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# Controllability of Lumped Parameter Chemical Reactors\*

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A methodology for the evaluation of control strategies and for the preliminary assessment of controllability of nonlinear control affine systems was proposed. 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. Also, there is no condition for the selection of controller used; therefore the methodology can be applied to *any* control structure selected for this process. An industrial system, fluidised bed catalyst regenerator, was used to illustrate application of this methodology.

The choice and pairing of control and manipulate variables in lumped parameter chemical reactors, usually Continuous Stirred Tank Reactors (CSTR), is not an easy task because of the lack of methodologies for a systematic evaluation of control schemes in nonlinear systems. Furthermore, intrinsic nonlinearities of this kind of systems could provoke responses to control actions that are difficult to predict. The classical procedure to identify stable operating steady states in CSTR does not help in the evaluation of the “easiness to control” (called controllability) at each desired operating state. It is important to note that controllability problems could cause an increase of operating costs, which are nonconvenient from the economic viewpoint. Nonetheless, there is an interesting feature of CSTR, they present control affine structure; *i.e.* manipulate variables affect the process dynamics in a linear way. In this work, advantage of this feature will be taken to find a strategy to compare the performance of different pairings of control and manipulate variables.

## THEORETICAL

The first step to determine the “easiness” of control of a CSTR is to develop a mathematical model, which consists of mass and energy balances and equilibrium and constitutive relationships. Thus, for  $n$  system states and  $m$  available manipulate variables, the following model may be written

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{G}(\mathbf{x})\mathbf{u} \quad (1)$$

Here  $\mathbf{x} \in \mathbb{R}^n$  is the vector of states,  $\mathbf{f} \in \mathbb{R}^n$  is a vector that contains the nonlinear part of mass and energy balances (mainly reaction terms), and  $\mathbf{G}(\mathbf{x}) \equiv \{\mathbf{G} : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^n\}$  is a rectangular matrix that contains the linear terms of the balances.  $\mathbf{u} \in \mathbb{R}^m$  is the vector of manipulate variables, which are the action variables in the control scheme.

Now, it is necessary to look for the stability of the system's zero dynamics [1], *i.e.* the dynamics of the system's inverse [2]. However, sometimes it is impossible to find this inverse dynamics for industrial systems. Nevertheless, even presenting control affine structure, characterisation of the zero dynamics of such systems could be performed in an alternative way; for example by following the idea of the Internal Model Control that separates an invertible and a not invertible part [3]. Firstly, the state variables vector is divided into “direct controlled variables”,  $x_C$ , and “uncontrolled variables”,  $x_D$

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{G}(\mathbf{x})\mathbf{u} \rightarrow \begin{cases} \dot{x}_C = \mathbf{f}_C(\mathbf{x}) + \mathbf{G}_C(\mathbf{x})\mathbf{u} \\ \dot{x}_D = \mathbf{f}_D(\mathbf{x}) + \mathbf{G}_D(\mathbf{x})\mathbf{u} \end{cases} \quad (2)$$

Note that nonlinear functions ( $\mathbf{f}_C, \mathbf{f}_D$ ) and linear matrices ( $\mathbf{G}_C, \mathbf{G}_D$ ) depend on the complete vector of state variables  $\mathbf{x}$ . Also, the vector of manipulate variables,  $\mathbf{u}$ , is the same in both subsystems. It is necessary that square matrix  $\mathbf{G}_C(\mathbf{x}) \equiv \{\mathbf{G}_C : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}^n\}$  be invertible in order to perform this analysis; however, this is the common situation in mass and energy balances.

