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Controllability assessment approach for chemical reactors: nonlinear control affine systems

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Abstract

Although there have been several attempts to develop systematic evaluation of control schemes, the choosing and pairing of control variables in chemical reactors is not an easy task. Intrinsic nonlinearities of this kind of systems provoke dynamic responses that are difficult to predict. In this paper, a simple proposition for the evaluation of pairs of control and manipulated variables is developed for nonlinear control affine systems. It compliments the RGA analysis for nonlinear systems because is based on the relationship between zero dynamics and control stability. The resulting strategy is simple, easy to understand and easy to apply for the analysis of control schemes. Also, it is independent of the type of controller used. As an example, it is probed in the evaluation of four control options for industrial FCC regenerators; two of them applied in industry. The results obtained when evaluating the control strategies proposed in four different situations are coherent with industrial practice and operating experience.

Keywords: Control; Controllability; Dynamics; FCC; Reactors; Steady state

1. Introduction

Regulation issues of nonlinear processes are an open problem in the control community, mainly because of the industrial relevance of this kind of systems. In general, control problems in industrial plants are very complex, so industrial processes are, only, partially controlled. The complete stabilisation and regulation of this kind of systems is not assured, therefore the dynamic behaviour of the uncontrolled variables have to be studied in order to predict an approximation of global performance of the process. Meanwhile, it is common to find control affine schemes for CSTRs, which means that manipulated variables appear linearly in the model of the system, this situation provides some advantages, studied in this work.

Because of its complexity, the control of nonlinear systems has motivated the development of several researches in this field. In a nonlinear setting, the stability of the inverse of the system dynamics should be checked itself. Following the ideas of Morari and co-workers [1,2], from the control point of view, the perfect control for a process should present a dynamic behaviour that is given by the inverse of the dynamics of this process. However, due to the existence of time delays, this inverse is not realisable. Moreover, there are not explicit formulas for the inversion of general MIMO system dynamics. One important attempt is the realisation of a minimal order inverse dynamics, which has been defined as the zero dynamics [3]. In general, the construction of the zero dynamics involves complicated algorithmic procedures, which could be unsuccessful. According with Daoutidis and Kravaris [3], the analysis of the zero dynamics of nonlinear systems yields the same conclusions of the analysis of the zeros for linear ones. Zhao [4] analyses the zero dynamics of nonlinear control systems with symmetries, showing that the zero dynamics of a symmetric system is also symmetric and admits a special form of cascade decomposition. These local zero dynamics are always possible to be extended to the semi-global case. Aleksandrov and Platonov [5] worked on the stability of nonautonomous large-scale systems, where the stability of nonautonomous complex systems in closed-loop systems was investigated. An interesting idea used for chemical processes was to separate the nonlinear dynamics of the system into invertible and noninvertible parts, last one containing time delay terms [6].

The mentioned papers present very interesting theoretic frames, where some properties of the closed-loop performance of nonlinear systems are highlighted, however, the mathematical tools employed are complex and,

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Nomenclature

C_p	heat capacity at constant pressure (kJ/kmol K)
$\boldsymbol{f}$	vector of terms that are independent of the manipulated variable(s) (consistent)
F	volumetric flow (m^3/s)
$\boldsymbol{G}$	matrix of terms independent of manipulated variable(s) (consistent)
H	specific enthalpy (kJ/kmol)
m	mass flow (kg/s)
P	pressure (bar)
Q	heat flow (kW)
r	reaction rate (kmol/s kg_{cat}, kmol/s ${m_{gas}}^3$)
R_g	universal constant of ideal gases (bar m^3/kmol K)
T	temperature (K)
$\boldsymbol{u}$	vector of manipulable variables (consistent)
V	Lyapunov function (consistent)
W	catalyst mass hold up (kg)
$\boldsymbol{x}$	vector of states (consistent)
y	mole fraction (dimensionless)

Greek variables

ρ	mass density (kg/m^3)
ω	mass fraction (kg_{coke}/kg_{cat})

Subscript

C	control variable
cat	referred to catalyst
CRC	coke on regenerated catalyst
CSC	coke on spent catalyst
D	Uncontrolled or dynamic variable
dp	Referred to the regenerator dense phase
flue	Referred to regenerator stack gases
rgn	Referred to the whole regenerator

Superscript

i	inlet
sp	set point
T	transpose
-1	matrix inverse
·	time derivative

consequently, it is not possible to apply their methodologies to industrial plants yet. In order to be used as a simple test of controllability, in this work a simple methodology is proposed to analyse control options for nonlinear control affine systems.

2. Theoretical background

The procedure of design and control of chemical reacting systems provides a good target for the identification of stable operating steady states, which is a well-known topic (see [7], for example). Nonetheless, the easiness of the regulation of important states will depend on dynamic features related to operating conditions, design, control and the relationship among them. As it was pointed out, one of the most important characteristics that have to be analysed when a reacting system is to be controlled, is the stability of the zero dynamics [3].

A dynamic nonlinear model for the system under study, which consists of the mass balances, energy balances and equilibrium relationships (Eq. (1)) is the starting point:

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{G}(\boldsymbol{x})\boldsymbol{u} \tag{1}$$

Here

$$\boldsymbol{x} \in \Re^n, \qquad \boldsymbol{f}(\boldsymbol{x}) \equiv \{\boldsymbol{f} : \Re^n \to \Re^n\},$$
$$\boldsymbol{G}(\boldsymbol{x}) \equiv \{\boldsymbol{G} : \Re^n \to \Re^{nxm}\}, \qquad \boldsymbol{u} \in \Re^m$$

First of all, zero dynamics of a system are defined as the minimal order dynamics of its inverse [3,7]. For nonlinear systems the realisation of this inverse could be very complicated or even impossible. However, for control affine systems that are partially controlled, it is possible to asses the stability features of the zero dynamics following the dynamics of the uncontrolled (or dynamic) states, $\boldsymbol{x}_D$, while the system is regulated by the control of a subset of states, $\boldsymbol{x}_C$ (Eq. (2)):

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}) + \boldsymbol{G}(\boldsymbol{x})\boldsymbol{u} \to \begin{cases} \dot{\boldsymbol{x}}_C = \boldsymbol{f}_C(\boldsymbol{x}) + \boldsymbol{G}_C(\boldsymbol{x})\boldsymbol{u} \\ \dot{\boldsymbol{x}}_D = \boldsymbol{f}_D(\boldsymbol{x}) + \boldsymbol{G}_D(\boldsymbol{x})\boldsymbol{u} \end{cases} \tag{2}$$

