Chemical Engineering Journal 100 (2004) 181–186

Chemical Engineering Journal

www.elsevier.com/locate/cej

Short communication

Effect of modelling pressure gradient in the simulation of industrial FCC risers

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Received 7 November 2003; received in revised form 20 February 2004; accepted 16 March 2004

Abstract

Fluidised-bed catalytic cracking (FCC) is one of the most important processes in petroleum refining. FCC reactions occur in transported bed reactors, known as risers, exhibiting residence times between 2 and 4 s. Although the economical importance of catalytic cracking, simulation of operating conditions is rather empirical due to the complex interactions among operating variables.

In order to improve simulation techniques, FCC processes should be modelled as much accurately as possible. In this work, a one-dimensional model that considers plug-flow of solid and gaseous phases is analysed. Two different approaches are considered, in the first one, the model consists only of mass and energy balances; in the second one, momentum balance is included to consider the axial pressure profile. Prediction of yield to products and conversion improves when the pressure gradient is modelled. This simplified description of hydrodynamics shows that more complete modelling of the hydrodynamics of the system improves the prediction of the behaviour of FCC risers, however this approach has not exhibited continuity in the FCC modelling literature.

Keywords: Catalytic cracking; Modelling; Hydrodynamics; Pressure gradient; Riser reactor

1. Introduction

Fluidised-bed catalytic cracking (FCC) is one of the most important processes in petroleum refining. It converts heavy and low value oils into lighter and high value fuels, such as gasoline and light olefins. Although the economical importance of FCC processes, their simulation is rather empirical because of complex interactions among operating variables.

FCC reactions occur in transported bed reactors, known as risers, exhibiting residence times between two and four seconds. In order to improve simulation techniques, catalytic cracking processes should be modelled as much accurately as possible. In particular, the modelling of transport phenomena allows improving predictions of the behaviour of FCC units. For example, density, viscosity and void fraction change due to modifications in operating conditions (temperature and/or pressure) and because of mole generation during cracking. In order to obtain better predictions of conversion and product yields, these changes have to be taken into account when modelling risers.

For several years, modelling of riser reactors for catalytic cracking has followed several research lines. Even when operating variables are known since some time ago, modelling of the riser reactor has neglected the pressure gradient. Recently, Pareek et al. [1] proposed a comprehensive model for non-isothermal risers. This model accomplishes the volume expansion of the reacting mixture due to mole generation during cracking by defining heat transfer characteristic heights. Nevertheless, authors did not perform pressure balance to consider the change of partial pressure of hydrocarbons. Maya-Yescas et al. [2] proposed also a simplified dynamic model for a riser and did not consider the pressure gradient along this reactor. Ali and Rohani [3] and Ali et al. [4] studied the interaction of the riser with the regenerator, however did not perform a pressure balance along the riser. Sungungun et al. [5] extended their previous works (e.g. Kolesnikov et al. [6]) to present a model that considers complex cracking kinetics depending on the partial pressure of hydrocarbons, but they did not perform pressure balances along the riser. Azkoiti et al. [7] presented another dynamic model for cracking units that considers the interaction between riser and regenerator, and did not evaluate the riser pressure gradient. The first one of a collection of papers on the modelling of cracking units by Arbel et al. [8] presented, also, a comprehensive model for the catalytic cracker, based

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doi:10.1016/j.cej.2004.03.001

Nomenclature

A_t	transversal area of the riser (m^2)
a_v	Specific interfacial area (m^{-1})
C/O	feed ratio catalyst/oil (dimensionless)
C_j	concentration of the jth component (j = feedstock, gasoline, liquid petroleum gas, dry gas, coke) ($kg\,m^{-3}$)
Cp	calorific capacity ($J\,kg^{-1}\,K^{-1}$)
C_{ref}	reference concentration ($kg\,m^{-3}$)
g	gravity acceleration ($m\,s^{-2}$)
$-\Delta H_{rxn,j}$	heat of reaction of the jth component ($kJ\,kg^{-1}$)
h_g	heat transfer coefficient ($W\,m^{-2}\,K$)
k_g	mass transfer coefficient ($m\,s^{-1}$)
L	height of the riser (m)
m_{cat}	feed catalyst rate ($kg\,s^{-1}$)
$m^{o}_{feedstock}$	feedstock rate ($kg\,s^{-1}$)
Mw_i	mass molecular weight (Da)
P	pressure (Pa)
$\Re_j$	reaction rate of the jth component ($kg\,m^{-3}\,s^{-1}$)
T	temperature (K)
u	velocity ($m\,s^{-1}$)
x_i	mass fraction of the ith component (dimensionless)
z	axial coordinate (m)

