac{C_{in}}{C_f}$$
$$for\ \ i = 1, 2, ..., N = 300$$

where $\overline{C}_i = C_i/C_f$ and $\overline{T}_i = T_i/T_f$ are the normalized concentration and temperature of the ith increment, $\overline{T}_{w,i} = T_{w,i}/T_f$ is the normalized temperature of the reactor wall of the ith increment, N is the number of increments in which the reactor is divided, T_f and C_f are normalization factors, and Δz is the length of the space increment. The variables are normalized in order to avoid possible numerical problems. The minimization problem that is solved by the optimization algorithm is defined as [1] :

$$\min_{\overline{T}_{j1},\overline{T}_{j2},\overline{T}_{j3}} \omega(\overline{C}_r - \overline{C}_N)^2 + (1 - \omega)\frac{1}{N}\sum_{i=1}^{N}(\overline{T}_{r,i} - \overline{T}_i)^2 \quad (5)$$

$subject\ to$

$$\text{steady state model given by (4)}$$

$$\frac{T_{jmin}}{T_f} \leq \overline{T}_{j1}, \overline{T}_{j2}, \overline{T}_{j3} \leq \frac{T_{jmax}}{T_f}$$

$$\overline{T}_i \leq \frac{T_{max}}{T_f}, \quad for\ \ i = 1, 2, ..., N = 300 \qquad (6)$$

where $\overline{C}_r$ is the desired concentration (normalized) at the reactor output, $\overline{T}_{r,i}$ is the desired temperature (normalized) inside the reactor of the ith increment, $\overline{C}_N$ is the concentration (normalized) at the reactor output, ω is a trade-off coefficient, T_{jmin} and T_{jmax} are the lower and upper temperature values of the fluids in the jackets, and T_{max} is the maximum allowed temperature inside the tubular reactor. In this problem $\overline{C}_r$ was set to 0, $\overline{T}_{r,i}$ was selected equal to the normalized temperature of the feeding flow ($\overline{T}_{in} = T_{in}/T_f$) for $i = 1, 2, ..., N$. The trade-off parameter ω can take values from 0 to 1. To solve the optimization problem described by (5) a sort of Sequential Quadratic Programming was proposed by [1].
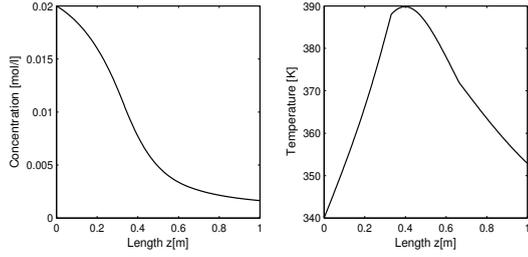
Fig. 2. Steady-state concentration and temperature profiles (Operating Profiles) whit $T_{J1} = 374.6K, T_{J2} = 310.1K$ and $T_J3 = 325.2K$.

The algorithm was executed using different initial conditions. Along the experiments, three local minima were found. The selection of the optimal temperature and concentration profiles was done by checking the value of the cost function and the deviation of the temperature at the reactor output with respect to the temperature of the feed flow.

From the three local minima it was adopted the operating point $T_{J1} = 374.6$ $K, T_{J2} = 310.1$ K and $T_{J3} = 325.2$ K, since it has the smallest cost function value and a small temperature deviation at the reactor output. The optimal concentration and temperature profiles can be observed in Figure 2.

2.2 Linear Model

The linear model of the tubular chemical reactor is obtained by linearizing (1) around the jacket's temperatures and the operating profiles presented in Figure 2. This linear model is given by,

$$\frac{d\overline{C}_i^{\Delta}}{dt} = -\frac{v}{\Delta z}\left(\overline{C}_i^{\Delta} - \overline{C}_{i-1}^{\Delta}\right) - \alpha_{A,i}\overline{C}_i^{\Delta} - \alpha_{B,i}\frac{T_f}{C_f}\overline{T}_i^{\Delta}$$

