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Comparison of two dynamic models for FCC units

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Abstract

Modelling of FCC units has been an interesting activity because of the complexity of the system and the economic incentives associated. Models have been classified depending on either the used kinetic scheme or the proposed reactor configuration. The main problems to assess are the elimination of coke when catalyst is regenerated and the delicate interaction between reactor and regenerator due to the global energy balance. In this work two models, each one using a different kinetic scheme, a different formulation for the catalyst activity and a different conception of the regenerator are compared when simulating the same FCC unit. Steady-state predictions and dynamic phenomena such as stability and multiplicity are simulated. In order to emphasise the ability for predicting the dynamic phenomena, the obtained results are compared in terms of accuracy and computing resolution time. It is pointed out that even though the complexity of a model could be a limiting factor for control purposes, in the case of dynamic studies this factor is not a constraint and it is possible to use more complex models. It is also emphasised that the most useful model will be the one which fulfils the requirements of the researcher, the situation to be modelled and the results that could be necessary.

Keywords: FCC; Lumped kinetic scheme; Mathematical modelling; Reaction kinetics; Reactor dynamics; Steady-state multiplicity

1. Introduction

Modelling of industrial FCC units has been of interest to workers in academia and industry because of their complexity and the economic incentives associated, particularly, with the increasing need for the processing of heavier oil fractions. Three main points could be classified while modelling FCC units. Firstly, depending on the type of the kinetic scheme and on the conception of the reactor–regenerator system, different kinds of models could be identified. Secondly, catalyst deactivation by coke deposition is a key feature which should be accounted for during the evolution of the cracking reaction rates [1]; it has been usually described by an exponential relation in terms of the catalyst residence time in the riser [2], without any explicit relation to the mass and heat balances. Thirdly, the description of the FCC reactor system is complicated mainly because of the heterogeneity of the reacting mixture and the fluid-catalyst contacting in both, riser reactor and regenerator (e.g., Venuto and Habib [3]). This feature of FCC units causes strong interaction between reactor and regenerator, which is difficult to model and characterises the dynamic behaviour of the unit.

On the other hand, reliable estimates of transport and kinetic parameters rest on a large amount of bench

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scale reactors and industrial operating data, however, when available, these are proprietary and therefore not so widespread. Hence, modelling of FCC units has been done using several simplifications and, in some cases, drastic assumptions. In this paper, a comparison between predictions of two different models to data from an industrial FCC unit are presented; the first considers a three-lump kinetic scheme and a moving bed regenerator with recycle, whereas the second model describes a CSTR regenerator and a five-lump scheme using an explicit relationship between catalyst activity and kinetic and transport phenomena. In both cases the cracking reactor is considered as a two-phase riser, where steaming has been neglected. A description of the problem is given in the following parts.

1.1. *Lumped kinetic schemes and catalyst deactivation*

The first problem found when modelling FCC units is the selection of the kinetic scheme. One approach to deal with multicomponent mixtures, like typical gasoils that contain more than 10 000 different species [4], is the continuous description of the mixtures, where all reactants undergo irreversible first-order reactions [5]. Although this procedure has been useful it is lengthy and complicated. An alternative approach to overcome the complexity of considering reacting multicomponent mixtures is the formulation of lumped kinetic schemes. Wei and Kuo [6] proposed a complete lumping procedure for mono-molecular systems in order to gather together similar chemical entities into a lump, which is the one considered into the reaction stoichiometry. One of the pioneering kinetic schemes using this procedure for FCC reactions was proposed by Weekman and Nace [7], in terms of three observable lumps: gasoil, gasoline and coke plus light gases. Although this formulation has been widely used for more than 25 years, it has several disadvantages. Firstly, it is focused on the three more obvious entities, but it does not consider other important products such as light gasoil and light gases explicitly, therefore, stoichiometry cannot be satisfied, which is one of the first requirements for a proper lumped scheme [6]. Secondly, the third lump gathers together coke and light gases, however, coke is a key component in the description of the reactor's behaviour [1], and should be predicted as an independent entity in order to define unambiguously the inlet condition for the regenerator; prediction of light gases (C_1–C_4 gases) that leave the riser at the top is also important for the simulation and optimisation of the separation units downstream. On the other hand, because of the simplicity of the three-lump kinetics, it is always possible to fit easily the kinetic parameters to operating data.

In order to fulfil the requirements for a proper lump, several attempts to model the kinetics have been developed. One of them is the ten-lump scheme proposed by researches at Mobil [8], lumping the components that constitute typical gasoils, which satisfies the mass balances, making the kinetic parameters independent of gasoil composition. However, it requires a large number of experimental data to estimate the reaction rate parameters which, again, are proprietary. Although other schemes containing four [9–11] and five lumps [12,13] have featured coke as a separate entity, the coke itself is difficult to describe because it is a mixture of hydrocarbons, nitrogen and sulphur compounds whose composition and molecular weight depend on the type of gasoil used as well as reactor characteristics and operating conditions [14].

