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Mechanistic Dynamic Modelling of an Industrial FCC Unit

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Abstract

The aim of this study is to obtain a model that can simulate the performance of an industrial Fluidised Catalytic Cracking (FCC) unit in steady and dynamic state, and which will subsequently be used in studies of control and real time optimisation.
In this paper, a dynamic model for a R2R type FCC unit is presented. The model includes the riser, the stripper/disengager, the regeneration system and the catalyst transport lines. Mass, energy and pressure balances are performed for each of these sections. Simulation results for steady and dynamic states are presented and compared qualitatively with those from previous FCC models.

Keywords: Fluid Catalytic Cracking, Dynamic simulation, Mathematical modelling, Process control

1. Introduction

Fluidised Catalytic Cracking (FCC) is one of the most important processes in a refinery, and is sometimes referred to as the heart of the refinery. Several studies have been made on the modelling, simulation, kinetics, multiplicity of steady states, chaotic behaviour, on-line optimisation and control of FCC units. However, there are still large areas to be examined due to the complexity and to the economical importance of this process.
Several types of FCC units are currently in operation, using various designs. In this study, a dynamic model is presented for an R2R unit comprising a riser, a stripper, a disengager, two standpipes and a regeneration system composed of two regenerators linked by a lift.
The R2R process was initially developed by Total and is now licensed by Axens/IFP and Stone & Webster. This technology is used to process feedstocks with high residue content. The first regenerator (Regenerator 1) acts as a mild precombustion zone to achieve 40 to 70% of the coke combustion. The partially regenerated catalyst with less

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than 0.5 wt% coke is then air-lifted to the elevated second regenerator (Regenerator 2) where complete regeneration is achieved with slight air excess and under a low steam partial pressure in order to minimize catalyst deactivation. (Gauthier et al., 2000)

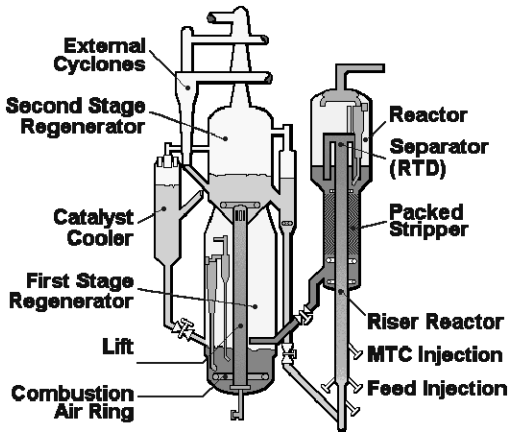

Figure 1. R2R Fluid Catalytic Cracking Process. (Gauthier et al., 2000)

2. Mathematical Model

The riser is considered to be in pseudo steady state, since it has a residence time in the order of a few seconds (2 to 5 s), while the regenerators and the stripper have characteristic times in the order of a few minutes. The riser hydrodynamics is modelled as a plug-flow reactor, while the cracking kinetics is described by a 6-lump model (Takatsuka et al., 1987), with a deactivation function depending on the catalyst coke content. The lumps considered are: Vacuum Gas Oil (VGO) + Decanted Oil (DO) (>360°C); Light Cycle Oil (LCO) (220 – 360°C); Gasoline (GLN) (C5 – 220°C); Liquified Petroleum Gas (LPG) (C3 and C4); Fuel Gas (FG) (H_2, C1, C2 and H_2S) and Coke. Besides the second order VGO cracking reactions, all reactions are first order.
Gas molar expansion as well as slip velocity between gas and solids is accounted for in the riser model. The stripper/disengager section is modelled as a CSTR without any cracking reactions occurring. Both regenerators are also modelled as CSTR reactors. The combustion kinetics considered in this model was previously studied at IFP (Vale, 2002). Coke is considered to be composed of carbon and hydrogen, although in practice sulfur and nitrogen are also present in small quantities. The combustion of carbon can be given by the following overall reaction:

$$C + \left(\frac{\sigma + 1/2}{\sigma + 1}\right) O_2 \rightarrow \left(\frac{\sigma}{\sigma + 1}\right) CO_2 + \left(\frac{1}{\sigma + 1}\right) CO \tag{1}$$

The lift is modelled as a plug-flow reactor where combustion reactions continue. Since the residence time in the lift is much smaller than in the regenerators, it is considered to be in pseudo steady state. Spent and regenerated catalyst standpipes are also modelled as being in pseudo steady state at incipient fluidisation with the solids and aeration gases moving in plug flow along the standpipes. Pressure balances in all the sections are made considering that the gases have ideal gas behaviour.