$$\frac{d\overline{T}_i^{\Delta}}{dt} = -\frac{v}{\Delta z}\left(\overline{T}_i^{\Delta} - \overline{T}_{i-1}^{\Delta}\right) - \alpha_{C,i}\frac{C_f}{T_f}\overline{C}_i^{\Delta} - \alpha_{D,i}\overline{T}_i^{\Delta} \quad (7)$$

$$+ H_r\overline{T}_{w,i}^{\Delta}$$

$$for \quad i = 1, 2, ..., N$$

$$\alpha_A(z) = k_0 e^{-\frac{E}{RT^*}}, \alpha_B(z) = k_0 C^* \frac{E}{RT^{*2}} e^{-\frac{E}{RT^*}}$$

$$(8)$$

$$\alpha_C(z) = -G_r e^{-\frac{E}{RT^*}}, \alpha_D(z) = -G_r C^* \frac{E}{RT^{*2}} e^{-\frac{E}{RT^*}} + H_r$$

With

$$\overline{C}_0^{\Delta} = \overline{C}_{in}^{\Delta}, \quad \overline{T}_0^{\Delta} = \overline{T}_{in}^{\Delta}$$

where $\alpha_{A,i} = \alpha_A(z_i), \alpha_{B,i} = \alpha_B(z_i), \alpha_{C,i} = \alpha_C(z_i), \alpha_{D,i} = \alpha_D(z_i)$ $z_i = i\Delta z$, C_i , T_i , $T_{w,i}$ are the concentration, temperature and reactor wall temperature of the ith increment,C_i^* ,T_i^* ,$T_{w,i}^*$ are the steady state concentration, temperature and reactor wall temperature corresponding to z_i ,C_{in}^* and T_{in}^* are the the steady state concentration and temperature of the feed flow, $\overline{C}_i^{\Delta} = (C_i - C_i^*)/C_f$,$\overline{T}_i^{\Delta} = (T_i - T_i^*)/T_f$, $\overline{T}_{w,i}^{\Delta} = (T_{w,i} - T_{w,i}^*)/T_f$ are the normalized deviations from steady state of the concentration, temperature and reactor wall temperature of the space increment, $\overline{C}_{in}^{\Delta} = (C_{in} - C_{in}^*)/C_f$, $\overline{T}_{in}^{\Delta} = (T_{in} - T_{in}^*)/T_f$

are the normalized deviations from steady state of the concentration and temperature of the feed flow, N is the number of space increments in which the reactor is divided, and Δz is the length of each increment.

The linear system (7) can be written as follows:

$$\dot{x}(t) = \mathbf{A}x(t) + \mathbf{B}u(t) + \mathbf{F}d(t) \quad (9)$$

Where $\mathbf{A},\mathbf{B}$ and $\mathbf{F}$ are the matrices describing the system, $x(t)$ is the state vector,$u(t)$ is the vector of the inputs and $d(t)$ is the vector of the disturbances.

Since the spatial domain of the reactor is divided into $N = 300$ sections, the number of states of (9) is equal to 600. Given that such large number of states makes the design and implementation of feedback controllers for the reactor difficult, in the next section a reduced order model will be derived using POD and Galerkin projection.

3. MODEL REDUCTION USING POD

Let $x(t) \in \Re^{2N} = [x_1(t), x_2(t), ..., x_{2N}]^T$ be the state vector of a given dynamical system, and let $X \in \Re^{2N \times N_d}$ with $N_d \geq 2N$ be the so-called snapshot matrix that contain a finite number of samples or snapshots of the evolution of $x(t)$ at $t = t_1, t_2, ..., t_{N_d}$. In POD, we start by observing that each snapshot can be written as a linear combination of a set of ordered orthonormal basis vectors (POD basis vectors) $\varphi_j \in \Re^N, \forall j = 1, 2, ..., N$:

$$x(t_i) = \sum_{j=1}^{2N} a_j(t_i)\varphi_j, \forall i = 1, 2, ..., N_d \quad (10)$$

where $a_j(t_i)$ is the coordinate of $x(t_i)$ with respect to the basis vector φ_j (it is also called time-varying coefficient or POD coefficient). Since the first n most relevant basis vectors capture most of the energy in the data collected, we can construct an nth order approximation of the snapshots by means of the following truncated sequence

$$x(t_i) = \sum_{j=1}^{n} a_j(t_i)\varphi_j, \forall i = 1, 2, ..., N_d, n \ll 2N \quad (11)$$

This is the essence of model reduction by POD.