In all kinetic schemes catalyst deactivation by coke deposition during the cracking reactions is a key phenomena in the modelling of FCC units. One of the most used non-phenomenological predictions of the amount of coke deposited on the catalyst (C) as a function of the catalyst time-on-stream (t) as $C = at^m$ was proposed by Voorhies [2]. An empirical prediction of the coke production is obtained, independently of the transport and reaction phenomena. It can be observed that parameters 'a' and 'm' depend on the operating conditions and the composition of gasoils and should be fitted experimentally.

1.2. *Contacting gas–solid in FCC units*

Another important consideration is the modelling of the two reactors in the FCC unit: riser and regenerator. For some FCC units, such as the Model IV, the cracking reactor has been considered as a fluidised bed [15] or a combination of transported and fluidised beds [16]. For other units, such as the Flexicracker, the UOP and the Orthoflow F, the reactor has to be modelled as a transported bed or "riser" reactor

[15]. The presented analysis is based on this kind of units, so the last type of model will be used.

At the riser inlet hot catalyst coming from the regenerator encounters the cold gasoil feed, and full vaporisation takes place together with the cracking reactions. This mixture travels towards the riser outlet where the gaseous compounds are separated and some other are desorbed by steaming. Measurements have been performed in cold riser reactors (for example Schrunmans [18]) to estimate the initial volumetric fraction, or void fraction, occupied by the reacting mixture. In the riser catalyst and the mixture of hydrocarbons travel together at different velocities, depending on the relation of their densities and on the catalyst to gasoil feed ratio (C/O). Void fraction and velocities change along the riser modifying the relationship among characteristic residence times, transport and kinetics, as well as the gas contacting patterns [3]. For this reason, these parameters should be estimated during the modelling of the riser reactor.

In all FCC units, the regenerator is a fluid-bed reactor where the hydrodynamics of the gas–solid mixture is difficult to describe. For purposes of steady-state modelling several details could be considered, but for studies on the dynamics and control the complexity of the non-linear model could be a limiting factor, and model simplifications have to be considered [17,19]. CSTR models have typically been used for control studies [16,20], because they are easy to implement, however, they lack the ability of predicting observed axial- and radial-temperature gradients. Other authors had developed bubble-bed models [21], and two-phase moving bed reactors with recycle [17], to estimate the order of magnitude of axial gradients and to assess their importance, but computing time used to integrate the model could be highly increased [17].

1.3. Reactor models

The models used in this work to predict, in the open-loop mode, the dynamic behaviour of FCC units have been described elsewhere [13,17]; their main characteristics are summarised below. Due to the transport of solid catalyst between riser and regenerator, and the key role of coke on catalyst, mass and energy balances are coupled, so an emphasis on heterogeneity has been considered. For both kinetic schemes, the parameters were estimated using data from an industrial FCC unit operating in the range of typical conditions (see Table 1). Great sensitivity of the models to the mass transfer and activity parameters was found. Due to the lack of knowledge of the real reactor's behaviour, the transport phenomena inside the catalyst are lumped together with the reaction terms obtaining an effective kinetic scheme. This is commonly assumed in most of the riser models and was also assumed in this work.

Table 1
Dimensions and operating conditions of the unit [17]

Riser (bottom diameter,	0.8 m
top diameter,	1.2 m
length)	30.0 m
Regenerator (volume)	2408 m^3
Catalyst hold up in riser	12 300 kg
Catalyst hold up in regenerator	128 800 kg
Gasoil feed rate	66.34 kg/s
Gasoil feed temperature	584 K
Catalyst/gasoil ratio	6.94
Air flow rate	26 kg/s
Air feed temperature	529 K

1.3.1. Model I

This model [17] considers a three-lump kinetic scheme [7]. The riser has been modelled as an heterogeneous tubular reactor where both phases, solid catalyst and fully vaporised hydrocarbon feed, are in contact moving upwards in plug flow presenting a slip velocity. Catalyst deactivation, resulting from the endothermic cracking reactions along the riser, follows an exponential decay in terms of the catalyst time-on-stream [7]. Stand pipes connecting both, riser and regenerator, are considered with the same time-delay, with no reaction taking place. The regenerator is described as a fluid co-current moving bed with recycle. Oxygen is transferred from the bubble to the emulsion phase to burn off the coke to CO and CO_2, and the CO transferred to the bubble phase reacts with oxygen to produce CO_2. Complete coke combustion is assumed. Heat losses to the environment and heat used in gasoil vaporisation are neglected and the freeboard region is included in the dense phase.

