

Temperature Control in an Industrial SO₂ Converter

Chaouki Bendjaouahdou¹ and Mohamed Hadi Bendjaouahdou²

¹ Department of Industrial Chemistry, Biskra University, Algeria

² Department of Mathematics, Constantine Mentouri University, Algeria

Email : chawk052000@yahoo.fr

Abstract: This study addresses the problem of controlling the magnitude of the maximal catalyst temperature, or hot spot, in a four catalyst beds SO₂ converter by manipulating the reaction mixture volumetric flow rate. The control of the maximal catalyst temperature is carried out in order to avoid the occurrence of a hot spot inside the catalyst mass and to keep high catalyst efficiency. Command algorithm used is the generalised predictive control (GPC) with off line process identification. The performance and robustness of the GPC controller are evaluated for the case of a kinetic complex and reversible exothermic reaction. The results obtained by numerical simulation show the possibility of the regulation of the hot spot temperature below a pre-specified value despite the occurrence of strong perturbations.

Keywords: SO₂ converter, packed bed, catalyst, process control, hot spot, simulation.

Introduction

Temperature control is crucial when designing a catalytic reactor for exothermic reactions because hot spots affect conversion, selectivity and lifespan of catalysts. In this study we focus on the control of the catalytic fixed beds reactor because it is very used in the industrial practice for the production of various and important chemicals (Kolios et al., 2000; Vanden Bussche et al., 1993).

The operation of the catalyst fixed beds reactor presents many challenges, such as a strong dependence of temperature and concentration profiles on the inlet conditions, the possible appearance of a maximum in the temperature profile (hot spot) and the possibility of temperature runaway (Varma, 1999). The occurrence of excessive temperatures can obviously have detrimental consequence on the operation of the reactor, such as catalyst deactivation, undesired side reactions, and thermal decomposition of the product. These considerations motivate the need for energy management strategies for such reactor. In this optic, control strategies that regulate the intensity of the hot spot temperature are of crucial importance.

It is well known that the control of the catalytic fixed bed reactors often represents very complex problem. The control problems are due to the process nonlinearity, its distributed nature and high sensitivity of the state and output variables to input changes. In addition, the dynamic characteristics may exhibit a varying sign of the gain in various operating points, the time delay as well as non-minimum phase behavior. Therefore, the process with such properties is hardly controllable by conventional control methods and its effective control requires the application of control advanced methods. It was proposed the use of adaptative control (Oderwater et al, 1988), linear optimal control (Kozub et al., 1987) and nonlinear control methods (Hua and Jutan, 2000) based on lumped approximations of the reactor model. Methods for distributed control in hyperbolic partial differential equation systems can be used for this purpose despite the fact that they require multiple heating/cooling zones, and as a consequence they are complex to implement in practice (Christofides and Daoutidis, 1998).

This work is a contribution related to the study of the control of the magnitude of the catalyst hot spot temperature in an industrial SO₂ converter. The studied reactor is running adiabatically with no flow reversal and it is used for the highly exothermic SO₂ oxidation in order to produce the sulfuric anhydride (SO₃). The sulfuric anhydride will be further used for the synthesis of the sulfuric acid (H₂SO₄). In order to reach high degree of SO₂ conversion, a cascade or a serial of catalytic fixed beds must be used. As a consequence, the industrial reactor is constituted, generally, of a serial of four catalytic fixed beds (Gosiewski, 1993). The control of this kind of reactor aims to avoid the occurrence of a hot spot inside the catalyst beds. This can be done by the use of a control loop for each catalytic bed in order to stabilize the maximal catalyst temperature to a specific and fixed value. The control objective is to avoid the occurrence of hot spot inside the catalytic bed and then prevents the catalyst from deactivation or sintering (Trambouze et al., 1984). From the mathematical point of view, this type of reactor belongs to the class of systems with distributed parameters (Gosiewski, 1993). The control of such process by conventional methods with fixed parameters of the controller could be a problem, mainly in the cases

where the operating point changes or reactor dynamic is affected by various changes of the inlet stream parameters. This inconvenience should be overcome with the use of some of recent control strategies such as adaptive control, predictive control etc. On the other hand, the adiabatic catalytic fixed bed is very challenging to control, relatively to cooled catalytic fixed bed, because there are not many control variables available. In this study, the inlet gas volumetric flowrate is used as manipulated variable in order to control this kind of reactor. For this purpose, the dynamic model of the process (adiabatic catalytic bed) will be integrated using the data related to its nominal operating point (Gosiewski, 1993), afterwards, the generalized predictive algorithm (GPC) with off line recursive least-squares identification will be applied to this model.