The most relevant equations for the riser and the regenerator are presented below.

2.1 Mass, force, energy and pressure balances in the Riser (RS)

$$\frac{\partial F_i}{\partial z} = \Omega_{RS}\varepsilon_c \hat{r}_i \qquad \hat{r}_i = \sum_j \hat{r}_{ji} - \sum_j \hat{r}_{ij} \qquad r_{ij} = \Phi A_{ij}\, exp\left(-\frac{E_{ij}}{RT}\right)\hat{C}_i^{n_{ij}} \tag{2}$$

$$\frac{\partial F_{cat}}{\partial z} = 0 \Leftrightarrow \frac{\partial\left(\Omega_{RS} v_c \rho_{cat} \varepsilon_c\right)}{\partial z} = 0 \Leftrightarrow \frac{\partial \varepsilon_c}{\partial z} = -\frac{\varepsilon_c}{v_c}\frac{\partial v_c}{\partial z} \tag{3}$$

$$\frac{\partial v_g}{\partial z} = \frac{\varepsilon_c \sum_i r_i}{C_t} - \frac{v_g(1-\varepsilon_c)}{C_t}\frac{\partial C_t}{\partial z} \tag{4}$$

$$C_D \frac{\rho_g (v_g - v_c)^2}{2}\frac{\pi d_{cl}^2}{4} + \rho_g \frac{\pi d_{cl}^3}{6} g - \rho_{cat}\frac{\pi d_{cl}^3}{6} g = 0 \tag{5}$$

$$\frac{\partial T_{RS}}{\partial z} = \frac{\Omega_{RS}\varepsilon_c \Delta H_{crk} r_{DO}}{\sum_i F_i C_{p_i}} \tag{6}$$

$$\frac{\partial P_t}{\partial z} = -\rho_{av} g \qquad \rho_{av} = \varepsilon_c \rho_{cat} + \varepsilon_g \rho_g \tag{7}$$

2.2 Mass, energy and pressure balances in the Regenerators (RG)

$$V_{bed}\frac{\partial C_{i,RG}}{\partial t} = N_{i,in}^g - N_{total,out}^g \times C_{i,RG} + V_{bed}\left(\varepsilon_g \sum_j \left(r_j^g \upsilon_{ji}^g\right) + \varepsilon_c \rho_{cat} \sum_j \left(r_j^s \upsilon_{ji}^s\right)\right) \tag{8}$$

$$\frac{W_{c,RG}}{M_{w,i}}\frac{\partial Y_{i,RG}}{\partial t} = \frac{F_{c,in}}{M_{w,i}} Y_{i,in} - \frac{F_{c,out}}{M_{w,i}} Y_{i,RG} + V_{bed}\varepsilon_c \rho_c \sum_j \left(r_j^s \upsilon_{ji}^s\right) \;, \quad i = C \; or \; H \tag{9}$$

$$\frac{\partial L_{RG}}{\partial t} = \frac{F_{c,in} - F_{c,out}}{\rho_c \varepsilon_c \Omega_{RG}} \tag{10}$$

$$\frac{\partial W_{g,RG}}{\partial t} = F_{g,in} - F_{g,out} + \sum_i \left(F_{c,in} Y_{i,in}\right) - \sum_i \left(F_{c,out} Y_{i,RG}\right) \tag{11}$$

$$\frac{\partial\left(W_c C_{p_c} T_{RG} + W_g C_{p_g} T_{RG}\right)}{\partial t} = F_{g+c,in} H_{in} + Q_r^{\circ} - F_{g+c,out} H_{out} \tag{12}$$

$$P_{RG_{bottom}} = P_{g,RG} + \rho_c \varepsilon_c L_{RG} g \tag{13}$$

3. Simulation Results and Discussion

In this section, the simulation results for the steady and dynamic states are presented and discussed. Figure 2 shows the influence of the steady state catalyst-to-oil ratio

(COR) on some process variables. It can be seen that increasing the COR leads to an increase in riser outlet temperature, since a larger amount of catalyst enters the riser for a same quantity of hydrocarbons. The increase in COR also leads to a lower coke content on the spent catalyst. Because of the higher catalyst flowrate, the residence time of the catalyst in the regenerators is lower, leading to lower regenerator temperatures for a given heat release. These temperature evolutions with COR are in agreement with the results presented by Malay et al. (1999). However, no maximum was found in the regenerators' temperature curves, as presented in the works of Arbel et al. (1995) and Han and Chung (2001). Nevertheless, it is important to remind that the regeneration system in all these works is different from the one presented here.