In order to apply the methodology given in [1], it

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is necessary to find the values of entries of the manipulate variables vector that ensure that controlled variables are steady at the set-point

$$\dot{\mathbf{x}}_C^{\text{SP}} = 0 \Leftrightarrow \mathbf{u}^{\text{SP}} = -\mathbf{G}_C^{-1}(\mathbf{x}) \mathbf{f}_C(\mathbf{x}) \quad (3)$$

If the dynamic evolution of the uncontrolled variables

$$\Rightarrow \dot{\mathbf{x}}_D = \mathbf{f}_D(\mathbf{x}) - \mathbf{G}_D(\mathbf{x}) \mathbf{G}_C^{-1}(\mathbf{x}) \mathbf{f}_C(\mathbf{x}) \quad (4)$$

exhibits negative sign (for the vector  $\mathbf{u}^{\text{SP}}$  determined from the control variables), it is possible to conclude that the system's zero dynamics is stable and, therefore, the control at this steady state will perform as expected [2]. For a discussion of this stability implication following Lyapunov functions see [1].

If evolution of the dynamic behaviour of uncontrolled variables is not stable, when operating under this particular set of inputs,  $\mathbf{u}^{\text{SP}}$ , *i.e.* it exhibits positive sign, it is possible to conclude that the zero dynamics is not stable as well [4]. Therefore, in order to ensure complete stability of the zero dynamics and the control, each balance for uncontrolled variables should exhibit negative sign at the desired set point, which will ensure the Lyapunov stability, too [1]. It is possible to notice that evaluation of the dynamics of vector of free 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 manipulate variables [5]. The difference is that, in this case, the initial assumption is that manipulate variables vector  $\mathbf{u}$  is already paired to the corresponding outputs. The RGA methodology, when used in nonlinear systems, yields relative gains that rather depend on the steady state analysed, and are not constant. Also, 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.

There are no limits to the type of controller used, which could be PI, PID, or any other. Furthermore, because linearization around the set point was not necessary, this methodology can be used at any operating point in control affine systems.

## EXPERIMENTAL

The analysis mentioned above was used to evaluate two control options applied to catalyst regenerators of fluidised-bed catalytic cracking units. This type of industrial CSTR is used in petroleum refining to convert a heavy feedstock (mainly vacuum gas oil) into high-value fuels, in the presence of synthetic catalysts. These units could be operated following different objectives, one of them is maximising LP gas ( $C_3$ – $C_4$  hydrocarbons) production, which means that the riser

outlet temperature is changing from 525°C up to the unit design limit; a good description of this reacting system and its features can be found in [6].

Due to current environmental constraints, these units are operated following complete combustion mode [7], *i.e.* it is necessary to ensure that the flue gases are free of carbon monoxide ( $y_{CO} = 0$ ). In this work a mathematical model for this system that was developed recently [1] is used

$$\begin{aligned} \dot{\mathbf{x}} = & \\ = & \begin{pmatrix} r_{\text{coke}} + m_{\text{cat}} \left( \frac{r_{O_2} (\omega_{\text{CSC}} - \omega_{\text{CRC}})}{W_{\text{rgn}}} \right) \\ r_{\text{CO}} \\ \frac{Q_{\text{steam}}^i + m_{\text{cat}} C_{p_p} (T_{\text{cat}}^i - T_{\text{dp}}) + \sum_{j=1}^{j=3} (-\Delta H_r)_j r_j}{W_{\text{rgn}} C_{p_p}} \end{pmatrix} \\ + & \begin{pmatrix} (y_{O_2}^i - y_{O_2}) \\ 0 \\ (y_{CO}^i + y_{CO}) \\ \frac{C_{p_g} (T_g^i - T_{\text{dp}})}{W_{\text{rgn}} C_{p_p}} \end{pmatrix} F_{\text{air}} \end{pmatrix} \quad (5)$$

The vector of state variables consists of oxygen concentration, coke on regenerated catalyst, carbon oxide concentration, and dense bed temperature,  $\mathbf{x} = (y_{O_2} \ \omega_{\text{CRC}} \ y_{CO} \ T_{\text{dp}})^T$ ; all variables are known for  $t = 0$ .

Data necessary for evaluation of variables were obtained from [8], using the riser outlet temperature as a parameter; additional details cannot be supplied because operating data are proprietary.

The following examples compare two different options to control the unit considering the industrial production objective. The model given by eqn (5) and the strategy of evaluation of controllability were used to follow the trend of uncontrolled variables. It is assumed that  $F_{\text{air}}$  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. Because there were no specific requirements on the controller used, the methodology can be applied to any control affine structure.