Greek letters

α	activity factor ($g_{ck}^{-1}\,g_{cat}$)
δ	slip velocity factor dimensionless
ε	void faction (dimensionless)
ρ	density ($kg\,m^{-3}$)
Φ	catalyst deactivation function (dimensionless)
ω_{CSC}	instantaneous mass of coke adsorbed to the catalyst surface ($g_{ck}\,g_{cat}^{-1}$)
ω_{CRC}	mass of coke adsorbed to the equilibrium catalyst surface specific to the mass of catalyst ($g_{ck}\,g_{cat}^{-1}$)

Subscripts

g	gas mixture (continuous phase)
p	catalyst particles (disperse phase)

on the 10-lump kinetic model by Jacob et al. [9], which does not consider the pressure drop along this reactor. Zheng [10] used a five-lump kinetic model for cracking units that considers also a reaction rate dependence on pressure and does not include a pressure balance inside the riser reactor.

It is important to note that chemical reactions in gas phase are very influenced by the total pressure inside the reacting system. Especially for riser reactors, consideration of this gradient has been evaluated for some other reacting systems [11]. This research line has been followed in catalytic cracking, too. An important work that exposed this situation more than 10 years ago is due to Theologos and Markatos [12]; however, these authors emphasised the fact that there is wall friction more than the pressure gradient due to solids distribution along the riser. Arandes et al. [13] used the 10-lump kinetic model [9] to predict steady states and dynamics of cracking units, the original model was completed with pressure balance in the riser, however it is considered only at the riser outlet. Derouin et al. [14] considered the impact of hydrodynamics during catalytic cracking by extending previous works by the same research group [15,16]. Nonetheless, in their last paper they do not include an explicit pressure balance along the riser, as it was the case in the paper by Van Landeghem et al. [15]. In the modelling of the previous generation of cracking units, that also included a riser, the only reference to a pressure balance inside this reactor is due to McFarlane et al. [17].

Hence, even when the influence of the riser pressure gradient has been considered important, there is not continuity in the development of models to consider it. In this work, a simplified description of the pressure gradient of an FCC riser is proposed. A one-dimensional (axial description) model that considers plug-flow of solid and gaseous phases is complemented by a momentum balance that considers the axial pressure profile. The model considers variations in transport properties (mainly density and velocity), due to mole generation during cracking. In addition, variable slip velocity between the gaseous mixture and the catalyst particles is modelled. These first results try to understand and to exhibit the differences obtained when the behaviour of this system is predicted, modelling or neglecting the riser pressure gradient. Numerical solution of this model are used to characterise the industrial operating region and to find feasible operating points, results are compared to industrial ones. The main characteristics of the industrial unit used as case study are listed in Table 1.

1.1. *Riser model*

The riser is considered an heterogeneous, adiabatic, transported bed reactor. The reaction process starts at the point where the preheated feedstock and the hot active catalyst are in contact at the bottom of the riser. The inlet temperature of the liquid is about 450 K, while the catalyst temperature is

Table 1
Industrial FCC unit studied

Type	Adiabatic
Technology	Side-by-side, revamped
Operating mode	Full combustion
Feedstock type	Gas oils blend
Feedstock capacity, BPD	25,000
Feedstock inlet temperature (K)	450.0
Catalyst type	Synthetic, microspherical
Particle diameter (average) (m)	7.0×10^{-5}
Riser outlet temperature (average) (K)	794.0

close to 900 K, so when the feedstock is in contact with the catalyst, it is assumed that the liquid is vaporised instantaneously. Regenerated catalyst transfers the heat required for endothermic cracking reactions; reaction temperature after feed vaporisation is about 840 K.