The effect of COR on VGO conversion and product yields presented in this paper is also in agreement with the results presented by Malay et al. (1999). Higher temperatures promote higher conversion rates and, at the same time, a higher COR also means more catalyst, and hence more active centres available for reaction leading again to higher conversions and light product yields.

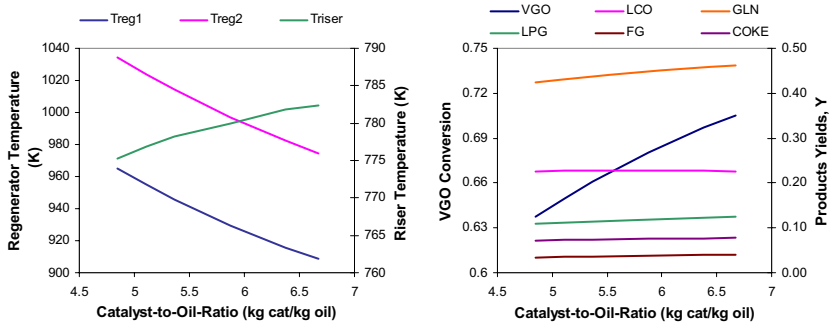

Figure 2. Effect of COR on temperatures, conversion and product yields.

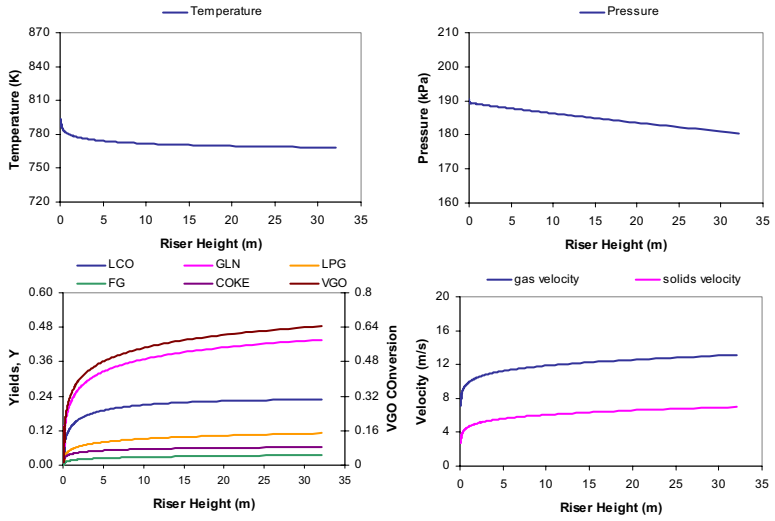

Figure 3. Steady state profiles along the axial coordinate in the riser.

Figure 3 shows the profiles of some important process variables along the axial coordinate in the riser. It can be seen that most of the cracking reactions occur in the first meters of the riser. This is an expected result when one considers the highest temperatures and lowest catalyst coke content are encountered at the riser inlet. The velocity profiles clearly show that there is a slip factor between the two phases, which rapidly tends to a value of 2.