The idea is to find the vector of manipulated inputs $\boldsymbol{u}$ assuming that the regulated variables will remain steady at the desired set point (Eq. (3)):

$$\dot{\boldsymbol{x}}_C^{sp} = 0 \Leftrightarrow \boldsymbol{u}^{sp} = -\boldsymbol{G}_C^{-1}(\boldsymbol{x})\boldsymbol{f}_C(\boldsymbol{x}) \tag{3}$$

Then it is possible to substitute the vector of manipulated variables, $\boldsymbol{u}^{sp}$, into the balances for dynamic variables (Eq. (4)):

$$\dot{\boldsymbol{x}}_D = \boldsymbol{f}_D(\boldsymbol{x}) - \boldsymbol{G}_D(\boldsymbol{x})\boldsymbol{G}_C^{-1}(\boldsymbol{x})\boldsymbol{f}_C(\boldsymbol{x}) \tag{4}$$

$$\boldsymbol{x}_D \in \Re^{n-m}, \qquad \boldsymbol{f}_D(\boldsymbol{x}) \equiv \{\boldsymbol{f}_D : \Re^{n-m} \to \Re^{n-m}\},$$
$$\boldsymbol{G}_D(\boldsymbol{x}) \equiv \{\boldsymbol{G}_D : \Re^{n-m} \to \Re^{(n-m)m}\}, \qquad \boldsymbol{u}^{sp} \in \Re^m$$

If the evolution of the dynamic behaviour of the uncontrolled variables is not stable when operating under this particular set of inputs $\boldsymbol{u}^{sp}$, it is possible to conclude that zero dynamics are not stable, as well [8]. Therefore, in order to ensure complete stability of the zero dynamics and of the control, each balance for the uncontrolled variables should tend to an attractor at the desired set point. The proposed policy is to ask for all the balances $\dot{\boldsymbol{x}}_D$ to have negative sign at the operating set point [8].

Proposition. *The controller of the system* $\dot{\boldsymbol{x}}$ *will be stable* $\forall t > 0$, *if and only if* $\boldsymbol{f}_D(\boldsymbol{x}) + \boldsymbol{G}_D(\boldsymbol{x})\boldsymbol{u}^{sp} < 0$ i.e. $\dot{\boldsymbol{x}}_D < 0\ \forall \boldsymbol{x}_D \in \boldsymbol{x}_D$.

Proof. Consider the closed-loop performance of the uncontrolled variables:

$$\dot{\boldsymbol{x}}_{\mathrm{D}} = \boldsymbol{f}_{\mathrm{D}}(\boldsymbol{x}) + \boldsymbol{G}_{\mathrm{D}}(\boldsymbol{x})\boldsymbol{u}^{\mathrm{sp}}$$

Now, define the Lyapunov function that follows:

$$V = \boldsymbol{e}^{\mathrm{T}} P \boldsymbol{e} = \|\boldsymbol{e}\|_{\mathrm{P}}^{2} > 0, \quad \boldsymbol{e} = (\boldsymbol{x}_{\mathrm{D}} - \boldsymbol{x}_{\mathrm{D}}^{\mathrm{sp}}) \Rightarrow \dot{\boldsymbol{e}} = \dot{\boldsymbol{x}}_{\mathrm{D}}$$

By applying the stability criterion of Lyapunov, the system $\dot{\boldsymbol{x}}_{\mathrm{D}}$ will be stable if the scalar function V is positive definite and its derivative is negative definite in some domain. Computing the derivative and substituting the expression for $\dot{\boldsymbol{e}}$, the following expression is obtained:

$$\dot{V} = \nabla V \cdot [\boldsymbol{f}_{\mathrm{D}}(\boldsymbol{x}) + \boldsymbol{G}_{\mathrm{D}}(\boldsymbol{x})\boldsymbol{u}^{\mathrm{sp}}] < 0$$

Because $\nabla V > 0\ \forall t$, and $\boldsymbol{u}^{\mathrm{sp}} \geq 0$, the system will be stable, $\forall t > 0$, if and only if:

$$\boldsymbol{f}_{\mathrm{D}}(\boldsymbol{x}) + \boldsymbol{G}_{\mathrm{D}}(\boldsymbol{x})\boldsymbol{u}^{\mathrm{sp}} < 0$$

i.e.

$$\dot{\boldsymbol{x}}_{\mathrm{D}} < 0\ \forall \boldsymbol{x}_{\mathrm{D}} \in \boldsymbol{x}_{\mathrm{D}} \qquad \square$$

Remarks. Notice that the full nonlinear model was used without linearisation or any other simplification. The vector of manipulated variables was defined as a function of the control policy, in terms of other process variables, and is evaluated at the *desired* set point, whatever it is. Due to these characteristics, the methodology can be used for *any* operating point that would be chosen as set point. Also, there were no restrictions to the type of controller used. Therefore, this methodology is applicable to *any* system that has control affine structure, in particular to CSTR systems.

It is possible to see that evaluation of the dynamics of vector of manipulate variables follows a procedure similar to the computing of elements of the relative gain array (RGA) by using partial derivatives of the process model with respect to manipulated variables [9]. The difference is that, in this case, the initial assumption is that manipulate variables vector $\boldsymbol{u}$ is already paired to the corresponding outputs. The RGA methodology, when is used in nonlinear systems, yields relative gains that rather depend on the steady state analysed, and are not constant. Following the methodology proposed in this paper, dynamic behaviour of uncontrolled states, influenced by interactions with controlled states, is obtained without the evaluation of the complete RGA. Moreover, in contrast to RGA, this methodology analyses uncontrolled states instead of controlled ones. Therefore, this methodology could be considered as complementary to the RGA analysis for nonlinear systems with control affine.