1.3.2. Model II

This is a model considering a kinetic scheme with five observable lumps: heavy gasoil (gol), light gasoil

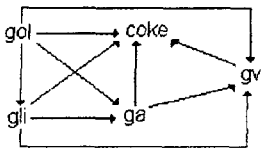

Fig. 1. Five-lumps kinetic scheme.

(gli), gasoline (ga), light gases (gv) and coke (Fig. 1). Average molecular weights for each lump were estimated and stoichiometric coefficients for the reactions were proposed [13]. They are necessary to estimate the generation of moles during the cracking reactions. Second-order kinetics were considered for the reactions where gasoil takes place and first-order kinetics for the rest [4].

In an attempt to have a more fundamental expression, a relationship (Eq. (1)) among catalyst activity (Φ) and some features of coke production, such as the mass fraction of coke that fully deactivates the catalyst ($\omega c\infty$); the current mass fraction of gasoil (μ_{gol}), and an adjustable parameter α related to the "coking" of the catalyst are proposed. The coke on the catalyst surface is evaluated by an independent mass balance which is the closure condition for the mass balances, and in this way catalyst activity, as a function of coke content, is explicitly included in the mass and the energy balances. It is important to note that μ_{gol} may include a contribution of the non-burned coke after regeneration, taking into account a possible remnant mass fraction of it.

$$\Phi|_z = \left| \frac{\alpha(\mu_{gol}|_z - 1)}{\omega_{c\infty} - \mu_{gol}|_z} \right| \tag{1}$$

The model for the riser considers different diameters at bottom and top, as in real practice. Movement in plug flow of gaseous and solid phases was considered including a slip velocity. This model describes the mass balances for each lump in the gaseous phase (Eq. (2)), around the catalyst particles (Eq. (3)), and the energy balances for both phases (analogous to the mass balances). The density (Eq. (4)), void fraction (Eq. (5)) and velocity of both phases (Eq. (6)) are also computed. The slip velocity was estimated at the riser inlet using the void fraction measured by Schrunmans [18] and the proposed C/O relationship (Eq. (7)). Because of the difference between riser and regenerator time constants, the assumption made by Kurihara [20] of a pseudo-steady riser is used. Some equations of Model II are reproduced here only for the sake of clarity.

$$u_g \frac{\partial C_{Ag}}{\partial z} + \frac{(1-\varepsilon_1)}{\varepsilon_1} k_g a_v (C_{Ag} - C_{Ap}) = 0 \tag{2}$$

$$u_s \frac{\partial C_{As}}{\partial z} - k_g a_v (C_{Ag} - C_{Ap}) = \Phi R_A \tag{3}$$

$$\rho_g = C_{ref} \sum_i \chi_i PM_i \tag{4}$$

$$\varepsilon_1 = \frac{1}{1 + (m_{cat}/m^0_{gol})(\rho_g/\delta\rho_{cat})} \tag{5}$$

$$u_g = \frac{m^0_{gol}}{\rho_g A_t \varepsilon_1} \tag{6}$$

$$\delta|_{z=0} = \frac{C/O}{(1-\varepsilon_1|_{z=0})} = \frac{us}{u_g} \tag{7}$$

The regenerator is modelled as a two-phase CSTR. The kinetics are considered first order with respect to gaseous oxygen and coke density. Combustion of coke to CO and CO_2 is lumped into one non-catalytic heterogeneous reaction, hence the density of the solid coke is constant until the end, when it suddenly changes to zero. To avoid accounting for the combustion when coke has been depleted, an independent mass balance for it is added. Oxidation of CO to CO_2 in both phases is also considered. Although afterburning in the upper part of the regenerator is one of the problem when temperature control has to be achieved, the modelling of the freeboard is included into the single CSTR model. The gaseous phase is considered pseudo-stationary and the emulsion phase in a dynamic state [22]. The regenerator model describes mass balances for each compound in both phases and energy balances for both phases, so a simultaneous differential-algebraic equations system is obtained. It is important to note that the total mass balance for solids will take an important role in the management of energy inside the FCC unit, so it is taken into account within an overall dynamic mass balance.

At the riser inlet, hot catalyst finds cold gasoil and instantaneous vaporisation occurs. Since there are available measurements of temperature, catalyst and gasoil mass flow rates, it was possible to develop an energy balance at this point using the vaporisation

enthalpy of gasoil as an adjustable parameter. The stand pipes between both reactors are simply modelled as time delays.