The POD basis Functions are determined from simulation or experimental data (Snapshot matrix) of the process. The dynamic model for the first n time varying coefficients can be found by means of the Galerkin projection [4].

The derivation of a reduced order model of (9) was done in 5 steps. These steps are described in the following subsections.

A. ***Generation of the Snapshot Matrix***. We have created a snapshot matrix $X_{snap} \in \Re^{600 \times 1500}$ from the system response where independent step changes were made in the input $u(t)$ and perturbation $d(t)$ signals of the nonlinear model (1)
$$X_{snap} = [x(t = \Delta t), x(t = 2\Delta t), ..., x(t = 1500\Delta t)]$$

B. ***Derivation of the POD basis vectors***. The POD basis vectors are obtained by computing the SVD of the snapshot matrix X_{snap},
$$\mathbf{X_{snap} = \Phi \Sigma \Psi^T}$$

where $\mathbf{\Phi} \in \Re^{600 \times 600}$ and $\mathbf{\Psi} \in \Re^{1500 \times 1500}$ are unitary matrices, and $\mathbf{\Sigma} \in \Re^{600 \times 1500}$ is a matrix that contains the singular values of X_{snap} in a decreasing order on its main diagonal. The left singular vectors, i.e. the columns of $\mathbf{\Phi}$ are the POD basis vectors.

C. **Selection of the most relevant POD basis vectors.** It was done by checking the singular values of X_{snap}. The larger the singular value the more relevant the basis function is. The first 20 basis functions associated to the first 20 largest singular values were selected. The 20th order approximation of $x(t)$ is given by

$$x(t_i) = \sum_{j=1}^{20} a_j(t_i)\varphi_j = \mathbf{\Phi_n a}(\mathrm{t}) \qquad (12)$$

D. **Construction of the model for the first n=20 POD coefficients.** The Galerkin projection is the most common way of deriving the dynamical model for the POD coefficients, and it will be the method used in this paper. Let us define a residual function $R(x)$ for equation (9) as follows:

$$R(x) = \dot{x}(t) - \mathbf{A}x(t) - \mathbf{B}u(t) - \mathbf{F}d(t), \qquad (13)$$

and we replace $x(t)$ by its nth order approximation $x_n(t) = \mathbf{\Phi}_n \mathbf{a}(\mathrm{t})$ in equation (13), the Galerkin projection states that the projection of $R(x_n)$ on the space spanned by the basis functions Φ_n vanishes. That is,

$$\langle R(x_n), \varphi_j(z_d) \rangle = 0; j = 1, ...n \qquad (14)$$

Replacing $x(t)$ by its nth order approximation $x_n(t) = \mathbf{\Phi}_n \mathbf{a}(\mathrm{t})$ in equation (9), and applying the inner product criterion (Galerkin projection) to the resulting equation we have:

$$\dot{\mathbf{a}}(t) = \mathbf{\Phi}_n^T \mathbf{A} \mathbf{\Phi}_n \mathbf{a}(\mathrm{t}) + \mathbf{\Phi}_n^T \mathbf{B} u(t) + \mathbf{\Phi}_n^T \mathbf{F} d(t)$$
$$x_n(t) = \mathbf{\Phi}_n \mathbf{a}(\mathrm{t}) \qquad (15)$$

and we obtain the model for the first n POD coefficients.