3. Case study: adiabatic FCC regenerators

Because of the large yield of products and their added value, fluid catalytic cracking units (FCC) are one of the most important process units in oil refineries. This process generates about 40% of the gasoline in the refinery pool; consequently any small benefit in this process is very profitable. One of the most important parts of the FCC is the catalyst regenerator-reactor, because in this vessel the cokised-spent catalyst is regenerated in order to recover catalytic activity. A very comprehensive description of FCC processes is in the classical paper by Venuto and Habib [10]. Regeneration consists of the burning-off of the deposited coke using atmospheric air, in a fluidised bed reactor that is considered as CSTR. The energy generated by the exothermic reactions is employed to vaporise the feedstock and to support the endothermic cracking reactions, which take place in the riser reactor [11]. Considering the exothermic nature of the regeneration reactions and the characteristics of the combustion kinetics, which can be described by consecutive reactions, it is expected the dynamic behaviour of the regenerator to be very complex. Some phenomena such as steady state multiplicity, inverse response to control actions (Fig. 1) and unstable operating zones might appear. An interesting feature of the system is that linear approximation of the model exhibits eigenvalues with positive real part (Fig. 2), which is an indication of instability of the closed-loop internal dynamics [3]. This instability will be reflected by control problems around these states [14].

One of the most common problems reflected when controlling adiabatic FCC units is the insufficient understanding of regenerator dynamics. Although fluidised beds have been a topic of study for many years, they are difficult to model and, therefore, the interpretation of operating results is not completely used to understand the dynamic behaviour of this kind of reactors [12].

Due to restrains in mechanical design, operating conditions and control actions are limited. Therefore, it is necessary to study stability and dynamic resilience taking into account these physical limits [13]. Since the riser is a plug flow reactor that carries out only endothermic reactions and feedstock vaporisation, it presents only one stable steady state for each operating condition. Hence, it is necessary to analyse the dynamics of the regenerator, exclusively [14].

Additionally, in adiabatic FCC regenerators there are very few manipulated variables, problem that limits the control design options [15]. The most common variables to manipulate are flow of air supplied to regenerator (F_{air}), mass flows of catalyst between reactors (m_{cat}) and preheat temperature of the feedstock (T_{feed}). In more sophisticated units it is also possible to manipulate the oxygen concentration in the air supplied to the regenerator and regenerator cooling rate, however, these cases will not be discussed in this paper. Then, the problem of control design yields a "pairing game" between a small set of manipulated variables and a large set of control targets on a narrow and constrained operating window [10].

As any reacting system, FCC regenerators are nonlinear systems. Research related to dynamic performance of FCC units has pointed out that operating in partial combustion mode (CO is present in regenerator flue gases) is

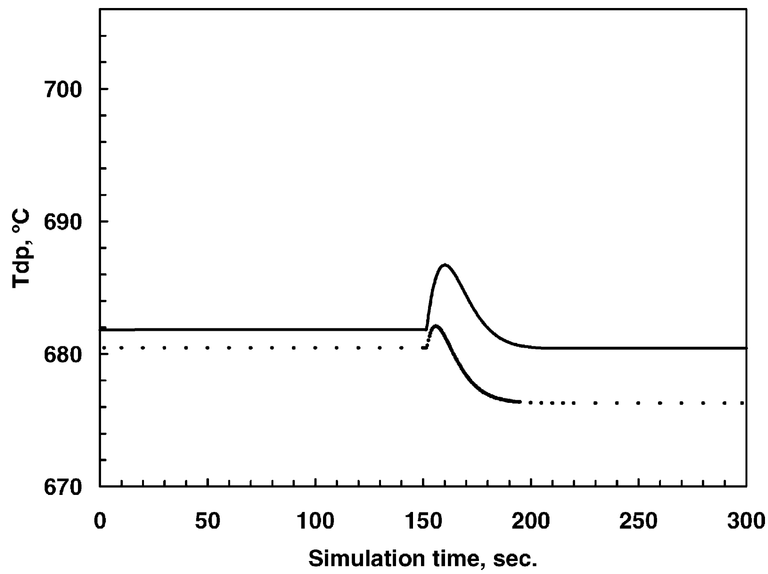

Fig. 1. Regenerator temperature inverse response at commercial operating conditions. Change from $F_{air} = 0.90F_{air}^{Base\ case}$ to $F_{air} = F_{air}^{Base\ case}$ (solid line) and from $F_{air} = 0.83F_{air}^{Base\ case}$ to $F_{air} = 1.05F_{air}^{Base\ case}$ (dotted line).

pseudo-stable [16,17]. Also, it has been said that a change to full combustion mode, by increasing the airflow rate, could eliminate steady state multiplicity at industrial operating conditions [16]. This phenomenon has been described by a convergence of the intermediate steady state to the ignited one [12]. This is also in agreement with the idea that an increase in the operating temperature of the regenerator dense phase is able to stabilise the system in most cases, even when operating in partial combustion mode [15]. Again, it is necessary to follow, as precisely as possible, the dynamics of the energy balance at the regenerator.

An industrial FCC unit is used as example; its main characteristics are summarised in Appendix A. The states that are followed are oxygen concentration at dense phase, carbon on regenerated catalyst, CO concentration at dense phase and dense phase temperature; all of them important operation variables. So, the vector of states is defined as $\boldsymbol{x} = (y_{O_2}\ \omega_{CRC}\ y_{CO}\ T_{dp})^T$. (See nomenclature section for definition of variables).

A nonlinear mathematical model of the process is developed in order to apply the methodology proposed. Introducing the dynamics of the gaseous entities in the dense

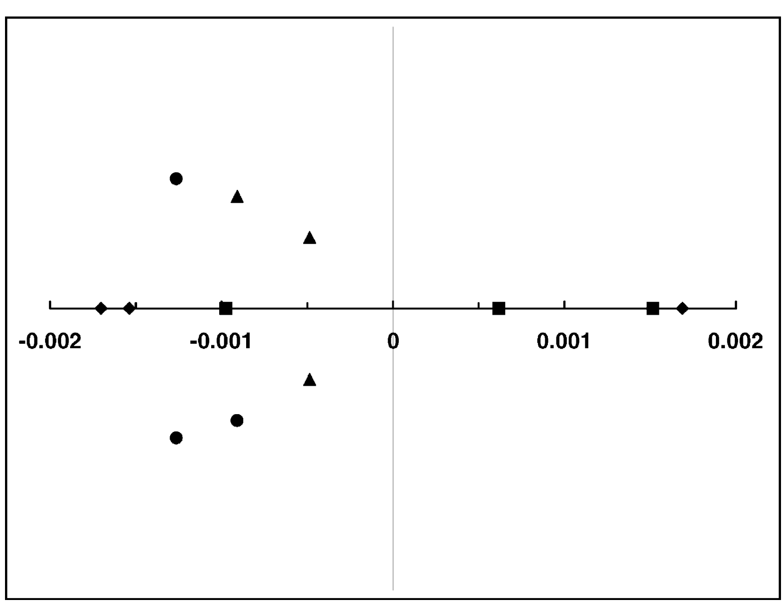

Fig. 2. Eigenvalues for linearised approximations of the model at commercial operating conditions: (◆) $F_{air} = 0.75F_{air}^{Base\ case}$, (■) $F_{air} = 0.90F_{air}^{Base\ case}$, (▲) $F_{air} = F_{air}^{Base\ case}$, (●) $F_{air} = 1.50F_{air}^{Base\ case}$.