1.4. Multiplicity and stability

The models proposed in the preceding section were resolved to represent the steady state and dynamic features of the behaviour of FCC units. One of the important characteristics, that has been under discussion for more than 25 years, is the possibility of multiplicity of the steady state at typical industrial operating conditions. It is important to distinguish this issue from the input multiplicity when the system is operating under the action of a controller. In this work only the first kind of multiplicity is addressed. Iscol [23] proposed that open-loop multiplicity does exist and the operating point of a FCC unit corresponds to the pseudostable point. Three years later, Lee and Kugelman [24] proposed that for the standard operating conditions and considering that the unit operates under the influence of a controller, it is not possible to find multiplicity around the operating point. However, they confused both concepts, input- and open-loop multiplicities. They also said that Iscol's conclusion was a consequence of the particular representation of the activation energy of the combustion reactions as a third-order polynomial.

After studying the industrial FCC operation, Edwards and Kim [25] proposed that the standard operating point could be pseudo-stable because of the presence of afterburning reactions in the gaseous phase. This reactions may be able to increase the temperature at the catalyst recovering cyclones inside the regenerator, changing the operating steady state. Their proposition is that the ignited steady state is obtained if, due to the afterburning reactions, complete oxidation of the CO is achieved. They also made an analysis of input multiplicity that is outside the scope of this paper.

By using a bubbling bed model for the regenerator, Elshishini and Elnashaie [26] found that it is possible to predict pseudo-stability and, furthermore, the shift between operating points by changing the catalyst circulation rate when operating at the standard steady state. These authors also found that it is difficult to predict the total combustion of CO because it can present bifurcation and, in this way, the unit can be ignited even without this restriction in the CO concentration. In a recent paper, Arbel et al. [27] developed a model which is able to predict steady-state multiplicity of the regenerator when operating around the standard conditions. In their work, the authors said that there are only two possibilities when a FCC unit is operating: to have one trivial steady state, the quenched one, or to obtain three states, two of them (the quenched and the ignited) stable and the one at the middle unstable. In a second paper [28], the same authors performed an analysis for the three steady states. By linearisation of the model, they concluded that the regenerator temperature eigenvalue is positive in the middle steady state, therefore, it is not possible to operate the unit in open loop mode in this state. Their predictions of the operating temperature for the middle and the ignited steady state are below the values obtained in this work and by Elshishini and Elnashaie [26]. These results will be compared later.

As it can be seen, although several studies have been performed, it has not been said anything clear about the stability of the operating point. Nevertheless, one of the most exhaustive models available in the literature for Model IV type units [16] considers explicitly the possibility of a shift of steady state. It includes a constraint for the maximum temperature that corresponds to a limit in the operating conditions for the cyclones zone in the freeboard of the regenerator.

2. Results and discussion

In this work steady state and open loop dynamic simulations for the FCC unit were performed. Since the riser was considered as a plug flow reactor and the reactions that are taking place are endothermic, it was found that there are neither multiplicity nor bifurcation in this reactor at the standard operating conditions. Because there have been several discussions about the possibility of multiplicity of steady states of FCC units, for example, Iscol [23]; Lee and Kugelman [24]; Edwards and Kim [25], Arbel et al. [27,28], in this work it is considered that the regenerator, which is the vessel of the exothermic reactions and can present internal mixing, is responsible for the multiplicity and the lack of stability, if present, of the whole unit, so the phenomenon is referred exclusively to the regenerator.

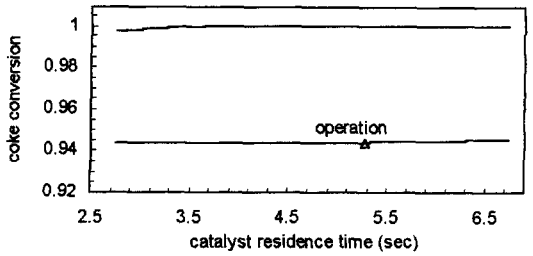

Fig. 2. Steady-state multiplicity at the regenerator [22].

Table 2
Operating case studies

1. A 3% step decrease in gasoil feed rate and step re-establishment of the original steady-state conditions after 60 min.
2. A 3% step increase in catalyst circulation rate and step re-establishment of the original steady-state conditions after 120 min.
3. A step increase of 3% in gasoil feed rate for 60 min and step re-establishment of the original steady-state conditions after 60 min (only for model II).

The FCC unit dimensions and operating conditions are shown in Table 1.