Feedstock cracks into products while the catalyst—feedstock mixture flows upward through the riser. During this time, the catalyst becomes deactivated, mainly by coke deposition. Gaseous products are separated from the coked catalyst by cyclones located at the top of the riser and sent to a fractionation column. The coked catalyst is stripped of entrapped and other volatile hydrocarbons and sent to the catalyst regenerator. The riser top temperature is about 794 K.

The model considers, explicitly, the heterogeneity of the process, i.e. gas and solid phases are modelled independently. It implies the description of transport phenomena: mass and energy for each phase, these parameters were evaluated using previous works [12,18]. Later, this model is complemented by taken into account a simplified modelling of the pressure drop inside the riser. Here, momentum balance considers the contribution of the hydrostatic head of solids, ignoring acceleration effects and friction at the walls.

The advantage of modelling the heterogeneity of the process is to consider, directly, the influence of the catalyst-to-oil ratio (C/O), which is one of the main operating variables. In addition, C/O determines conversion of feedstock and yield to products, so these two effects could be taken into account explicitly in the model. This model was discretized in 2000 intervals; this number was proposed in order to evaluate continuous changes of parameters.

Momentum balance in the riser is based on equations for the disperse phase (catalyst particles) and energy and mass equations for both phases (continuous and disperse). The main assumptions are:

- gas and solid phases follow a plug-flow regime;
- feedstock is vaporised instantaneously when it is in contact with regenerated catalyst;
- gaseous mixture has a behaviour of an ideal gas;
- cracking reactions are catalytic;
- the riser does have neither lateral inlets nor lateral outlets.

1.1.1. *Pressure balance*

The momentum balance (Eq. (1)) is simplified to the term of total pressure gradient of the system. The terms of momentum transfer at the interface gas–particle are simplified as a first approximation of the model.

$$\frac{\mathrm{d}P}{\mathrm{d}z} = -\rho_\mathrm{p} g(1-\varepsilon) \tag{1}$$

$$P(z=0) = P_\mathrm{o} \tag{1a}$$

where P is the total pressure of the system, ρ_p the catalyst density, g the gravity acceleration, and ε the void fraction. Eqs. (1) and (1a) are taken into account in the approach that includes the hydrodynamics of the system.

1.1.2. *Mass balances*

(a) *Continuous phase (gaseous mixture)*:

$$u_\mathrm{g}\frac{\mathrm{d}C_{j\mathrm{g}}}{\mathrm{d}z} + k_\mathrm{g} a_v[C_{j\mathrm{g}} - C_{j\mathrm{p}}] = 0 \tag{2}$$

$$C_{j\mathrm{g}}(z=0) = C_{j\mathrm{go}} \tag{2a}$$

Here u_g is the average velocity of the gaseous mixture, $C_{i\mathrm{g}}$ is concentration of the jth (j = feedstock, gasoline, liquid petroleum gas, dry gas, coke) component in the gaseous mixture, k_g is the mass transfer coefficient of the gas and a_v is the interfacial area of the catalyst particles.

(b) *Disperse phase (catalyst particles)*:

$$u_\mathrm{p}\frac{\mathrm{d}C_{j\mathrm{p}}}{\mathrm{d}z} - k_\mathrm{g} a_v[C_{j\mathrm{g}} - C_{j\mathrm{p}}] = \varepsilon\rho_\mathrm{g}\frac{\mathrm{C}}{\mathrm{O}}\Phi\mathfrak{R}_j \tag{3}$$

$$C_{j\mathrm{p}}(z=0) = 0 \tag{3a}$$

where u_p is the average velocity of the catalyst, $C_{j\mathrm{p}}$ the concentration of the jth component at the surface of the solid phase, Φ the catalyst deactivation function, and $\mathfrak{R}_j$ the reaction rate of the jth component.

1.1.3. *Energy balance*

(a) *Continuous phase (gaseous mixture)*:

$$u_\mathrm{g}\frac{\mathrm{d}T_\mathrm{g}}{\mathrm{d}z} - \frac{h_\mathrm{g} a_v}{\mathrm{Cp}_\mathrm{g}\rho_\mathrm{g}}[T_\mathrm{p} - T_\mathrm{g}] = 0 \tag{4}$$

$$T_g(z=0) = T_{\mathrm{go}} \tag{4a}$$

where T_g is the temperature of the gaseous mixture, h_g the heat transfer coefficient, and Cp_g the specific heat of the gaseous mixture.