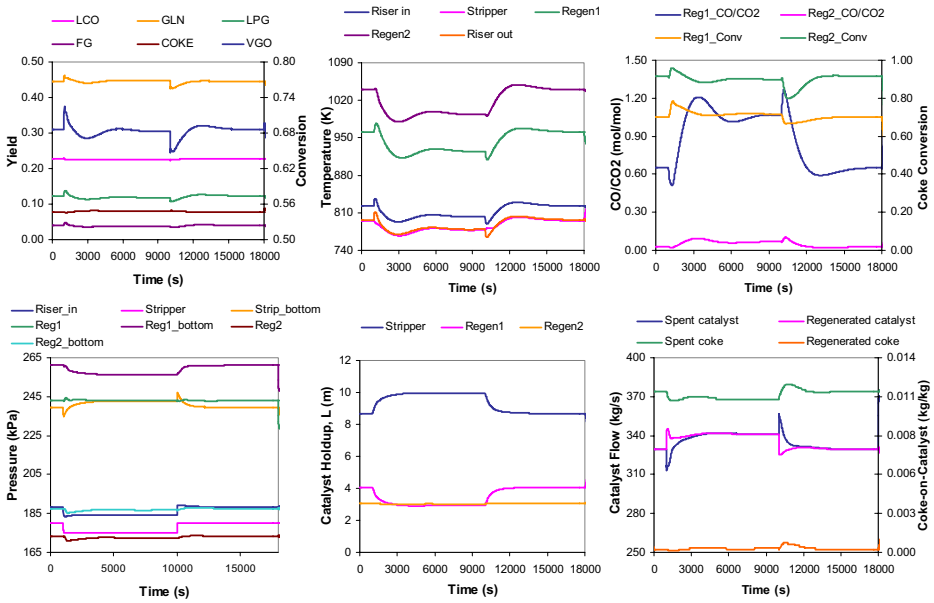

Figure 4. Open loop dynamic response to a step perturbation of –5% in the fresh feed flowrate, followed by a step perturbation to the previous value of fresh feed flowrate.

Figure 4 shows the dynamic response of the system to a step perturbation in the gas oil feed rate.

Decreasing the fresh feed flowrate initially results in a steep increase of the riser temperature due to a higher COR. This immediately leads to a steep increase in conversion. On the other hand, a lower concentration of hydrocarbons leads to a pressure decrease in the stripper, which causes a steep decrease in the flowrate of spent catalyst and an increase in the regenerated catalyst flowrate. The evolution to the new steady state is achieved through a pressure balance compensation caused by a decrease of the catalyst level in regenerator 1 and an increase of the stripper catalyst level. Coke-on-catalyst decreases, due to a lower feed flowrate. After a small initial increase, the temperature in regenerator 1 also decreases, since the coke content decreased as well as the residence time of catalyst (lower catalyst holdup). The CO/CO_2 ratio shows an inverse behaviour from temperature with steeper decreases and increases, which is expected since the literature shows that σ decreases exponentially with temperature (Vale, 2002). Due to lower temperatures in the regenerators, the temperature in the riser eventually decreases as well as the conversion.

After the second perturbation to the previous value of fresh feed flowrate, all variables return to their initial steady state.

4. Conclusions

A mechanistic dynamic model has been developed for the simulation of the steady state and dynamic behaviour of a R2R type FCC unit. The model includes a riser reactor, a stripper, a disengager, a regeneration system and catalyst transport lines.
From the simulation results presented it can be seen that the model shows a behaviour that is consistent with the experimental data and literature results. In future work, the model will be used for studies of advanced control and real time optimisation.

Nomenclature

A_{ij}: Pre-exponential factor of the reaction i→j (s^{-1} or $m^3s^{-1}kg^{-1}$); E_{ij}: Activation energy (J/mol); $\hat{C}_i$: Mass concentration of component *i* (kg/m^3); C_i: Molar concentration of component *i* (mol/m^3); C_D: Drag coefficient for a particle on an infinite medium; C_p: Specific heat capacity ($Jkg^{-1}K^{-1}$); d_{cl}: Catalyst cluster mean diameter (m); D: Diameter (m); F_i: Mass flow rate of component i (kg/s); g: Gravity acceleration (m/s^2); $H_{k,j}$: Enthalpy of phase k in stream i (J/kg); L: Length (m); M_w: Molar mass (kg/mol); n_{ij}: Order of reaction; N_i^g: Molar flow rate of component *i* in the gas phase (mol/s); P: Pressure (Pa); Q_r: Global reaction heat (J/s); r_i: Rate of formation of lump i ($kgm^{-3}s^{-1}$); r_{ij} : Rate of reaction i→j ($kgm^{-3}s^{-1}$); r_j: Rate of the reaction j ($molm^{-3}s^{-1}$ or $molkg^{-1}s^{-1}$); R: Universal gas constant ($Jmol^{-1}K^{-1}$); t: Time (s); T: Temperature (K); v: Velocity (m/s); V: Volume (m^3); W: Inventory (kg); Y_i: Component *i* (in coke) content of catalyst (kg/kg); z: Axial coordinate (m); ΔH_{crk}: Heat of cracking per kg of VGO (J/kg); ε: Volume fraction; Φ: Deactivation function; π: constant Pi; ρ: Density (kg/m^3); σ: Intrinsic CO_2/CO molar ratio; υ_{ji}: Stoichiometric coefficient of component i with respect to the reaction j; Ω: Cross section (m^2); $_g$: gas; $_c$: catalyst; $_s$: solid

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