Using a CSTR model for the regenerator, it was possible to predict multiplicity of the steady state by changing either the catalyst circulation rate or the amount of supplied air. The standard operating point was found in the so called "pseudo-stable region". There is a stable region which corresponds to the state known as "ignited state" and another corresponding to the quenching of the unit (not shown) (Fig. 2), as predicted by Model II. The temperature of the regenerator when operating in the standard and ignited steady states depend on the evolution (see dynamic cases below), it was found to be 925 K for the standard steady state and for the ignited one to be between 1012 and 1162 K. In contrast, Arbel et al. [28] found that the temperature for the unstable state is 886.5 K and for the ignited state is 952 K. Because the standard operating temperature for the regenerator in Models I and II is 925 K [17], we supposed that they are considering that the unit operates in the ignited steady state and that there is no chance for shifting to occur. The possibility of shifting of steady states after a change in the catalyst circulation rate has been reported previously [26] where a bubbling bed model was used for the regenerator.

The analysis of the steady states zero dynamics stability yielded that the ignited state has a stable zero dynamics; in contrast, there are some problems in the zero dynamics of the standard steady state, although it can be reached by simulation. This situation is able to cause inverse response after a change either in the catalyst circulation rate or in the flow of air supplied. The main cause of inverse response identified was the interaction between the energy balances of both reactors. When catalyst flow is changed, the energy hold up of the reactor changes in opposite way to the one in the regenerator. This situation generates a conflict between the production and the elimination of energy, because of the couple by means of the catalyst circulation, and the response to control actions can be non ideal [22]. Arbel et al. [28] found the same inverse response behaviour after a change in catalyst circulation rate despite the fact they are proposing that the unit operates in the ignited state, which has stable zero dynamics. Our conclusion is that, possibly there are more feasible steady states, some of them presenting stable zero dynamics. An analysis in this way is recommended.

In order to model the open-loop dynamics of the FCC unit, the changes shown in Table 2 were simulated after the standard steady state was reached. One of the important variables analysed was the catalyst activity. In this work, because the expression of the remnant activity as a function of the gasoil conversion was proposed in Model II, there is a new parameter which is able to change dramatically the behaviour when the unit is subjected to disturbances affecting the coke generation.

Responses after a decrease in gasoil feed rate, situation that uses less energy to evaporate the gasoil and to heat the reacting mixture, are very different when the catalyst activity is evaluated by using different models (Figs. 3 and 4). If the activity is considered simply as a function of the residence time in the riser and full depleting of the coke is assumed (Model I), because the reacting mixture is hotter than in the original standard operating point, it is possible to obtain a better conversion of gasoil (Fig. 3c). The conversion is not affected by the coke generation, which should also be increased. The riser temperature shows a small peak due to the instantaneous availability of more energy for the cracking reactions (Fig. 3a), but finally the unit remains as before the

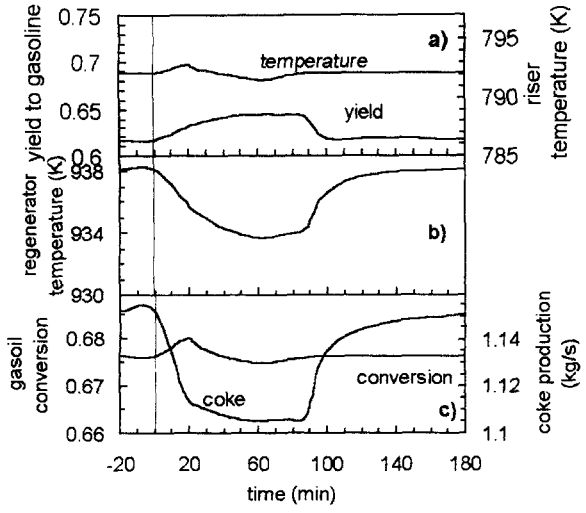

Fig. 3. Responses to a decrease of the gasoil feed rate. Model I (see text).

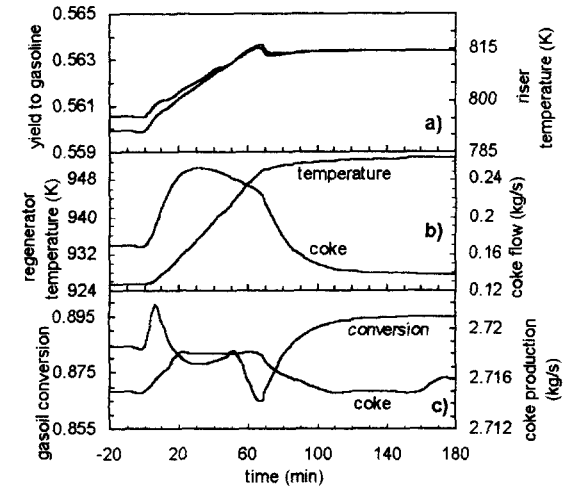

Fig. 4. Responses to a decrease of the gasoil feed rate. Model II (see text).

perturbation. After the re-establishment of the original conditions the unit operates in the same steady state.