phase, (Eq. (5)), complements the model proposed by Arbel et al. [11]. The kinetic scheme and parameters proposed by Arandes et al. [18] were used. A comparison of the easiness to control is performed for different operating steady states, when either T_{dp} or y_{O_2} is chosen as control target.

$$\dot{x} = \begin{pmatrix} (y^{i}_{O_2} - y_{O_2})F_{air} + r_{O_2} \\ r_{coke} + m_{cat}\dfrac{\omega_{CSC} - \omega_{CRC}}{W_{rgn}} \\ (y^{i}_{CO} - y_{CO})F_{air} + r_{CO} \\ \dfrac{Q^{i}_{steam} + (C^{i}_{p_g}T^{i}_{g} - C_{p_g}T_{dp})F_{air} + \sum_{j=1}^{j=3}(-\Delta H_r)_j r_j + m_{cat}C_{p_p}(T^{i}_{cat} - T_{dp})}{W_{rgn}C_{p_p}} \end{pmatrix} \quad (5)$$

(control of either y_{O_2} or T_{dp}) are studied using the methodology developed in the Section 2 of this paper, in order to characterise the dynamics at different operating steady states. Note that both control policies are analysed using the same operating data, so the different control problems exhibited by the system are consequence, only, of the variable pairing.

4. Results and discussion

In order to obtain the desired operating points, a commercial simulator/optimiser (KBC-Profimatics FCC-Sim, Version 99) was tuned, against some industrial data, and used to simulate operating regions for two different objective functions: maximum C_4-olefins production and maximum gasoline production. Industrial and simulation results are plotted against riser outlet temperature, which is the industrial reference set point in industrial operation (Figs. 3 and 4). Results taken from the simulator are the set points of the riser outlet temperature and some of the dependent operating variables. After that, the dynamic model described previously is used to determine the sign of the mass balances for y_{O_2}, ω_{CRC}, y_{CO} and the energy balance for T_{dp}, when applicable. The aim is to regulate the regenerator during normal operating conditions. Hence, the two control policies described

4.1. Example 1: only one manipulable variable is available

For the first example, it is assumed that F_{air} is the only variable available to regulate the regenerator, as it is the case in industrial practice. Therefore, it is possible to regulate only one control target. The following operation policies analyse the effect of two different elections of this control target.

4.1.1. First operating policy

The first case study is the analysis of the dynamic behaviour of the FCC regenerator when an arbitrary initial steady state is changed to the maximum C_4-olefins

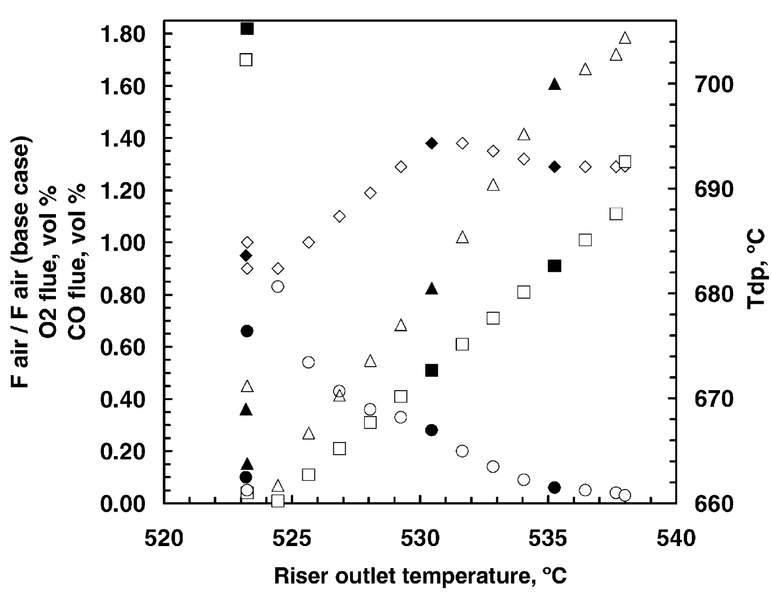

Fig. 3. Operating (solid) and simulated (void) steady states in the region of maximum olefin production: (◆) F_{air}, (▲) T_{dp}, (●) y_{CO}, (■) y_{O_2}.

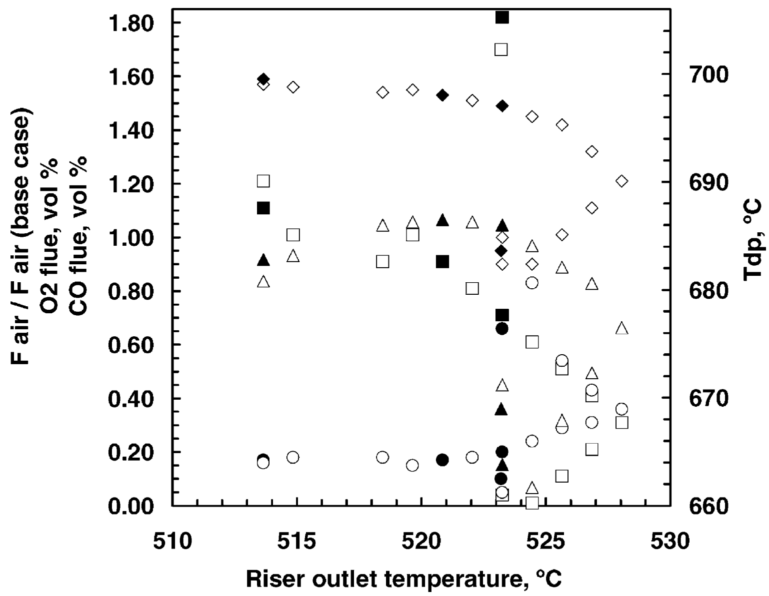

Fig. 4. Operating (solid) and simulated (void) steady states in the region of maximum gasoline production: (◆) F_{air}, (▲) T_{dp}, (●) y_{CO}, (■) y_{O_2}.