(b) *Disperse Phase (catalyst particles)*:

$$u_\mathrm{p}\frac{\mathrm{d}T_\mathrm{p}}{\mathrm{d}z} + \frac{h_\mathrm{g} a_v}{Cp_\mathrm{p}\rho_\mathrm{p}}[T_\mathrm{p} - T_\mathrm{g}] = \frac{\varepsilon\rho_\mathrm{g}\mathrm{C/O}\Phi\mathfrak{R}_j}{\mathrm{Cp}_\mathrm{p}\rho_p}\sum_j(-\Delta H_{\mathrm{rxn},j}) \tag{5}$$

$$T_\mathrm{p}(z=0) = T_{\mathrm{po}} \tag{5a}$$

where T_p is the temperature of the solid phase, Cp_p the specific heat of the catalyst, and $\Delta H_{\mathrm{rxn},j}$ the specific enthalpy of the jth reaction.

1.1.4. *Reaction kinetics*

Due to the complexity of feedstock (more than 10,000 different species), it is not possible to define a fundamental reaction mechanism. This problem has another inconvenient; the catalyst deactivation mechanism due to coke produced by cracking is neither defined. A five-lump kinetic scheme [19] is used (Fig. 1). In order to be able to use kinetic data

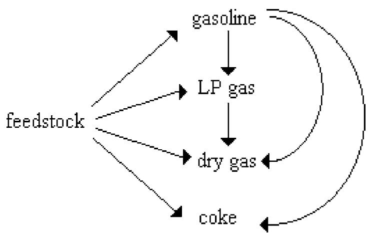

Fig. 1. FCC kinetic scheme.

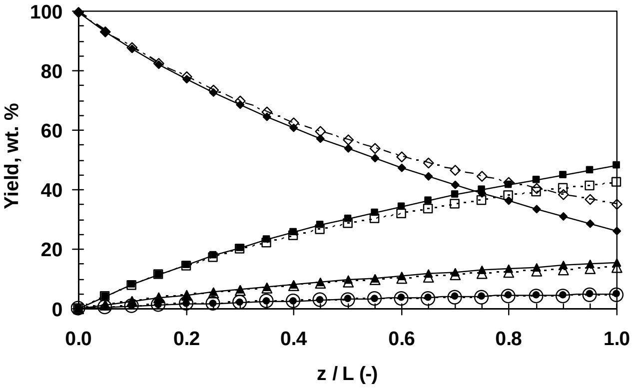

Fig. 2. Axial profile of mass fractions: (◆) feedstock, (■) gasoline, (▲) LP gas, (●) dry gas. Considering pressure profile (solid markers), without considering pressure profile (void markers).

obtained in laboratory devices for the modelling of industrial units, it is necessary to transform them (e.g. [20]); this transformation was performed. These five lumps are defined by their boiling points. Feedstock (bp $> 615\,\mathrm{K}$), which is the heavier entity present in all the reactions; it produces gasoline ($303\,\mathrm{K} < \mathrm{bp} < 492\,\mathrm{K}$), gases, and coke. Gases are separated into dry gas (hydrogen, methane, ethane and ethylene) and liquid petroleum gas (LPG: propane, propylene, butanes and butenes). In addition, gasoline can crack to produce dry gas, LPG or coke. Rates of reaction depend on temperature following the Arrhenius law and on hydrocarbons partial pressures.

Second-order kinetics has been proposed for the cracking of feedstock and first-order for the other components. Catalyst deactivation is modelling using an hyperbolic expression (as suggested by Froment and Bischoff [21]; Van Landeghem et al. [15]) for the deactivation factor (Eq. (6)).