When catalyst activity is a function of gasoil conversion (Model II), the initial response of the system is again the increase in gasoil conversion (Fig. 4c). However, due to the faster lost of activity by coke formation, some minutes later there is a drop in the conversion of gasoil. This situation enables the temperature of the riser to increase due to the availability of more energy (Fig. 4a). The situation continues to be the same until the gasoil feed is recovered. Due to the larger amount of gasoil, the energy necessary to evaporate and heat the feed is larger and the riser temperature is dropped (Fig. 4b). A new drop in gasoil conversion is shown because of the temperature change. However, because the coke production is also decreased, gasoil conversion is able to recover until its original level, followed by the coke production that reaches the original level. The temperature is high enough to maintain the unit in the new state, so it is possible to notice that, in fact, a theoretical shift of the steady state has been predicted. It is important to see that the response of the regenerator temperature is highly influenced by the riser temperature at the beginning. However, due to the coke accumulation and because the combustion of this entity is the main source of energy of the unit, the temperature increase is promoted by this last phenomenon. Hence, after a few minutes, coke burning is responsible for increasing the temperature of both reactors.

Although the last modelled case is mainly a theoretical one, an activity that is not affected by the kinetics at all versus a model which is very sensitive to the gasoil conversion, show that results at the exit of the unit are not sufficient to predict the global behaviour. Moreover, response to real perturbations of the unit when operating close to the standard steady state could be non trivial and difficult to perdict, depending on the functionality and the close relationship among variables such as temperature, activity and conversion. On the other hand, the ability of the CSTR model for the regenerator in the prediction of multiple steady states is one of the cause for the shift towards the ignited steady state. If the model of the regenerator predicts that the unit is operating in a stable steady state such as the ignited one, it will not be able to represent situations of violations of constraints in operating conditions if the actual unit is operating in a middle state.

The second case study, is a common control action that is used in FCC units. In order to set the yield to gasoline and the gasoil conversion, energy management is applied by increasing the catalyst circulation rate. The changes in energy hold-up produced by this action increase the energy circulating along the riser and reduce the accumulation of energy in the regenerator. When the regenerator is modelled as a moving

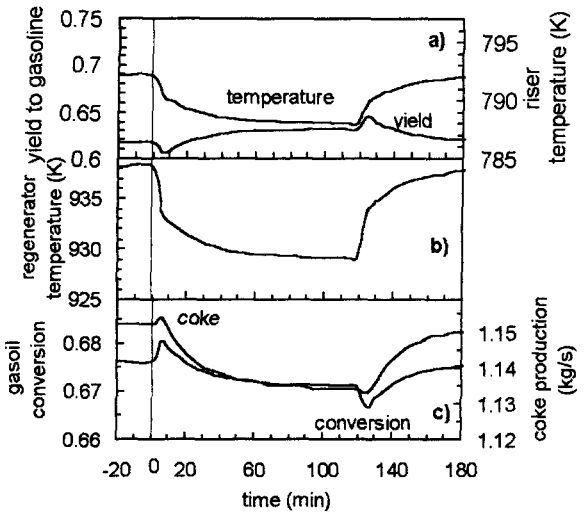

Fig. 5. Responses to an increase of the catalyst circulaton rate. Model I (see text).

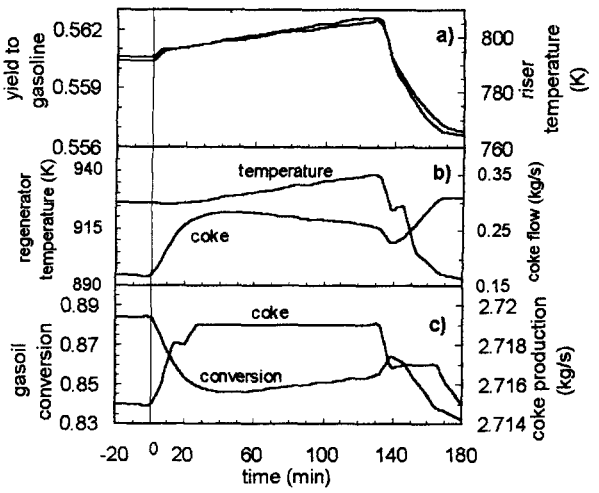

Fig. 6. Responses to an increase of the catalyst circulation rate. Model II (see text).

bed, the effect of a 3% increase in catalyst circulation rate is not appreciable (Fig. 5). The regenerator temperature continues in its original value (Fig. 5b) and, following it, the riser temperature (Fig. 5a). The gasoil conversion (Fig. 5c) and the gasoline yield are not affected because they are a function of the temperature. However, once the original conditions are recovered, i.e., there is more energy accumulated in the regenerator, the situation is reflected by a larger amount of CO_2 and lesser one of O_2 (not shown), due to the enhancement of the combustion rate, reflected by an increase in the regenerator temperature (Fig. 5b). This trend is followed by the riser temperature, and conversion of gasoline (Fig. 5a) and gasoil (Fig. 5c) are increased. Finally, the steady state is reached and it is predicted that the unit will continue operating in the standard steady state. It is important to notice that this moment is reflected by inverse response behaviour in all the variables.