The industrial SO₂ converter

A schematic flowsheet of the industrial multiple catalytic fixed beds reactor is illustrated in Figure 1 (Gosiewski, 1993). This reactor is a series of four catalytic fixed beds disposed vertically. Heat exchangers are disposed between two consecutive catalytic beds in order to avoid the decrease of the conversion by cooling the gas before being fed into the next bed. The diameter of each bed is equal to 8.6 m. Each catalytic bed is formed by a compact and fixed stack of vanadium catalyst pellets (Gosiewski, 1993). The inlet gas is fed through the whole reactor from the top to the bottom as illustrated in figure 1. Before the inlet gas is fed, the catalytic beds are preheated to a certain high temperature value which is greater than the catalytic ignition temperature. Then, the inlet gas with low SO₂ concentration is fed into the reactor. Each catalytic stage possesses its nominal run state or operating point specified by the physical parameter values related to the gas (the value of the inlet gas temperature is clearly predefined) and to the catalytic bed (the catalyst mass is rigorously calculated). In order to track the conversion adiabatic path and then to reach the expected conversion value at the exit of each bed, it is necessary to cool the gas at the exit of each bed. Such cooling is done by the use of heat exchangers disposed between two consecutive beds (fig.1). The catalyst bed is made adiabatic by recovering its inside wall by a thermal insulating (firebrick) layer (Gosiewski, 1993).

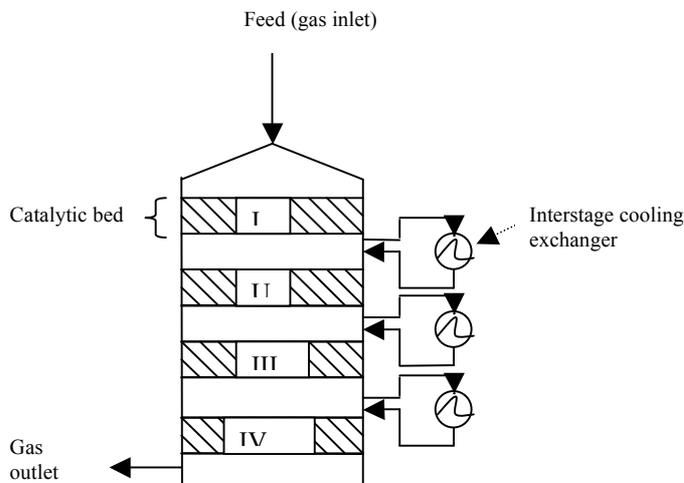


Figure 1. Schematic flowsheet of the industrial multi-staged catalyst fixed bed reactor used for SO₂ oxidation with intermediary cooling.

The catalyst characteristics, reaction rate and inlet gas composition

The SO₂ oxidation is done by the use of a vanadium pentoxide (V₂O₅) based catalysts. The catalyst pellets have 6 to 8 wt % V₂O₅ (Trambouze et al., 1984). The catalyst is active only between 400 and 650 °C (Gosiewski, 1993). Beyond 650°C, the catalytic efficiency decrease gradually and the catalyst begins to be destroyed (Gosiewski, 1993; Trambouze et al., 1984).

The oxidation of SO₂ is a very exothermic reaction. The enthalpy related to this reaction is approximately constant between 400 and 600 °C (Gosiewski, 1993). The kinetic of SO₂ expression was studied by many authors (Dunn et al., 1999; Villiermaux, 1990). In this study, the Calderbank expression rate was used (Calderbank, 1952) in which T (expressed in Kelvin) means the temperature of the catalytic solid phase, the

kinetic constants K_1 and K_2 are expressed in mol^{-1} , the component partial pressure P_i are expressed in atmosphere, and the used value of the perfect gas constant R is $8.31 \text{ J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$.

$$r = K_1 \cdot (P_1 P_2 / P_1^{1/2}) - K_2 \cdot (P_3 \cdot P_2^{1/2} / P_2^{1/2})$$

$$K_1 = e^{[(130000/R.T) + 12.07]}$$

$$K_2 = e^{[(220000/R.T) + 22.75]}$$

In the expression of the reaction rate, the intrinsic kinetic, r is expressed in kmol of $\text{SO}_3/\text{kg}\cdot\text{hr}$. the inlet gas fed to the first catalytic bed must have a temperature greater than $430 \text{ }^\circ\text{C}$, and its molar composition is : 79 % of N_2 , 11 % of O_2 and 10 % of SO_2 (Gosiewski, 1993). Table I gives additional parameter values related to the reaction rate, catalyst and the reactor.