$$\Phi=\begin{cases}\Phi_0 & \omega_{\mathrm{CRC}}\le\omega_{\mathrm{CSC}}<\omega_{\mathrm{CSC\,min}}\\ \dfrac{\Phi_0}{1+\alpha(\omega_{\mathrm{CSC}}-\omega_{\mathrm{CSC\,min}})} & \omega_{\mathrm{CSC}}\ge\omega_{\mathrm{CSC\,min}}\end{cases}\qquad(6)$$

where $\Phi_0 = 70$ wt.% is the MAT activity of equilibrium catalyst, $\omega_{\mathrm{CRC}} = 0.066$ wt.% the mass of coke adsorbed to the equilibrium catalyst surface specific to the mass of catalyst, ω_{CSC} the instantaneous mass of coke adsorbed to the catalyst surface, $\alpha = 1013.8\,g_{\mathrm{ck}}^{-1}\,g_{\mathrm{cat}}$ an activity factor, and $\omega_{\mathrm{CSC\,min}} = 0.01315\,g_{\mathrm{ck}}\,g_{\mathrm{cat}}^{-1}$ is the minimum coke amount that provokes the catalyst to show deactivation. Activity parameters were determined experimentally in our laboratories.

Kinetic parameters were taken from literature [19,22] and transport parameters were evaluated using correlations [12,23]; they correspond to operating data of industrial FCC units. Kinetic parameters include frequency factors, activation energies and reaction enthalpies for each one of the cracking reactions shown in the kinetic scheme (Fig. 1). In addition, molecular weights and stoichiometric coefficients for each lump were assigned [18]. Transport parameters, such as mass and heat transfer coefficients, and interfacial area of the catalyst were estimated [12].

The model consists of five equations and 22 unknown variables P, ε, C_{jg}, C_{jp}, u_{g}, u_{p}, Φ, $\Re_j$, T_{g}, T_{p}; these unknowns are estimated by the kinetic expressions and the following relations (Eqs. (7)–(10)). Estimation of the slip velocity as a function of mass fraction and void fraction in the riser:

$$\delta = \frac{u_{\mathrm{p}}}{u_{\mathrm{g}}} = \frac{\rho_{\mathrm{g}}\varepsilon}{(\mathrm{C/O})\rho_{\mathrm{p}}(1-\varepsilon_1|_{z=0})}\qquad(7)$$

Here the void fraction at the riser entrance is $\varepsilon_1|_{z=0} = 0.90$, according to [23]. Gaseous mixture velocity is expressed by:

$$u_{\mathrm{g}} = \frac{m^{\mathrm{o}}_{\mathrm{feedstock}}}{\rho_{\mathrm{g}}A_{\mathrm{t}}\varepsilon}\qquad(8)$$

where A_{t} is the variable transversal surface of the riser. The change of density in the reaction mixture, due to moles generation, has an effect in the contact time. Assuming ideal gas behaviour, gaseous mixture density is described by:

$$\rho_{\mathrm{g}} = C_{\mathrm{ref}}\sum_i x_i Mw_i\qquad(9)$$

where x_i is the mass fraction of the ith component. Void fraction occupied by the gas is:

$$\varepsilon = \frac{1}{1+[(\mathrm{C/O})(\rho_{\mathrm{g}}/\delta\rho_{\mathrm{p}})]}\qquad(10)$$

2. Results and discussion

Operating conditions used to quantify the effect of the modelling of the pressure gradient are: feedstock rate $36.82\,\mathrm{kg\,s^{-1}}$ and $\mathrm{C/O} = 8$, as it was observed during industrial operation. Comparative profiles for both approaches are shown with respect to axial non-dimensional coordinate of the riser (Z/L). Profiles inside the riser are theoretic, because there are not experimental results at these points.

Axial profiles of mass fractions are shown for both simulation approaches, considering the axial pressure profile and without this consideration (Fig. 2). Profile of mass fraction of feedstock shows the typical behaviour of a reactant, which is not generated inside the riser but is consumed in order to generate products. It is important to note that the conversion predicted is higher when the pressure balance is included

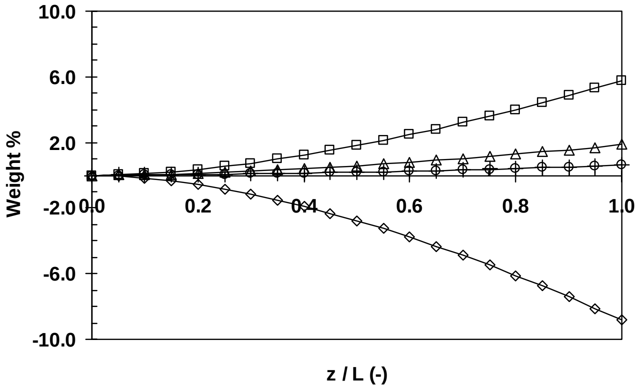

Fig. 3. Mass fraction differences when modelling the pressure balance: (◇) feedstock, (□) gasoline, (△) LP gas, (○) dry gas.

in the model; consequently, yields to products predicted are higher.