production point. The first control policy to be analysed is the proposed for full combustion regenerators, i.e. y_{O_2} is the control target. Following the methodology proposed (Eq. (2)); the vector of states is divided into controlled and uncontrolled variables (Eq. (6)):

$$\boldsymbol{x}_{C} = (y_{O_2}), \qquad \boldsymbol{x}_{D}^{T} = (\omega_{CRC}\ y_{CO}\ T_{dp}) \tag{6}$$

Following the methodology (Eq. (3)), the value of the manipulated variable is then calculated for the desired set point (Eq. (7)):

$$\boldsymbol{u}^{sp} = F_{air}^{sp} = -\frac{r_{O_2}}{y_{O_2}^{i} - y_{O_2}^{sp}} \tag{7}$$

Once the manipulated variable is known, it is possible to calculate the dynamics of the uncontrolled variables (as it was done in Eq. (4)), when the unit is operating following this control policy (Eq. (8)):

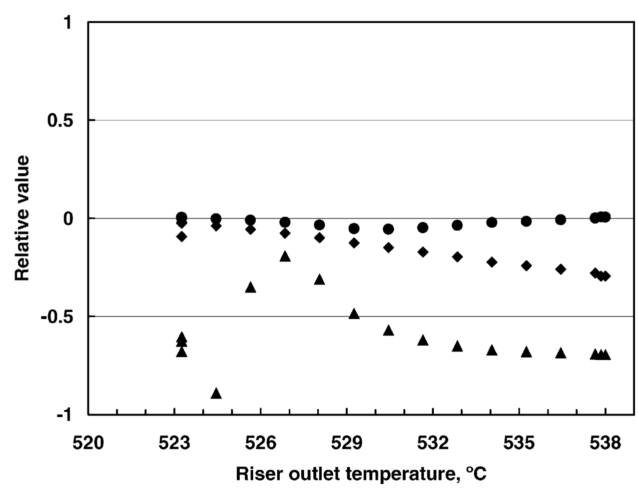

Fig. 5. Values of the balances for $\dot{\boldsymbol{x}}_D$ when controlling y_{O_2} in the region of maximum olefin production: (▲) T_{dp}, (◆) ω_{coke}, (■) y_{CO}.

$$\dot{\boldsymbol{x}}_D = \begin{pmatrix} r_{coke} + \dfrac{\omega_{CSC} - \omega_{CRC}}{W_{rgn}} m_{cat} \\ r_{CO} - \dfrac{(y_{CO}^{i} - y_{CO})}{(y_{O_2}^{i} - y_{O_2}^{sp})} r_{O_2} \\ \left\{ Q_{steam}^{i} + \sum_{j=1}^{j=3} (-\Delta H_j) r_j + m_{cat} C_{p_p} (T_{cat}^{i} - T_{dp}^{sp}) - \dfrac{C_{p_g}^{i} T_g^{i} - C_{p_g} T_{dp}}{(y_{O_2}^{i} - y_{O_2}^{sp})} r_{O_2} \right\} \dfrac{1}{W_{rgn}} \end{pmatrix} \tag{8}$$

The relative values of the balances for $\dot{\boldsymbol{x}}_D$ for different steady states, when maximum olefin production is required are shown in Fig. 5.

As it can be seen, at the first three operating states, the unit was predicted to be around a difficult operating point. This was due to the fact that the air supplied was not enough. In fact, the CO concentration in flue gases was higher, which means that there is partial combustion. From the fourth state the air amount was increased, changing the operating conditions to more favourable ones. As it can be noticed in Fig. 4, this operating region presents local problems of stability of the zero dynamics, because of the positiveness of some eigenvalues. This situation is found during operation because at this operating point temperatures tend to change 'too fast' and sometimes to the undesired direction. This is also reflected by the possibility of inverse response in this range of F_{air} values (Fig. 1). Once the airflow is increased these problems disappear.

This case illustrates the common industrial control policy. Because this unit operates at full combustion, the control policy should be the regulation of y_{O_2}. Once the air amount is incremented, this operating problem disappears. Therefore, it is possible to note that between 525 and 535 °C the unit works satisfactorily.

The change of signs of CO balance at about 536 °C was discussed with the refinery operators. They said that there is a 'kind of limit' in riser outlet temperature, which is reflected by control problems if it is exceeded. Their rule of thumb is to establish, *a priori*, a maximum temperature and never cross over it. This analysis provides this maximum temperature simply following the time evolution of the signs of mass and energy balances. The actual maximum temperature limit depends on operating conditions and would not be easily estimated *a priori*, however, using this methodology this limit is predicted from steady state simulations.

4.1.2. Second control policy

This control policy is the one proposed for partial combustion regenerators, i.e. T_{dp} is the control target. Following the proposed methodology, the vector of states is divided into controlled and uncontrolled variables (Eq. (9)):

$$\boldsymbol{x}_C = (T_{dp}), \qquad \boldsymbol{x}_D^T = (y_{O_2}\ \omega_{CRC}\ y_{CO}) \tag{9}$$

Now, the value of the manipulated variable is calculated for the desired set point (Eq. (10)):

$$\boldsymbol{u}^{sp} = F_{air}^{sp} = -\frac{Q_{steam}^{i} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j + m_{cat}C_{p_p}(T_{cat}^{i} - T_{dp}^{sp})}{C_{p_g}^{i}T_g^{i} - C_{p_g}T_{dp}^{sp}} \tag{10}$$

Once the manipulated variable is known, it is possible to calculate the dynamics of the uncontrolled variables, when the unit is operating under this control policy (Eq. (11)):

$$\dot{\boldsymbol{x}}_D = \begin{pmatrix} r_{O_2} - \dfrac{Q_{steam}^{i} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j + m_{cat}C_{p_p}(T_{cat}^{i} - T_{dp}^{sp})}{C_{p_g}^{i}T_g^{i} - C_{p_g}T_{dp}^{sp}}(y_{O_2}^{i} - y_{O_2}) \\ r_{coke} + \dfrac{\omega_{CSC} - \omega_{CRC}}{W_{rgn}}m_{cat} \\ r_{CO} - \dfrac{Q_{steam}^{i} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j + m_{cat}C_{p_p}(T_{cat}^{i} - T_{dp}^{sp})}{C_{p_g}^{i}T_g^{i} - C_{p_g}T_{dp}^{sp}}(y_{CO}^{i} - y_{CO}) \end{pmatrix} \tag{11}$$

Following this control policy, the relative values of the balances for $\dot{\boldsymbol{x}}_D$, using the same operating data of the first operating policy, are shown in Fig. 6.