## RESULTS AND DISCUSSION

The first control policy was proposed for partial combustion regenerators, with  $T_{\text{dp}}$  as the control target. Following eqn (2), the vector of states was divided into controlled and uncontrolled variables

$$\begin{aligned} \mathbf{x}_C &= (T_{\text{dp}}) \\ \mathbf{x}_D^T &= (y_{O_2} \ \omega_{\text{CRC}} \ y_{CO}) \end{aligned} \quad (6)$$

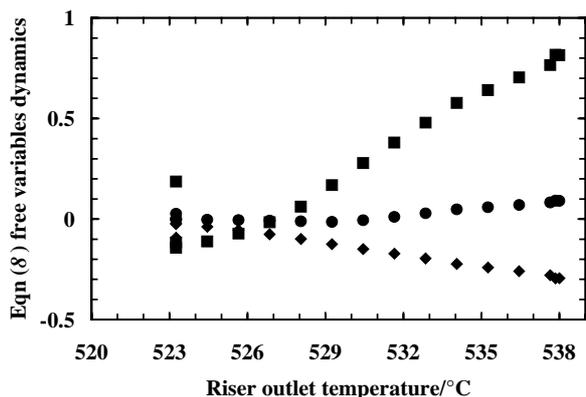


Fig. 1. Relative values of  $\hat{x}_D$  when controlling  $T_{dp}$ : ■  $y_{O_2}$ , ♦  $\omega_{CRC}$ , ●  $y_{CO}$ .

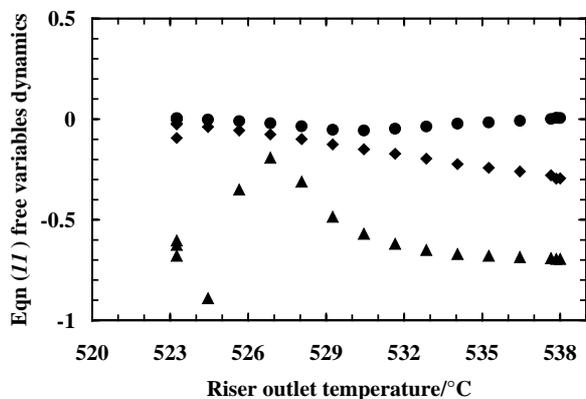


Fig. 2. Relative values of  $\hat{x}_D$  when controlling  $y_{O_2}$ : ♦  $\omega_{CRC}$ , ●  $y_{CO}$ , ▲  $T_{dp}$ .

and the theoretical value of manipulate variable was calculated for the desired set point following eqn (4)

$$u^{sp} = F_{air}^{sp} = \frac{Q_{steam}^i + \sum_{j=1}^{j=3} (-\Delta H_j) r_j + m_{cat} C_{pP} (T_{cat}^i - T_{dp}^{sp})}{C_{p_g}^i T_g^i - C_{p_g} T_{dp}^{sp}} \quad (7)$$

Once the value of manipulate variable was known, it was possible to calculate the dynamics of uncontrolled variables, when the unit is operating under this control policy

$$\hat{x}_D = \begin{pmatrix} r_{O_2} - \frac{Q_{steam}^i + \sum_{j=1}^{j=3} (-\Delta H_j) r_j + m_{cat} C_{pP} (T_{cat}^i - T_{dp}^{sp})}{C_{p_g}^i T_g^i - C_{p_g} T_{dp}^{sp}} (y_{O_2}^i - y_{O_2}) \\ r_{CO} - \frac{Q_{steam}^i + \sum_{j=1}^{j=3} (-\Delta H_j) r_j + m_{cat} C_{pP} (T_{cat}^i - T_{dp}^{sp})}{C_{p_g}^i T_g^i - C_{p_g} T_{dp}^{sp}} (y_{CO}^i - y_{CO}) \end{pmatrix} \quad (8)$$

Values of the balances for  $\hat{x}_D$ , relative to its base case when maximising LP gas production, are shown in Fig. 1.