E. **Validation of the reduced order model.** For validating the reduced order model of the reactor, we applied constant input signals $\overline{T}_{J1}^{\Delta}(t) = 0.125$ $(T_{J1}^{\Delta}(t) = 10 \ K), \overline{T}_{J2}^{\Delta}(t) = 0.25$ $(T_{J2}^{\Delta}(t) = 20K)$ and $\overline{T}_{J2}^{\Delta}(t) = 0.25$ $(T_{J2}^{\Delta}(t) = 20K)$ and constant perturbation signals $\overline{C}_{in}^{\Delta}(t) = 0.05$ $(C_{in}^{\Delta}(t) = 10^{-3}mole/l)$ and $\overline{T}_{in}^{\Delta}(t) = 0.0625$ $(T_{in}^{\Delta}(t) = 5K)$ to both the full order model (1) and the reduced order model (15), and afterwards we compared their responses. Figure 3 show the temperature and concentration deviation profiles of the reactor at different time instants for each model. From the previous results we can conclude that the reduced order model with only 20 states provides an acceptable approximation of the full order model (600 states). The discrete-time version of (15) that is used for designing the digital controller, was obtained using the discretization method known as zero-order hold (ZOH) with a sampling time of 0.2s,

$$\mathbf{a}(k+1) = \tilde{\mathbf{A}}\mathbf{a}(\mathrm{k}) + \tilde{\mathbf{B}}u(k) + \tilde{\mathbf{F}}d(k)$$
$$x_n(k) = \mathbf{\Phi}_n \mathbf{a}(\mathrm{k}) \qquad (16)$$
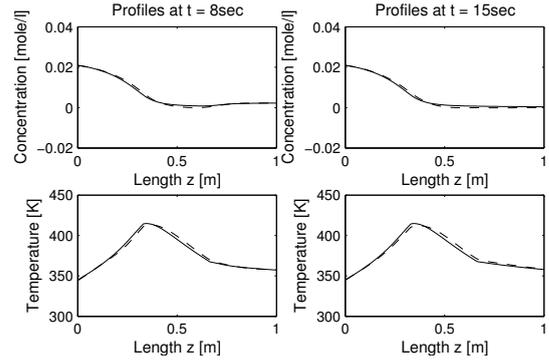
Fig. 3. Temperature and concentration deviation profiles at $t = 8s$ and $t = 15s$. Solid line - full order Model. Dashed line - reduced order model.

where $\tilde{\mathbf{A}}, \tilde{\mathbf{B}}$ and $\tilde{\mathbf{F}}$ are the matrices describing the new system. A modeling approach frequently adopted in model predictive controller (MPC) considers a discrete-time state-space model in the incremental form (see [2]), hence model(16) can be represented in the following form:

$$\begin{bmatrix} x^s(k+1) \\ x^d(k+1) \end{bmatrix} = \begin{bmatrix} I_{ny} & 0 \\ 0 & P \end{bmatrix} \begin{bmatrix} x^s(k) \\ x^d(k) \end{bmatrix} + \begin{bmatrix} D^s \\ D^d \end{bmatrix} \Delta u(k)$$
$$+ \begin{bmatrix} F^s \\ F^d \end{bmatrix} \Delta d(k) \qquad (17)$$

$$y(k) = \begin{bmatrix} C^s & C^d \end{bmatrix} \begin{bmatrix} x^s(k) \\ x^d(k) \end{bmatrix} \qquad (18)$$

where $x^d(k) = V_1\mathbf{a}(k), x^s(k) = V_2\mathbf{a}(k-1), \Delta u_k = u_k - u_{k-1}$ is the input increment $\Delta d_k = d_k - d_{k-1}$ is the disturbances increment and V_1, V_2 are transformation matrices. In the state equation defined in (17), the state component x^s corresponds to the integrating poles produced by the incremental form of the model, and $x^d(k) = \mathbf{a}(k)$ corresponds to the system modes. For stable systems, it is easy to show that when the system approaches steady state, component x^d tends to zero. P is a diagonal matrix with components corresponding to the poles of the system

4. EXTENDED INFINITE HORIZON MODEL PREDICTIVE CONTROL

MPC is usually based on a discrete state-space model as shown in Eqs. (17) and (18). The IHMPC cost can be defined as follows:

$$J_{k,\infty} = \sum_{j=1}^{\infty} (e_{k+j} - \delta_k)^T Q (e_{k+j} - \delta_k)$$
$$+ \sum_{j=1}^{m-1} \Delta u_{k+j}^T R \Delta u_{k+j} + \delta_k^T S \delta_k \qquad (19)$$