In contrast, when the regenerator is modelled as a CSTR the response of the unit is rather complex (Fig. 6). Immediately after the disturbance is supplied, due to the availability of a larger amount of energy coming with the catalyst, the riser temperature is increased (Fig. 6a). The coke production is accelerated by this situation and consequently the gasoil conversion drops (Fig. 6c), even though the yield to gasoline is increased following the temperature trend, but not its conversion. At the regenerator there is an accumulation of coke (Fig. 6b), due to the high production rate of this entity in the riser. Because the temperature in this reactor is not very high, and there is not accumulation of energy, the burning rate of coke cannot be maintained and the coke starts accumulating in the regenerator (Fig. 6b). When the disturbance is taken out the response is drastic, as expected because of the sensitivity of this model. In this case, coke in the regenerator (Fig. 6b) and gasoil conversion (Fig. 6c) experience a favourable change for a few minutes, followed by inverse response. The temperature of both reactors drop (Fig. 6a and b) stopping the reaction rates. Therefore, coke is accumulated in the riser and in the regenerator and stops conversion of gasoil. The combination of the last two factors is known as the 'snow-ball effect' [25] and usually takes the unit to its quenching, which is one of the stable steady states [22].

In this second case study it was possible to see that the change in the catalyst circulation rate, which is a control action, could present a non-ideal behaviour. In both models, the decrease of the circulation rate presented more drastic influence on the system response. In Model I, which considers a constant activity decay rate, the final steady state is the same as before the disturbance. However, for Model II it is possible to note that the catalyst activity lost during the

time the disturbance has been taking place, and when the original conditions are re-established, the system is not able to recover the previous steady state. This simulation showed a topic that was pointed out more than 30 years ago by Pohlenz [1]: the coke is a very complex variable to follow and it is not an independent one because it depends on the history of the system. The proposition here is that the high interaction between both reactors, additionally to the energy interchange, depends on the catalyst activity as one of the main parameters. This variable is able to affect the reaction conditions and, therefore, to change the dynamics of the unit.

The third case study presented is the simulation of an increment of the gasoil feed rate. This disturbance is simulated by using only Model II, that incorporates a CSTR as regenerator and the complex activity function. For Model I the expected behaviour is not very exciting.

For Model II, when the increment in gasoil feed rate is supplied, there is an increment in the energy necessary to evaporate and heat the reacting mixture. The first obvious response is the cooling of the reactor (Fig. 7a), situation that causes the cooling of the regenerator (Fig. 7b). The coke starts accumulating in the regenerator and, simultaneously, is travelling back to the riser, so it receives a catalyst that is partially deactivated. Due to this situation, gasoil

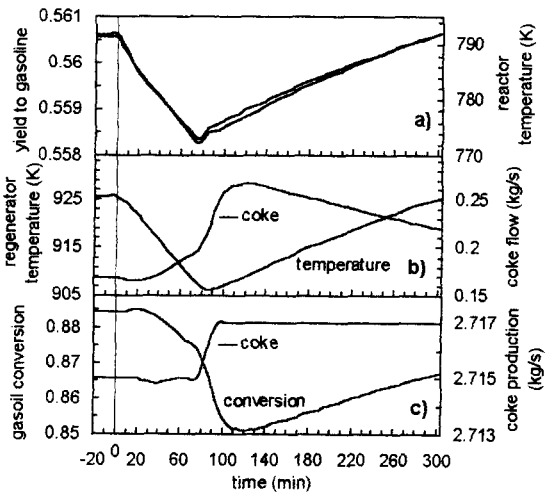

Fig. 7. Responses to an increase of the gasoil feed rate. Model II (see text).

conversion drops during the time the disturbance applies (Fig. 7c). Before reaching the shift to the quenching state, the standard operating conditions were re-established. The system is changed to move towards the original steady state. Due to the increase in temperature in the riser (Fig. 7a), the regenerator temperature is also increased and the coke combustion is enhanced (Fig. 7b). This situation causes the heating-up of the unit. The final result is that, even when coke is burned-off slowly, the FCC unit is able to recover and to operate in the standard steady state again. This situation is an important evidence of the different influences that causes disturbances in gasoil feed rate – which are very likely to occur – may present, depending on direction of the disturbance, i.e., whether the feed rate decreases or increases.