As it is possible to note, it is expected that the control of  $T_{dp}$  will not perform adequately. This is theoretically right, because in order to operate under full combustion mode, it is necessary to ensure the CO burn-off; therefore temperature should be free. If  $T_{dp}$  is set to a specific value and complete combustion is required, the reactor exhibits problems of inverse response of temperature after changes of  $F_{air}$ , which are closely related to this control instability [1, 4]. Such problematic operating regions were predicted using this methodology of analysis based only on the operating data for the steady states given in [8].

The second control policy was proposed for full combustion regenerators, where  $y_{O_2}$  was the control target. Following the proposed methodology, eqn (2), the vector of states was divided into controlled and uncontrolled variables

$$\begin{aligned} x_C &= (y_{O_2}) \\ x_D^T &= (\omega_{CRC} \quad y_{CO} \quad T_{dp}) \end{aligned} \quad (9)$$

and the value of manipulate variable was calculated for the desired set point

$$u^{sp} = F_{air}^{sp} = -\frac{r_{O_2}}{y_{O_2}^i - y_{O_2}^{sp}} \quad (10)$$

Once the value of manipulate variable was known, it was possible to calculate the dynamics of uncontrolled variables (as it was done in eqn (4)), when the unit was operating following this control policy

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

Values, relative to its base case, of the balances for  $\hat{x}_D$  at different steady states are shown in Fig. 2, using the same operating data as those presented in Fig. 1. It is possible to note that between 525°C and 535°C the control performance should be satisfactory. In this case, control policy is adequate and able to follow the reactor dynamics (cf. Figs. 1 and 2).

There is a change of signs of  $y_{CO}$  balance at about 536°C, which was discussed with the operators. According to their knowledge, there is a “kind of limit” in riser outlet temperature, which, if exceeded, is reflected by control problems. Their rule of thumb is to establish, *a priori*, a maximum temperature and never overpass it. This analysis provides this maximum temperature simply following 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 the maximum temperature limit could be predicted from data of operation at steady state.

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## SYMBOLS

$C_{p_p}$	specific heat at constant pressure for catalyst particles	$\text{kJ kmol}^{-1} \text{K}^{-1}$
$C_{p_g}$	specific heat at constant pressure for gases mixture	$\text{kJ kmol}^{-1} \text{K}^{-1}$
$F_{\text{air}}$	volumetric airflow rate	$\text{m}^3 \text{s}^{-1}$
$\mathbf{f}$	vector of terms independent of manipulate variable(s)	
$\mathbf{G}$	matrix of terms independent of manipulate variable(s)	
$\Delta H_r$	heat of reaction	$\text{kJ kmol}^{-1}$
$m_{\text{cat}}$	rate of catalyst flow	$\text{kg s}^{-1}$
$m$	number of manipulate variables	
$n$	number of state variables	
$r_j$	$j$ -th reaction rate	$\text{kmol s}^{-1} \text{kg}_{\text{cat}}^{-1}$ $\text{kmol s}^{-1} \text{m}_{\text{gas}}^{-3}$
$Q_{\text{steam}}$	rate of heat flow	$\text{kW}$
$\mathfrak{R}$	set of real numbers	
$T$	temperature	$\text{K}$
$t$	time	$\text{s}$
$\mathbf{u}$	vector of manipulate variables	
$W_{\text{rgn}}$	catalyst mass hold-up	$\text{kg}$
$\mathbf{x}$	vector of states	
$y$	mole fraction	
$\omega$	mass fraction of coke relative to mass of catalyst particles	$\text{kg}_{\text{coke}} \text{kg}_{\text{cat}}^{-1}$

## Subscripts

C	related to controlled variables
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cat	related to catalyst
CO	carbon monoxide
coke	coke
CSC	coke on spent catalyst (before regeneration)
CRC	coke on regenerated catalyst
D	related to free variables
dp	related to regenerator's dense phase
g	related to gas phase
$j$	$j$ -th component
O <sub>2</sub>	related to oxygen

## Superscripts

-1	matrix inverse
i	at inlet
sp	set point
T	transpose of a vector

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