It is possible to note that the control of T_{dp} will perform adequately only for the bad operating points, i.e. when the unit is operating in partial combustion mode. This is theoretically right, because for FCC units that operate in partial combustion T_{dp} is always the control target. However, to operate under full combustion mode, it is necessary to ensure the burn of CO produced; therefore temperature should be free. The problems of inverse response in temperature and the positive eigenvalues illustrated by Figs. 1 and 2, respectively, are closely related to this control instability [8]. The signs of the balances also exhibit this problem, if T_{dp} is regulated, then O_2 and CO balances tend to move away from the desired steady state, hence there will be control problems. When full combustion is achieved, control of T_{dp} always exhibits controllability problems.

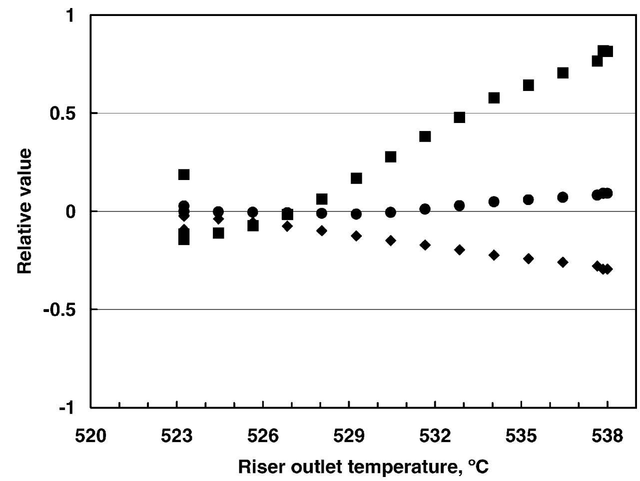

Fig. 6. Values of the balances for $\dot{\boldsymbol{x}}_D$ when controlling T_{dp} in the region of maximum olefin production: (■) y_{O_2}, (◆) ω_{coke}, (●) y_{CO}.

4.1.3. Second operating policy

The second operating policy to be analysed is the maximum gasoline production. Simulation results of some operating steady states are shown in Fig. 4.

The analysis of the control policies follows the same steps as in the case of the first operating policy. The first control policy analysed is the proposed for full combustion regenerators, i.e. y_{O_2} is the control target, and the second one is the use of T_{dp} as control target. The sign of the mass and energy balances of both control policies are shown in Figs. 7 and 8.

When optimising gasoline, the best operating policy is to take the reaction temperature to values smaller than the

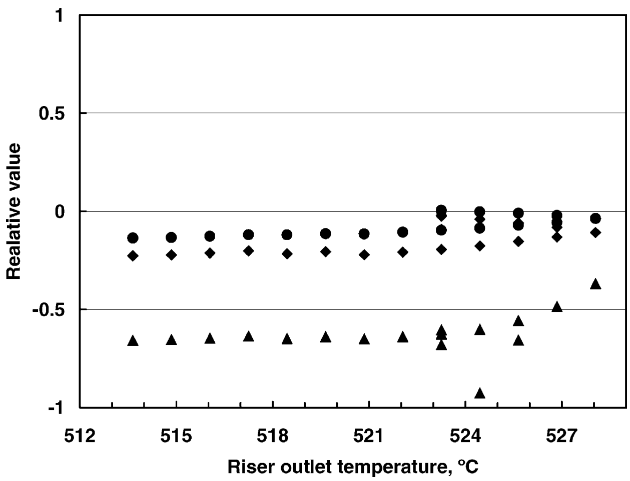

Fig. 7. Values of the balances for $\dot{x}_D$ when controlling y_{O_2} in the region of maximum gasoline production: (▲) T_{dp}, (◆) ω_{coke}, (●) y_{CO}.

base case. This situation arises because higher temperatures improve conversion to lighter products, such as LPG and dry gases. The first three steady states behave the same as in the other cases analysed, and later the control of y_{O_2} is always adequate (Fig. 7). In this case, between 513 and 526 °C, the system is working properly in a region that does not present controllability problems.

In contrast to the last analysis, control of T_{dp} always presents controllability problems (Fig. 8). This is the expected situation because of the industrial control mode, i.e. full combustion. It is important to notice that the maximum of gasoline production takes place at lower operating temperatures. And even for these 'softer' conditions, a wrong control policy will cause control problems during normal operation.

Again, following the signs of the balances it is possible to predict the best control policy for different operating conditions. For both situations, results are coherent with industrial experience. The methodology was able to explain the rule of thumb for maximum reaction temperature in this particular unit and, even better, was able to predict the value of the maximum temperature. Therefore, this rule of thumb is supported by this analysis of mass and energy balances.

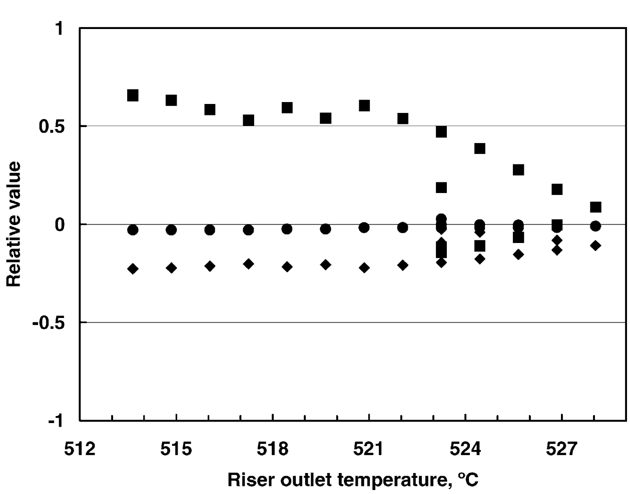

Fig. 8. Values of the balances for $\dot{x}_D$ when controlling T_{dp} in the region of maximum gasoline production: (■) y_{O_2}, (◆) ω_{coke}, (●) y_{CO}.