Table 1. Parameters for SO_2 oxidation in a multiple fixed bed reactor

Parameter	Nominal value
Heat of reaction (J/mole)	$-\Delta H = 8.89 \times 10^4$
Effective heat capacity of particle	$C_{p\text{keff}} = 2.1 \text{ kJ/kmole}$
Density of catalyst particle	$\rho_u = 620 \text{ kg/m}^3$
Mean diameter of catalyst pellets	$d_p = 0.0018 \text{ m}$
Specific outer surface area of catalyst pellets	$S = 568 \text{ m}^{-1}$
Effective thermal conductivity of catalyst pellets	$\lambda_e = 0.46 \text{ W}\cdot\text{m}^{-2}\cdot\text{K}^{-1}$
Gas-particle heat transfer coefficient	$\alpha = 151 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
Number of catalytic bed	$n = 4$
Depth of the catalytic bed	$L = 0.48 \text{ m}$
Diameter of the catalytic bed	$D = 8.6 \text{ m}$
Void fraction of the catalytic bed	$\epsilon_c = 0,5$
Inlet gas superficial molar flow (first bed)	$n_g = 13.24 \text{ mole m}^{-2} \cdot \text{s}^{-1}$
Inlet gas pressure (first bed)	$P_T = 1.2 \text{ atm}$
Initial bed temperature (first bed)	$T_{co} = 460 \text{ }^\circ\text{C}$
Gas feed temperature (first bed)	$T_{go} = 460 \text{ }^\circ\text{C}$
Steady state SO_2 conversion (exit of first bed)	$X_1 = 68 \%$

The dynamic model of the catalytic bed, Boundary and Initial Conditions

Dynamic model of the catalytic bed

In a catalytic fixed bed, the heat transfer between gas and particle phases is the most important, because the cold inlet gas has to be heated by the hot solids near the entrance of the bed and the cold solid is heated by the hot gas near the exit of the bed. As a consequence, in this model, the temperature and concentration differences between the gas and particle phases are accounted. The model equations were derived from the components transient continuity equations and the transient energy balance for both gas and solid phase. The used dynamic model of the catalytic fixed bed is a pseudo-homogeneous one and its related assumptions are those proposed by K. Gosiewski (Gosiewski, 1993).

$$n_g \cdot C_{pg} \cdot \frac{\partial T_g}{\partial x} + \alpha \cdot S \cdot (T_g - T_k) = 0 \quad (1)$$

$$\lambda_e \cdot \frac{\partial^2 T_k}{\partial x^2} - \rho_u \cdot C_{ps} \cdot \frac{\partial T_k}{\partial t} + \alpha \cdot S \cdot (T_g - T_k) + \Delta H \cdot r \cdot \rho_u = 0 \quad (2)$$

$$n_g \cdot \frac{\partial C_i}{\partial x} + v_i \cdot r \cdot \rho_u = 0 \quad (i = 1,2,3) \quad (3)$$

In the bed dynamic model, the effective axial conduction is taken into consideration since the effective axial conductivity (λ_e) used for the two phases expresses better the heat and mass transfer in the catalytic fixed bed (Gosiewski, 1993; Wakao and Kaguei, 1982; Nodehi and Mousavian, 2006; Toledo et al., 2011).

Boundary and initial conditions

Boundary conditions are (Gosiewski, 1993) :

- For $x = 0$

$$C_1(0, t) = C_{1in}(t)$$

$$C_2(0, t) = C_{2in}(t)$$

$$C_3(0, t) = 0$$

$$\lambda_e \left(\frac{\partial T_k}{\partial x} \right)_{x=0} = (1 - \epsilon_c) \cdot \alpha \cdot [T_k(0, t) - T_{gin}(t)]$$

$$T_g(0, t) = T_{gin}(t)$$

- For $x = L$

$$T_g(L, t) = T_{gout}(t)$$

$$\left(\frac{\partial T_k}{\partial x} \right)_{x=L} = 0$$

Initial conditions are (Gosiewski, 1993) :

$$T_k(x, 0) = T_{co}(x) \quad (0 \leq x \leq L)$$

$$T_g(x, 0) = T_{go}(x) \quad (0 \leq x \leq L)$$

$$C_i(x, 0) = 0 \quad (0 \leq x \leq L)$$

Solution of the dynamic model equations

The equations (1) and (2) are, respectively, the gas phase and the solid phase energy balance. The equation (3) expresses the component mass balances. The Equations (1) and (3) represent Cauchy differential problems, hence readily solvable by the fourth order Runge-Kutta method (Finalyson, 1980). The equation (2) represents a boundary values differential problem. This equation was solved by the Crank Nicholson method using an implicitness factor equal to 1/2 (Necati Özisik, 1993). Indeed, the equation (6) does not belong to the convection-diffusion problems, so, the convective numerical instability will not take place with our difference scheme. A uniform computational grid was used. The catalytic bed depth was divided into N_z equivalent parts ($N_z = 100$), therefore, the spatial discretization step (ΔX) used was equal to 0.49 mm. The time discretization step (Δt) used was equal to 1 second. The matrix coefficients resulting from the discretization of the equation (6) is tri-diagonal. Therefore, at each time step, the tri-diagonal Thomas algorithm ((Patankar, 1980) was applied.