All the open loop dynamic simulations have some common points. First of all, the set of parameters that define the model can predict a stable or an unstable steady state. In the first case, as shown by the Model I, the response to small disturbances could be not very drastic. However, it is possible to miss some important dynamic phenomena that could affect the behaviour in the case of a larger perturbation. If the predicted steady state zero dynamics is unstable, as in the case of Model II, it is possible to obtain different predictions for small disturbances that look very similar, for example an increase or a decrease in the gasoil feed rate. In one of them a shift of steady state is predicted, whereas in the other only a slow recovering of the unit is observed. Secondly, the functionality of the remnant catalyst activity with the gasoil conversion introduces another parameter and also increases the parametric sensitivity of the model, because small changes at the inlet conditions can yield the shifting of the steady state. Although, in this work, the proposition of this functionality is a theoretical one, this feature of the model enables the simulation to predict some complex relationships between, say for example, temperature and conversion, and temperature and yield to gasoline. Hence, introducing this new parameter it is possible to take into account fast responses that could affect other variables, such as gasoil conversion after coke production, even when the observed temperature has not changed too much. In fact, because Model I is not considering coke accumulation in the unit, responses to perturbations and control actions are not very dramatic compared to Model II. This could be a

deficiency of the model because, as it was pointed out, coke accumulations is one of the most important variables to take into account, due to the catalyst deactivation. In fact, Model I is not able to predict the show-ball effect for the parameters and conditions used in this simulation. Finally, if the modelled unit is working around a stable steady state which presents stable zero dynamics, it is not necessary to consider a complex model for its control. In this way, the co-current flow regenerator is not very useful for that purposes, even when it could predict that situation.

On the other hand, the complexity of the models should be considered depending on the analysed situation. If an accurate prediction of axial gradients is necessary, the most complex model could be very useful. However, in the case of a lack of experimental measurements in industrial FCC units, a simple model such as the CSTR could be sufficiently accurate for purposes of optimisation and control of the unit. In the particular case of Model II, an analysis of both, predictions and stability, were made. It was found that for this kind of regenerators it is alike to present inverse response behaviour, independently from the responses of the riser [29]. However, a model considering only the regenerator is not enough to predict the relationship among the riser variables and the whole energy management. Therefore, the model of an FCC unit should consider both reactors and their interactions if it is expected to simulate a partial representation of the dynamic phenomena that could take place in this kind of reactor units.

The last point that is important to emphasise is that the computing time required to resolve the model depends on the number of differential length intervals proposed times versus the time intervals [17]. In this way, when a moving bed model is proposed it is necessary to integrate it in both independent variables (time and length). Even if the model is pseudo-stationary it is necessary to integrate it for each length segment. In the case of a CSTR-type model it is necessary to perform only one integration in each time interval. The situation is different in the riser because both models are formulated in terms of axial gradients. However, the integration of any of them by using a Runge–Kutta method uses approximately the same time when the kinetic scheme consists of five or three lumps. Also, the complex functionality proposed for the catalyst activity does not make difference in the integration time. Hence, the solution time, which is a limiting factor for models developed for control purposes [30], is another point to consider while choosing FCC models. On the other hand, to study the dynamics of the system it is not necessary to have the responses as soon as the disturbances are supplied, so a complex model could be more useful because of its ability to predict some other phenomena such axial and radial gradients of temperature and composition.

3. Conclusions

In this work two very different models were used to simulate the behaviour of an industrial FCC unit. It was found that depending on the characteristics that is desirable to detail, different approximations could be useful. The modelling of chemical reactors continues being an area of uncertainty. Even if there are available industrial and experimental data, the conception and translation of the physical situation to equations depends on the researcher's criteria. We are conscious that the new trends lead to develop more accurate kinetic schemes, either lumped or continuous. However, the uncertainty in the estimation of kinetic and thermodynamic parameters, as well as the number of adjustable variables increase, and for the case of proprietary data this situation is not easy to manage.

For the particular simulations performed, it was found that there are several contradictory affirmations, such as the possible pseodu-stability of the operating steady state, that can be simulated by using two different formulations of the same phenomena. Although this situation is present when the study of steady states is performed, it is more obvious when open loop dynamics of the unit is considered. In this work only algebraic-differential equation models were used. It was found that the complexity of this kind of models can be varied in a wide range. However, depending on the desired results, the researcher has some flexibility when choosing among available options. It is important to note that due to the fast growing of the computing facilities, currently it is possible to use more complex models. Therefore, it is necessary to agree in the representation and validation of phenomena taking place in chemical reactors. This could be considered as the "raison de être" of reactor engineers.

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