Where $e_{k+j} = y(k+j) - y_{sp}, y(k+j)$ is the output prediction at time instant $k + j$ made at time k, y_{sp} is the desired output reference, $\delta_k \in \Re^{n_y}$ is a vector of slack variables, m is the control horizon, $Q \in \Re^{n_y \times n_y}$, $R \in \Re^{n_u \times n_u}$ and $S \in \Re^{n_y \times n_y}$ are positive definite weighting matrices. Observe that each slack variable refers to a given

controlled output. Weight matrix S should be selected such that the controller pushes to zero the slacks or at least minimize them depending on the number of inputs, which are not constrained. Most of the infinite horizon controller reduce to finite horizon controller by defining a terminal state penalty $\overline{Q}$. For the cost defined in (19) such a terminal penalty is computed by the following Lyapunov equation

$$\overline{Q} - P^T \overline{Q} P = P^T C^{d^T} Q C^d P \tag{20}$$

Since an infinite horizon is used and the model defined in (17) and (18) has integrating modes, terminal constraints must be added to prevent the cost from becoming unbounded. Hence constraints can be written as follows:

$$\overline{C}^s x^s(k) - y_{sp} + \overline{C}^s \tilde{D}^s \Delta u_k - \delta_k = 0 \tag{21}$$

Where

$$\tilde{D}^s = [\, D^s ... D^s \,]$$
$$\overline{C}^s = diag\,[\, C^s ... C^s \,] \tag{22}$$

Finally, the control optimization problem of the extended infinite horizon MPC can be formulated as:

$$\min_{\Delta u_k, \delta_k} J_{k,\infty} = \sum_{j=1}^{m} (e_{k+j} - \delta_k)^T Q (e_{k+j} - \delta_k) +$$
$$x^d_{k+j}{}^T \overline{Q} x^d_{k+j} + \sum_{j=1}^{m-1} \Delta u^T_{k+j} R \Delta u_{k+j} + \delta_k^T S \delta_k \tag{23}$$

$subject\ to\ (17),(18),(21)\ and$
$$-\Delta u^{max} \leq \Delta u_{k+j} \leq \Delta u^{max}$$

$$\Delta u_{k+j} = 0 \;\; ; \;\; j \geq m \tag{24}$$
$$u^{min} \leq u_{k-1} + \sum_{i=0}^{j} \Delta u_{k+i} \leq u^{max}; \;\; j = 0, 1, ..., m-1$$

The control objective is to reject the disturbances that affect the reactor, that is the changes in the temperature and concentration of the feed flow. In addition, the control actions must satisfy the input constraints of the process $(280K \leq T_{J1}(t), T_{J2}(t), T_{J3}(t) \leq 400K)$, and the control system should keep the temperature inside the reactor below $400K$.

4.1 (IHMPC-POD)-Formulation in terms of the POD coefficients

In this scheme, the control of the temperature and concentration profiles is achieved indirectly by controlling the POD coefficients. The references of these POD coefficients can be calculated by

$$\mathbf{a}_{ref} = \mathbf{\Phi}_n^T x_{ref}$$

where x_{ref} is the reference of the vector $x(t)$ and is equal to 0 since the control system has to keep the reactor operating around the profiles shown in Figure 2. The IHMPC controller, which uses model (17) to predict the future behavior of the reactor, is formulated as (23) and (24), where $C^d = I_{20 \times 20} V_1, C^s = \mathbf{0}_{20 \times 20} V_2$. Observe that the temperature constraint $T(z, t) \leq 400K$ of the reactor has not been included in this IHMPC formulation.