GPC Algorithm

The objective of the generalized predictive control (GPC) law is to compute, at each sample time t , a control signal $u(t)$ whom the objective is to lead the future plant output $y(t+j)$ ($j = N_1, N_2$) close to the set point $w(t+j)$ (Clarke et al., 1987). The control signal is then computed so to minimize a cost function J of the form (Clarke et al., 1987):

$$J(N_1, N_2) = \sum_{j=N_1}^{j=N_2} [y(t+j) - w(t+j)]^2 + \sum_{j=N_1}^{j=N_2} \lambda(j) \cdot [\Delta u(t+j-1)]^2$$

with $\Delta u(t) = u(t) - u(t-1)$

From the expression of the cost function J , it is clear that the objective of GPC control law is twice. On one hand, the control law minimizes, to least squares sense, the sum extended to the entire prediction horizon ($j = N_1, N_2$) of the future errors; on the other hand, this objective is realized so that to minimize the energy consumption. The control weighting vector $\lambda(j)$ is introduced into the control law in order to limit every activity excess of the command signal by a judicious choice of its components. Sometimes, to simplify it is assumed that $\lambda(j) = \lambda$ and therefore, λ will be called the control weighting coefficient. The coefficients λ , N_u , N_1 and N_2 are the main conception parameters of the GPC control algorithm (Clarke et al., 1987).

Results and Discussion

In this study we focused only on the control of one catalytic bed (first bed) of the industrial reactor (fig. 1), but, it is obvious that the results found are easily applicable to the other catalytic beds. The control of the catalytic stage

aims to stabilize the intensity of the hot spot in order to prevent the runaway or shutdown of the chemical reaction temperature. In this study, the controlled variable is the maximal catalyst temperature and the manipulated variable is the inlet gas volumetric flowrate. The perturbations considered were the inlet gas temperature, the reactant (SO_2 and O_2) inlet concentrations and the inlet gas pressure.

Open loop catalytic fixed bed

Figures 2 and 3 show that despite the occurrence of an intense perturbation related to SO_2 and O_2 inlet concentrations, the maximal catalyst temperature reaches (fig. 2) or does not exceed $650\text{ }^\circ\text{C}$ (fig. 3). This last value is generally the maximal temperature supportable by the V_2O_5 based catalysts. The results given by these figures can be explained by the fact that the reactants are strongly diluted by the inert component (N_2) in the inlet gas. These last figures show that after the inlet reactant concentrations have been turned back to the normal operating value, the maximal catalyst temperature reaches its original value.

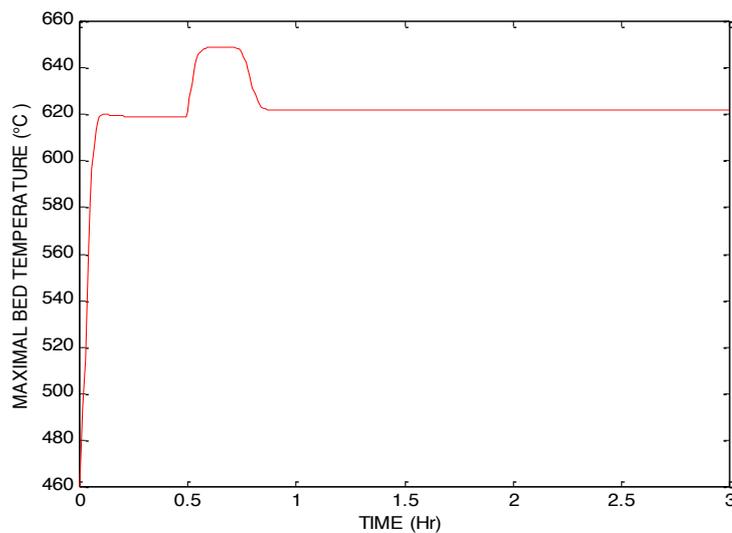


Figure 2. Process response to +25 % step change of C_{1in} ($C_{1in} = 0.1$) occurring at 0.5 hour during 10 minutes

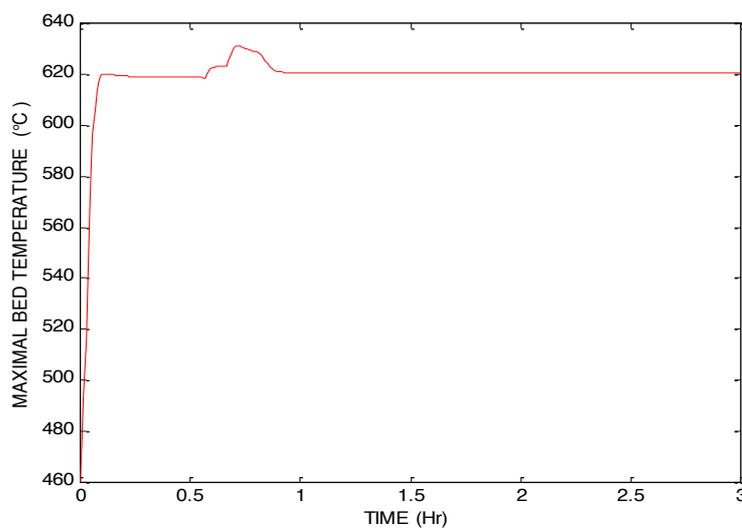


Figure 3. Process response to +25 % step change of C_{2in} ($C_{2in} = 0.11$) occurring at 0.5 hour during 10 minutes.