In order to make more evident the effect of modelling changes in pressure; Fig. 3 shows the difference between predictions for both cases as a function of the axial non-dimensional coordinate of the riser.

Mass fraction predictions at the riser outlet differ in more than 5% for feedstock and gasoline. As the reaction proceeds along the riser, the difference between both approaches increases. Moreover, this difference is directly proportional to product yields, which is undesirable for prediction of gasoline, LP gas and dry gas. The difference between the two approaches is due to the fact that reaction rates depend on partial pressures, which are consequence of the total pressure inside the riser. This pressure exhibits a drop of about −0.382 bar (Fig. 4), which are in agreement to experimental results [12]. This pressure drop represents more than 20% of the initial pressure; therefore, results predicted are clearly affected by this change.

Fig. 5 compares predicted and industrial results for conversion (remaining feedstock) and yields to gasoline, liquid petroleum gas, dry gas and coke against industrial results at the riser outlet. Data were taken at conditions shown in Table 1. As it is possible to note, modelling results are better if the pressure gradient along the riser is taken into account. This result was expected because of the importance of the pressure drop calculated along the riser; it shows how different the results of the two approaches could be.

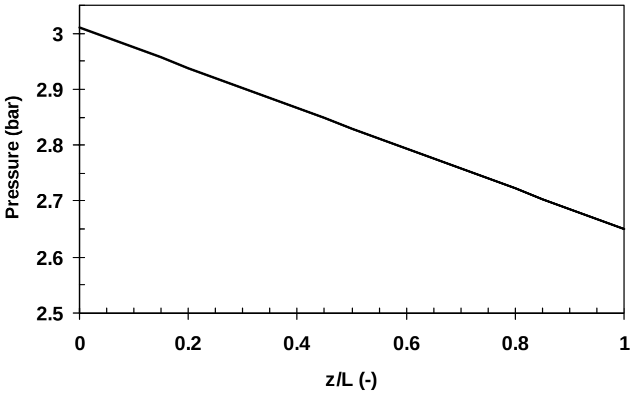

Fig. 4. Axial pressure gradient.

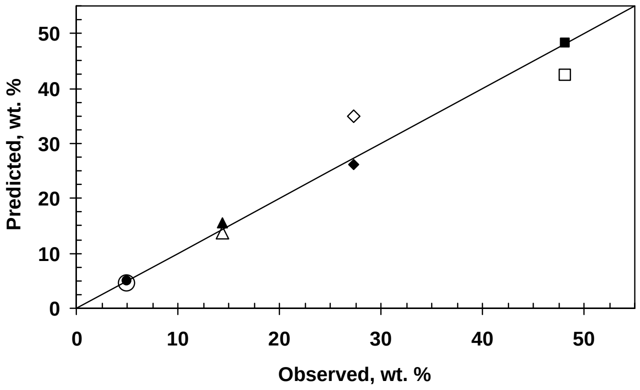

Fig. 5. Industrial and predicted mass fractions: feedstock (◆), gasoline (■), LP gas (▲), dry gas (●). Considering pressure profile (solid markers) and without considering pressure profile (void markers).

3. Conclusions

This work shows the impact of modelling pressure gradient during the simulation of mono-dimensional risers. The addition of a simplified momentum balance to the model, assuming that the only contribution to the axial pressure drop is the hydrostatic head of solids, improves prediction of feedstock conversion and yield to products. Even when this approach seems more adequate to describe catalytic cracking in FCC risers, there has not been continuity of this kind of models in the literature. This information can be extended to model bi-dimensional risers (axial and radial description) for more rigorous analysis of transport phenomena.

Acknowledgements

Authors thank economic support from the Research Program Tratamiento de Crudo Maya at the Instituto Mexicano del Petróleo. Authors are grateful with reviewers for their valuable comments.

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