Since the state vector $a(k)$ is unknown and the changes in the concentration of the feed flow $(d1(k) = C^\Delta_{in}(k))$ are not measured directly, they are estimated by means of an observer (in this case a Kalman filter) with the following formulation:

$$\begin{bmatrix} \hat{\mathbf{a}}(k+1) \\ \hat{d}_1(k+1) \end{bmatrix} = \begin{bmatrix} \tilde{\mathbf{A}} & \tilde{\mathbf{F}}_C \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \hat{\mathbf{a}}(k) \\ \hat{d}_1(k) \end{bmatrix} + \begin{bmatrix} \tilde{\mathbf{B}} \\ 0 \end{bmatrix} u(k)$$
$$+ \begin{bmatrix} \tilde{\mathbf{F}}_T \\ 0 \end{bmatrix} d_2(k) + \begin{bmatrix} \mathbf{L}_a \\ \mathbf{L}_d \end{bmatrix} (y(k) - \hat{y}(k)) \tag{25}$$
$$y(k) = C_{sel} \hat{x}_n(k) = C_{sel} \mathbf{\Phi}_n \hat{\mathbf{a}}(k)$$

where $\hat{\mathbf{a}}$ is the estimated vector of the POD coefficients, $\hat{d}_1(k)$ is the estimation $\overline{C}^\Delta_{in}$, $d_2(k)$ is the normalized temperature deviation of the feed flow $\overline{T}^\Delta_{in}(k)$, $y(k) \in \Re^4$ is a vector which contains the four temperature measurements (normalized deviations) along the reactor, $\hat{y}(k)$ is the estimate of $y(k)$, L_a and L_d are the submatrices of the observer gain (Kalman gain), F_C and F_T are the column vectors of $\tilde{F} = [\tilde{F}_C, \tilde{F}_T]$ and C_{sel} is a selection matrix which selects the measured temperatures from the vector $x_n(k)$.

The control horizon m was set to 10 samples u_{min} and u_{max} were selected according to the input constraints of the process and the operating temperatures of the jackets, and the weighting matrices in this way: $Q = 10 \cdot I_{20 \times 20}, R = 1000 \cdot I_{3 \times 3}, S = 1 \cdot I_{20 \times 20}$. The Kalman gain matrix was computed from the following covariance matrices: $R_w = 1000 \cdot I_{21 \times 21}, R_v = 10^{-6} \cdot I_{4 \times 4}$.

4.2 (IHMPC-PV)-Formulation in terms of physical variables

Unlike the previous control system, in this scheme the formulation of the MPC controller is in terms of physical variables. These variables are the temperature of some selected points along the reactor and the concentration at the reactor outlet. In this IHMPC formulation, the temperature constraint $(T(z, t) \leq 400K)$ of the system is imposed in the selected points. The IHMPC controller, which uses model (17) to predict the future behavior of the reactor, is formulated as (23) and (24), where $C^d = C_{sel_{C,T}} \mathbf{\Phi}_n V_1, C^s = \mathbf{0}_{n_l, 20} V_2$, the temperature constraint $T(z, t) \leq 400K$ of the reactor has been included in this IHMPC formulation, $C_{sel_{C,T}}$ is a selection matrix which selects the temperatures and concentration that will be controlled and n_l is the number of controlled variables. For estimating the state vector ($x^s(k)$ and $x^d(k)$) and the changes in the concentration of the feed flow ($d_1(k) = \overline{C}^\Delta_{in}(k)$), this control scheme employs the same observer used by the previous control system.

The parameters of the IHMPC controller were set as follows: The control horizon m was set to 10 samples u_{min} and u_{max} were selected according to the input constraints of the process and the operating temperatures of the jackets, and the weighting matrices in this way: $Q = 15 \cdot I_{20 \times 20}, R = 1000 \cdot I_{3 \times 3}, S = 1 \cdot I_{20 \times 20}$. The references for the variables were selected in this way: $\overline{T}^\Delta_{p,ref} = 0$, and $\overline{C}^\Delta_{p,ref} = 0$.
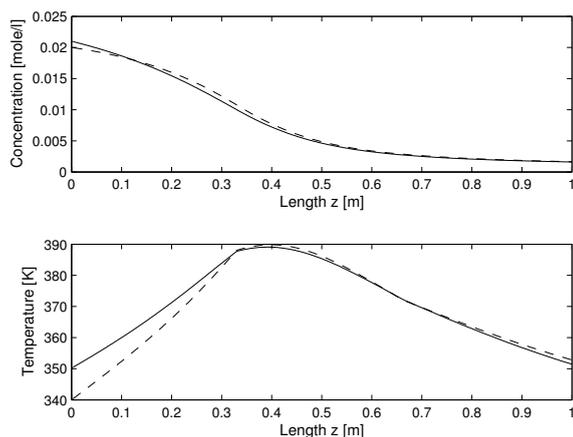
Fig. 4. Steady-state temperature and concentration profiles for Test. Dashed line - Nominal profile (reference).Solid Line -IHMPC-POD.