Fig. 4 shows that an intense perturbation related to the total pressure does not induce an important increase of the maximal catalyst temperature, (the maximal catalyst temperature remain less than 650 °C), this can be explained, according to Le Châtelier principle (Villermaux, 1990), by the weak value of the difference of the total molecules or moles number of the reaction between reactants and products, which is equal to $\frac{1}{2}$ ($\text{SO}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{SO}_3$).

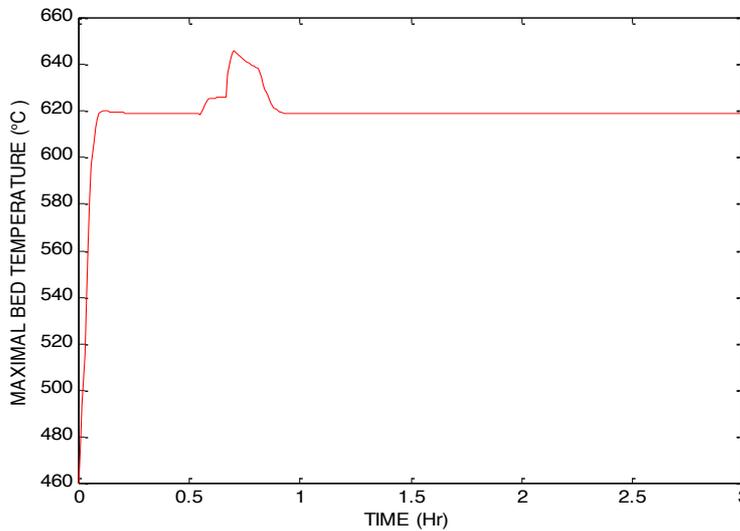


Figure 4. Process response to + 25 % step change of P_T ($P_T = 1.2 \text{ atm}$) occurring at 0.5 hour during 10 minutes.

Figures 5 and 6 illustrate the strong influence of gas inlet temperature on the value of the maximal catalyst temperature; this can be explained by the high exothermic effect of the reaction and also by the adiabatic run of the catalytic bed. It can be seen from these figures, that the maximal catalyst temperature exceed largely 650 °C, and consequently, the production capacity of the bed is expected to decrease due to the catalyst deactivity or sintering.

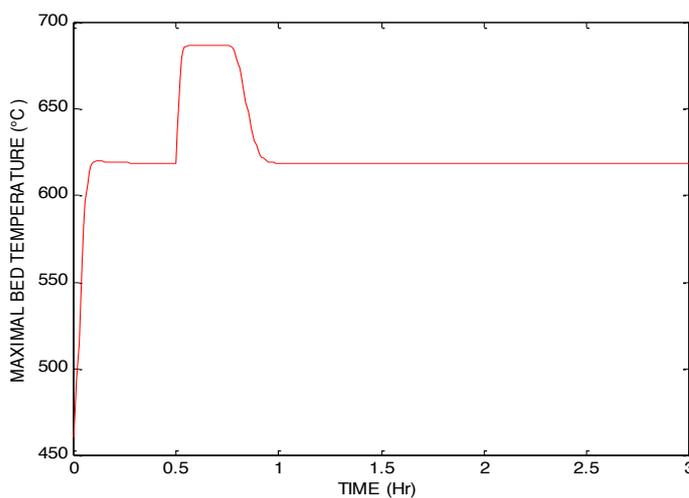


Figure 5. Process response to + 25 % step change of $T_{g_{in}}$ ($T_{g_{in}} = 440 \text{ °C}$) occurring at 0.5 hour during 10 minutes.

In figure 6, the phenomenon of the inverse response is observed, although it is of a small magnitude. This means that a very special care has to be taken if the gas inlet temperature is used as manipulated variable in a control loop. The inverse response can be explained by the fact that a sudden decrease in the inlet temperature will affect the bed temperature by two mechanisms: by the migration of temperature waves in the bed, which is a slow process; and by the changes in the concentration of chemical components, which is a relatively fast process

(Quina and Quinta Ferreira, 2000). As a consequence, there will be a loss of conversion in the whole bed and the bed temperature decreases (Morud and Skogestad, 1993). The inverse response usually causes difficulties of the stability in a control loop and a such phenomenon was observed for the SO₂ converter (Xiao and al., 1999). The prediction of the heterogeneous and the pseudo-homogeneous dynamic models are quite similar. The pseudo-homogeneous model assumes the same local temperature for the gas and the solids and hence, the time scale for heat transfer between the two phases is zero, whereas reaction time is finite. Thus the pseudo-homogeneous model can predicts better the inverse response or wrong way behavior when compared to the heterogeneous model (Quina and Quinta Ferreira, 2000). Since in the industrial practice, the magnitude of the perturbation of the parameters process does not exceed $\pm 20\%$ (Luyben, 2007; Toledo and al., 2001), so, it can claimed that for this kind of industrial reactor, the inlet gas temperature is the only parameter to be considered as a main perturbation for control purposes.