4.2. Example 2: two manipulable variables are available

The second example shows the result of the application of the methodology developed when another control scheme is analysed for the same unit. In this case, it is considered that it is possible to manipulate, as independent variables, both the airflow rate and the mass catalysis flow that arrive to regenerator, i.e. $\boldsymbol{u}^{T} = (F_{air}\, m_{cat})$. Although this example is not applicable in industry because m_{cat} is used to regulate riser outlet temperature, it will illustrate the different behaviour presented by the regenerator when control policies are changed, for the same operating conditions.

In this case, the first control target to choose is the carbon mass fraction on regenerated catalyst, ω_{CRC}. This variable is very important because sets the catalytic activity for cracking. Also, if ω_{CRC} grows up the unit would move to the 'snowball quenching', phenomenon that is well-known [17]. The second control target is chosen analogous to Example 1.

4.2.1. First operating policy

The first operating policy to be analysed is, again, the maximum C_4-olefins production. The operating steady states simulated are, obviously, the same of the first operating policy in Example 1 (Fig. 3).

The first control policy to be analysed is the proposed for full combustion regenerators, i.e. y_{O_2} is the control target. Following the proposed methodology, the vector of states is divided into controlled and uncontrolled variables (Eq. (12)):

$$\boldsymbol{x}_C^T = (y_{O_2}\, \omega_{CRC}), \qquad \boldsymbol{x}_D^T = (y_{CO}\, T_{dp}) \tag{12}$$

Now, the value of the manipulated vector of variables is calculated for the desired set point (Eq. (13)):

$$\dot{\boldsymbol{x}}_C^{sp} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \Leftrightarrow u^{sp} = \begin{pmatrix} F_{air} \\ m_{cat} \end{pmatrix}^{sp} = -\begin{pmatrix} y_{O_2}^{i} - y_{O_2}^{sp} & 0 \\ 0 & \dfrac{\omega_{CSC} - \omega_{CRC}^{sp}}{W_{rgn}} \end{pmatrix}^{-1} \begin{pmatrix} r_{O_2} \\ r_{coke} \end{pmatrix} \tag{13}$$

Once the manipulated vector is known, it is possible to calculate the dynamics of the uncontrolled variables, when the

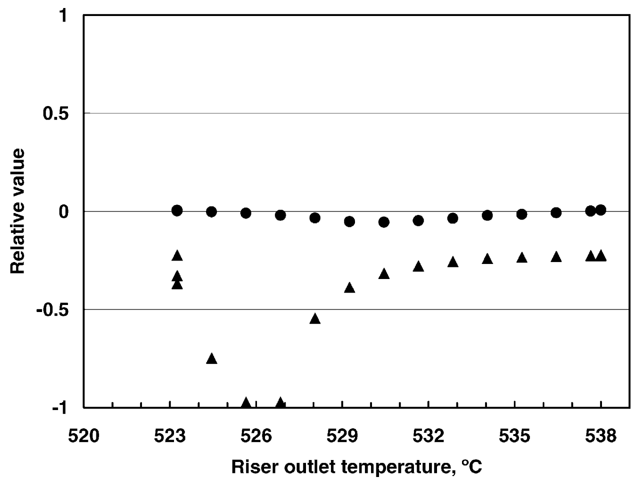

Fig. 9. Values of the balances for $\dot{x}_D$ when controlling y_{O_2} in the region of maximum olefin production: (▲) T_{dp}, (●) y_{CO}.

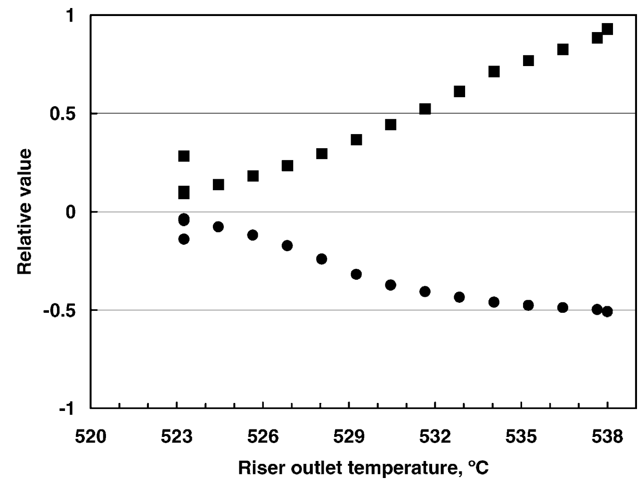

Fig. 10. Values of the balances for $\dot{x}_D$ when controlling T_{dp} in the region of maximum olefin production: (■) y_{O_2}, (●) y_{CO}.

unit is operating following this control policy (Eq. (14)):

$$\dot{x}_D = \begin{pmatrix} r_{CO} - \dfrac{y^i_{CO} - y_{CO}}{y^i_{O_2} - y_{O_2}}(r_{O_2}) \\ \dfrac{Q^i_{steam} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j}{W_{rgn} C_{p_p}} - \dfrac{C^i_{p_g} T^i_g - C_{p_g} T_{dp}}{(y^i_{O_2} - y_{O_2}) W_{rgn} C_{p_p}}(r_{O_2}) - \dfrac{(T^i_{cat} - T_{dp})}{\omega_{CSC} - \omega_{CRC}}(r_{coke}) \end{pmatrix} \tag{14}$$

Following this control policy, the signs of the balances for $\dot{x}_D$ during the optimisation of olefin production are shown in Fig. 9.

As it was expected, control of y_{O_2} was easier at steady states over 526 °C, i.e. when operating under full combustion mode. Again, a maximum in operating temperature was detected at about 536 °C, and control problems were predicted in the following simulations.