4.3 Simulation Results

In order to evaluate the performance of the control system, the following test was carried out: The temperature of the feed flow is increased $10K$ at the $10s$ and the concentration of the feed flow is increased $10^{-3}mole/L$ at the $5s$. This disturbances has a big impact on the temperature profile of the reactor.

The simulation results of the test are presented in figures 4 for IHMPC-POD and Figures 5 for IHMPC-PV. Furthermore, some quantities of interest are given in table II. In this table, T_{max} is the maximum temperature reached inside the reactor during the test, $\Delta C_{out}\% = (C_N - C_N^*)/C_N^*$ is the percentage of change of the concentration steady state at the reactor output with respect to its nominal value $(1.648 \cdot 10^3 mol/l)$ and C_N is the concentration at the reactor output steady state after the test.

Table 2. Performance parameters of the control systems

Quantities		IHMPC-POD	IHMPC-PV
T_{max}	[k]	389.1	387.4
ΔC_{out}	[%]	-2.6092	-1.8811

5. CONCLUSIONS

In this paper we have presented the results of applying POD and infinite horizon model predictive control techniques to the control of the temperature and concentration profiles of a non-isothermal tubular reactor.Thanks to the POD and Galerkin projection techniques, the high-dimensionality of the linearized model of the reactor has been significantly reduced making possible the control design. Two POD-based IHMPC control schemes have been proposed: a scheme where the formulation of the predictive controller is in terms of the POD coefficients (MPC-POD) and a scheme where the IHMPC is formulated in terms of physical variables (IHMPC-PV). The second IHMPC controller had better behavior for rejecting the disturbances and in addition the tuning was more intuitive.Due to the
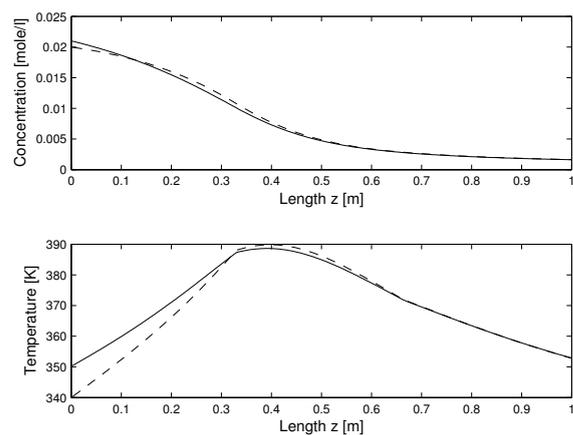
Fig. 5. Steady-state temperature and concentration profiles for Test. Dashed line - Nominal profile (reference).Solid Line -IHMPC-PV.
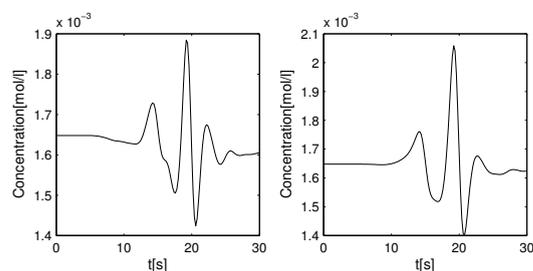
Fig. 6. Concentrations at the reactor output-IHMPC-POD and IHMPC-PV.

flexibility that this scheme provides, we gave more importance to the reduction of the concentration at the reactor outlet than to the reduction of the temperature deviations. In spite of the spatial discretization of the nonlinear PDEs that model the reactor, the linearization and the dramatic reduction order by means of POD, on which the controller is based, the controller performed well.

6. ACKNOWLEDGMENTS

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