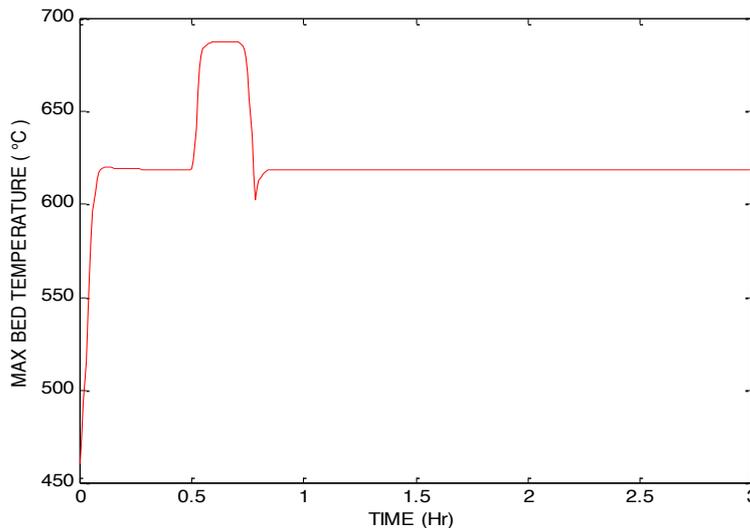


Figure 6. Process response to -25% step change of $T_{g_{in}}$ ($T_{g_{in}} = 440\text{ }^{\circ}\text{C}$) occurring at 0.5 hour during 10 minutes.

Closed loop catalytic fixed bed

The system (catalytic fixed bed) was identified in open loop mode using a pseudo-random binary sequence (PABS) with a sampling time equal to 20 seconds and a forgetting factor equal to the unity. The recursive least-squares identification method was applied to determine the discrete transfer function. It was found that the system is a second order one and its transfer function is as follows:

$$G(z^{-1}) = z^{-1} (0.417 + 0.34z^{-1}) / (1 - 0.988z^{-1} + 0.02z^{-2})$$

In order to control the maximal catalyst temperature, the GPC algorithm was used with the following values of its main parameters $N_1 = 1$; $N_2 = 8$; $\lambda = 4$; $Nu = 2$. These last values were determined by a trial and error procedure. The controlled variable (maximal catalyst temperature) will be given by a set of thermocouples disposed axially along the bed because the hot spot can move inside the bed (Yakhnin and Menzinger, 1998). The maximal catalyst temperature will be selected by a high selector device. This configuration of the thermocouples is frequently used in the practice and has been proven to give good measurements results (Cho and al., 1993; Chin et al., 2002). The control signal (inlet gas flow rate) will be given by a control valve disposed at the entrance of the bed. For all the simulations, the sampling period value used was equal to 30 seconds, the set point of the maximal catalyst temperature was $610\text{ }^{\circ}\text{C}$ and the control signal or the manipulated variable was limited between 5 and $37.45\text{ m}^3/\text{s}$. This control configuration is applicable for the four bed of the converter, and the results obtained for the first bed will be applicable for the other beds.

Figure 7 illustrates that the GPC controller successfully maintains the maximal catalyst temperature at its set value ($610\text{ }^{\circ}\text{C}$) despite the occurrence of perturbation. Furthermore the controller attenuates the disturbance very fast and the overshoots caused by this last one are minimal (figure 7 is to be compared with figure 2). From figure 8 it is shown that the GPC controller effectively regulates the maximal bed temperature to the set point value despite the occurrence of an perturbation related to the total operating pressure (P_T). The control signal varies regularly without the presence of dangerous peaks, detrimental for the control valve (figure 8 is to be compared with figure 4).