The second control policy, when operating at this operating policy to be analysed is the proposed for partial combustion regenerators, i.e. T_{dp} is the control target. Following the proposed methodology, the vector of states is divided into controlled and uncontrolled variables (Eq. (15)):

$$x^T_C = (\omega_{CRC}\ T_{dp}), \qquad x^T_D = (y_{O_2}\ y_{CO}) \tag{15}$$

Now, the value of the manipulated variable is calculated for the desired set point (Eq. (16)):

$$u^{sp} = -\begin{pmatrix} 0 & \dfrac{\omega_{CSC} - \omega^{sp}_{CRC}}{W_{rgn}} \\ C^i_{p_g} T^i_g - C_{p_g} T^{sp}_{dp} & C_{p_p}(T^i_{cat} - T^{sp}_{dp}) \end{pmatrix}^{-1} \begin{pmatrix} r_{coke} \\ Q^i_{steam} + \sum_{j=1}^{j=3}(-\Delta H_r)_j r_j \end{pmatrix} \tag{16}$$

Once the manipulated variable is known, it is possible to calculate the dynamics of the uncontrolled variables, when the unit is operating following this control policy (Eq. (17)):

$$\dot{x}_D = \begin{pmatrix} r_{O_2} - \dfrac{(y^i_{O_2} - y_{O_2})(Q^i_{steam} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j)}{C^i_{p_g} T^i_g - C_{p_g} T_{dp} - (y^i_{O_2} - y_{O_2}) C_{p_p}(T^i_{cat} - T_{dp}) r_{coke}} \\ r_{CO} - \dfrac{(y^i_{CO} - y_{CO})(Q^i_{steam} + \sum_{j=1}^{j=3}(-\Delta H_j)r_j)}{C^i_{p_g} T^i_g - C_{p_g} T_{dp} - (y^i_{CO} - y_{CO}) C_{p_p}(T^i_{cat} - T_{dp}) r_{coke}} \end{pmatrix} \tag{17}$$

Following this control policy, the evolution of the signs of the balances for $\dot{x}_D$ during the optimisation of olefin production are shown in Fig. 10.

As it was expected, control of T_{dp} exhibits a complete different behaviour. When two control targets are available, it is not adequate at all to follow this control policy for any operating conditions (Fig. 10). In this case, the O_2 balance reflects control problems for the whole range of operating

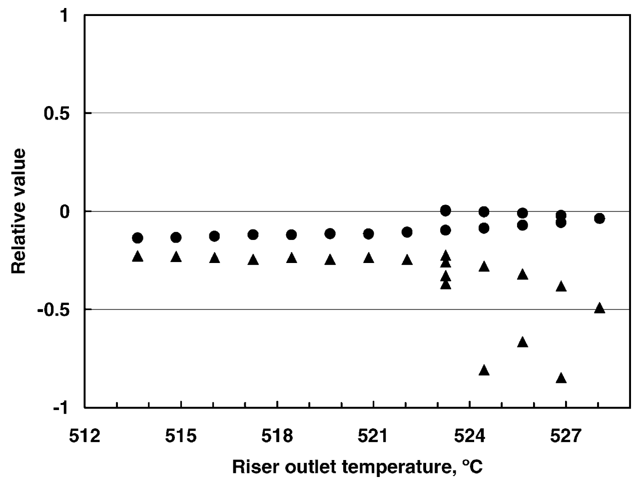

Fig. 11. Values of the balances for $\dot{x}_D$ when controlling y_{O_2} and m_{cat} in the region of maximum gasoline production: (▲) T_{dp}, (●) y_{CO}.

conditions. Hence, even for partial combustion operating regions, the control of T_{dp} will exhibit control problems. This result is different to the case when there is only one control target. Since operating conditions are the same, these different behaviours depend, only, upon the control scheme that was chosen.

4.2.2. Second operating policy

The second operating policy to be analysed is the maximum gasoline production. The analysis of the control policies follows the same steps of the first operating policy. The first control policy analysed is the proposed for full combustion regenerators, i.e. y_{O_2} is the control target, and the second one is the use of T_{dp} as control target. Following the methodology proposed, the evaluations of both control policies are shown in Figs. 11 and 12.

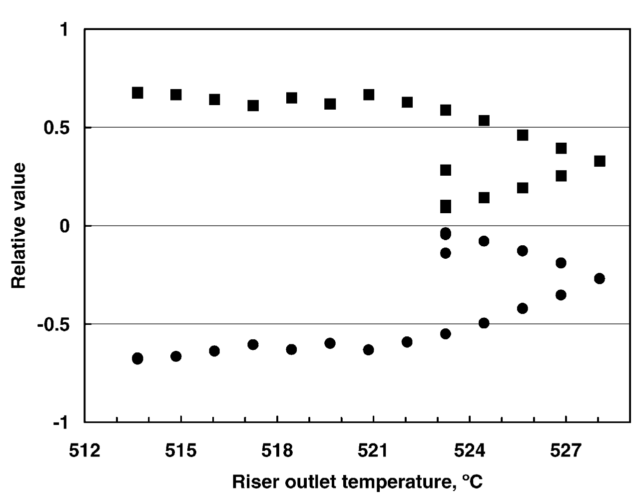

Fig. 12. Values of the balances for $\dot{x}_D$ when controlling T_{dp} and m_{cat} in the region of maximum gasoline production: (■) y_{O_2}, (●) y_{CO}.

The first three steady states show the same evolution of Figs. 9 and 10, and later the control of y_{O_2} is always adequate. Meanwhile, control of T_{dp} will always present control problems. This is the expected situation because of the industrial control mode and the results obtained when optimising for C_4-olefins production. Again, following the signs of the balances it is possible to predict the best control policy for different operating conditions.

For both operating policies (maximisation of either C_4-olefins or gasoline), it is noticed that the choosing of the pairing among control and manipulate variables is a key issue. The operating performance of the unit, even when operating at optimum steady states, will depend on control behaviour, i.e. on the controllability of the system. The results obtained were coherent with industrial practice and were able to predict the maximum operating temperature, a rule of thumb used by operators. Results for variables pairing gave similar results for two cases, one with only a single control target and the other with two control targets.

5. Conclusions

A methodology for the evaluation of control strategies, and for the preliminary assessment of controllability of nonlinear systems was proposed. It is applicable for any nonlinear system that presents control affine structure. Due to the fact that the full nonlinear model of the process is used, the methodology is applicable to any steady state that is chosen as the set point. In particular, CSTR systems are good targets to apply this methodology. The analysis proposed compliments the classical RGA for nonlinear systems.

Two examples of evaluation illustrated the predictions obtained. In both the results were coherent with industrial practice, rules of thumb and operators' experience. Therefore, the methodology predictions were accurate. For two cases, one or two possible control targets, analysed results were coherent with industrial experience. The methodology was able to explain the rule of thumb for maximum reaction temperature in this particular unit and, even better, was able to predict the value of this maximum temperature for two different control policies. Moreover, this methodology was very easy to understand, to evaluate and to apply during normal industrial operation.

Acknowledgements

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Appendix A. Description of the FCC unit

Main operating data of the FCC unit studied

Type of unit	Adiabatic
Operating mode	Full combustion
Unit feedstock capacity (BPD)	25,000
Average coke production (t/D)	160
Average air flow rate (m^3/h)	75,000

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