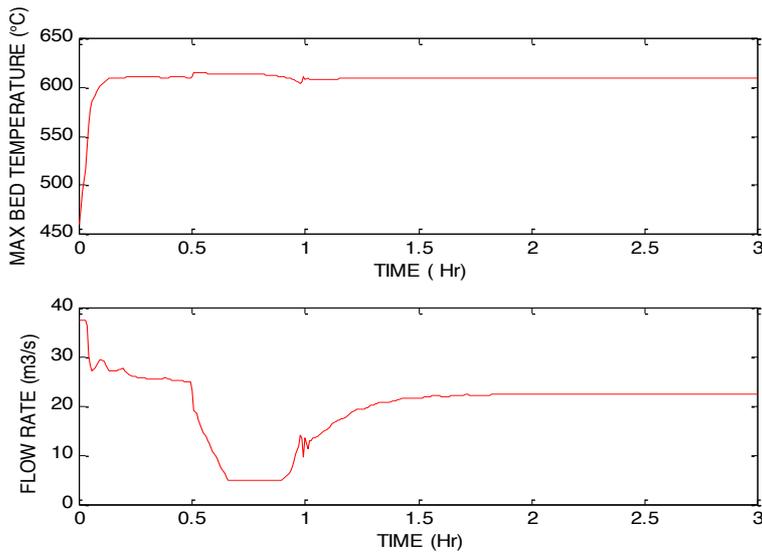


Figure 7. Process response and control signal to + 25 % step change of C_{1in} ($C_{1in} = 0.1$) occurring at 0.5 hour during 10 minutes with regulation of the temperature at 610 °C.

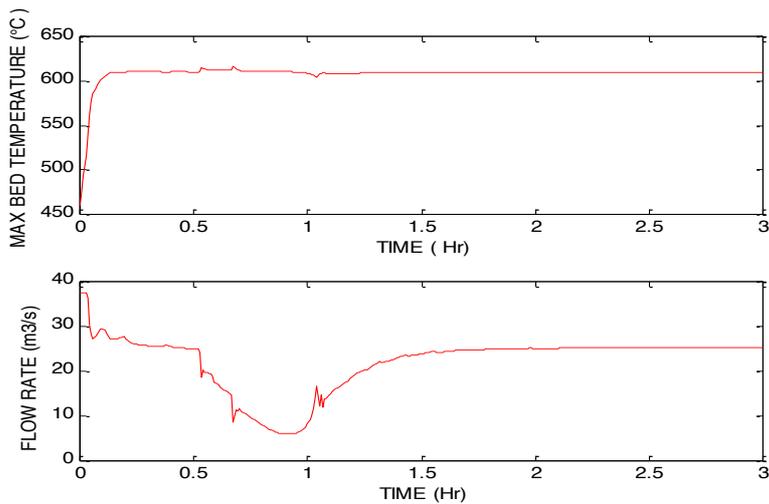


Figure 8. Process response and control signal to + 25 % step change of P_T ($P_T = 1.2$ atm) occurring at 0.5 hour during 10 minutes with regulation of the temperature at 610 °C.

Figures 9 and 10 show that the GPC controller efficiently stabilizes the maximal bed temperature with a great disturbance rejection capability and the control signal does not present very excessive variations (figures 9 and 10 are to be compared respectively with figures 5 and 6). Figure 11 shows the set point tracking of the maximal bed temperature when the desired temperature changes from 610 °C to 590 °C. It can be seen that the maximal catalyst temperature effectively follows the new value of the desired temperature and the control signal varies regularly. However, the new value of the desired temperature is not reached rapidly; this can be explained by the important thermal inertia of the bed conferred by its great thermal capacity due to the important catalytic mass.

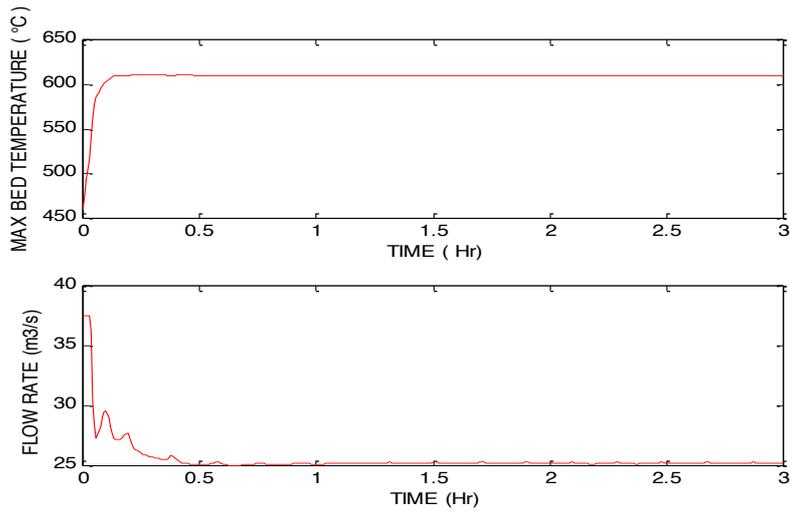


Figure 9. Process response and control signal to +25 % step change of $T_{g_{in}}$ ($T_{g_{in}} = 440\text{ }^{\circ}\text{C}$) occurring at 0.5 hour during 10 minutes with regulation of the temperature at $610\text{ }^{\circ}\text{C}$.

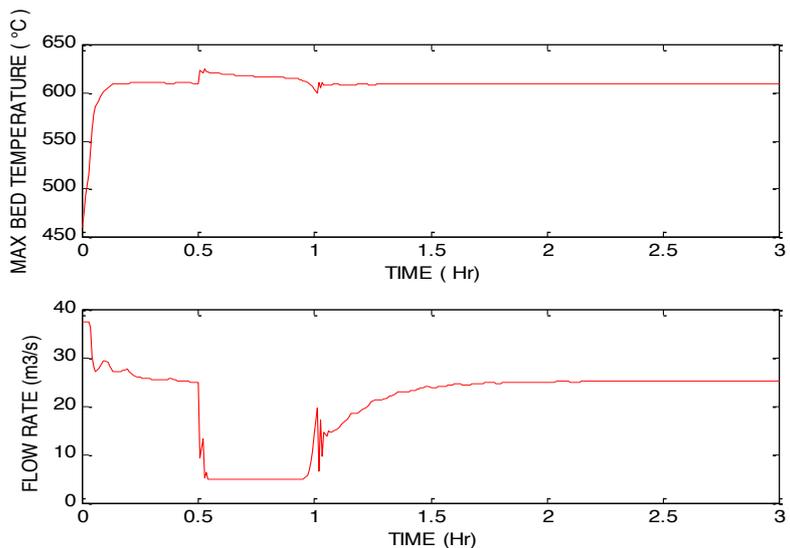


Figure 10. Process response and control signal to -25 % step change of $T_{g_{in}}$ ($T_{g_{in}} = 440\text{ }^{\circ}\text{C}$) occurring at 0.5 hour during 10 minutes with regulation of the temperature at $610\text{ }^{\circ}\text{C}$.

Conclusion

The results obtained in this study can be resumed as follows.

1. The finite difference method based on the Crank-Nicolson scheme was used to solve the dynamic model equations on uniform grid. This scheme was stable and provides satisfactory numerical results.
2. The controlled process (catalytic bed) was identified using a pseudo-random binary sequence (PABS) and the recursive least-squares identification method was applied to determine its discrete transfer function.
3. The open loop results showed that the maximal catalyst temperature or hot spot is very sensitive to the inlet temperature gas and insensitive to the inlet reactant concentration and total pressure of the gas. On the other hand, the inlet temperature gas cannot be used as a manipulated or control variable due to the inverse response phenomenon.
4. The closed loop results showed that the generalized predictive control (GPC) successfully and satisfactory controls the maximal catalyst temperature (hot spot) in regulation and set point tracking mode.

5. The control of the magnitude of the hot spot for a catalytic fixed bed is possible, by manipulating the inlet volumetric gas flow, in order to avoid the temperature runaway and the deactivation of the catalyst.

Nomenclature

C_i	molar fraction of species i , in the bulk phase gas, mole
C_{pg}	heat capacity of gas, J/mole.K
C_{ps}	heat capacity of solid, J/mole.K
D	catalytic bed diameter, m
j	predictive index
J	objective function or cost function
K_1, K_2	reaction rate constants
L	catalytic bed depth, m
n_g	superficial molar flow of gas, mole/m ² .s
N_1	minimum prediction horizon
N_2	maximum prediction horizon
N_u	control horizon
N_z	subdivision number of bed depth
p	Laplace variable
P_i	partial pressure of specie I , atm
P_T	total pressure, atm
r	intrinsic rate reaction, kmole of SO ₃ /(kg.hr)
S	specific outer surface area of catalyst pellets, m ² /m ³
T_g	temperature of the gas phase, (K)
T_k	temperature of the solid phase, K
$T_{g\ in}$	temperature of the gas at the entrance of the first bed, K
$T_{g\ out}$	temperature of the gas at the exit of the first bed, K
$T_{co}(x)$	initial bed temperature profil, K
$T_{go}(x)$	initial gas temperature profil, K
t	time, s
u	control signal
w	set point or reference signal
x	spatial coordinate computed from the entrance of gas phase in the catalytic bed, m
y	output or response process
z	sampling variable

Greek letters

ρ_u	density of solid, kg/m ³
ϵ_c	voidage of catalyst bed
α	gas –solid heat transfer coefficient, W/m ² .K
ΔH	heat of reaction, J/mol
Δt	step size of time discretization, s
Δx	step size of spatial discretization, m
$\Delta u(t)$	control signal increment at the current instant
λ_e	axial effective thermal conductivity of solid, Watt/(m. K)
λ	control weighting vector of the control signal
v_i	stoichiometric coefficient of specie i

Subscripts

1	sulfur dioxide (SO ₂)
2	molecular oxygen (O ₂)
3	sulfuric anhydride (SO ₃)
4	molecular nitrogen (N ₂)
g	gas phase
in	entrance of the first catalytic bed
i	chemical specie
k	catalytic or solid phase
out	exit of the first catalytic bed

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