The Importance of Using Three-Phase 3-D Model in The Simulation of Industrial FCC Risers

Gabriela Cantarelli Lopes[1], Leonardo Machado da Rosa[1], Milton Mori[1,*], José Roberto Nunhez[1], Waldir Pedro Martignoni[2]

[1] University of Campinas, School of Chemical Engineering
500 Albert Einstein Ave, 13083-970, Campinas, SP, Brazil, *mori@feq.unicamp.br

[2] PETROBRAS/AB-RE/TR/O
65 Republica do Chile Av, 20031-912, Rio de Janeiro, RJ, Brazil

An industrial riser reactor of a fluid catalytic cracking (FCC) unit was numerically studied in this work. A three-dimensional and three-phase Eulerian-Eulerian-Lagrangian flow model was used to predict the dynamic behavior of the reactor. To better understand the flow inside these reactors a rigorous model was applied and two different geometric configurations for the riser were tested. Results show that both the modeling of feedstock vaporization and the modification of the riser geometry, change the flow patterns and influence the reaction yields, emphasizing the importance of using sophisticated models in FCC process predictions.

1. Introduction

Fluid catalytic cracking (FCC) is the most important conversion process used in petroleum refineries. It converts in a few seconds the heavy distillation fractions into lighter and valuable hydrocarbon products such as gasoline, middle distillates and light olefins. Changes in feedstock requirements as well as the need to improve the reaction performance drive the advances in feed injection technology and the development of a highly active zeolite catalyst. A typical FCC unit consists of a side-by-side reactor regenerator configuration operating continuously for 2 to 3 years between shutdowns for routine maintenance. In this process, the preheated high-boiling liquid oil (at about 300 °C) is injected into a riser reactor, where is vaporized and cracked into smaller molecules of vapor by contact and mixing with the hot catalyst particles coming from the regenerator. The catalytic reactions result in coke deposition on the catalyst surface, which reduces catalyst activity and selectivity. The regeneration process, in addition to reactivating the catalyst pellets, provides the heat required by the feed vaporization and the endothermic cracking reactions in the riser. Since catalytic reactions can only occur after the vaporization of liquid feedstock, mixing of hydrocarbon droplets with catalyst must take place in the riser as quickly as possible.

Computational fluid dynamics tools have been widely used in chemical process engineering to predict and analyze the dynamic behavior of gas-solids flows. Bastos et al. (2008) showed heterogeneous structures and asymmetric behavior of the gas-solid flow in three-dimensional simulations of non-reactive systems. These characteristics

were also observed by Lopes et al. (2011) and Wang et al. (2010), in three-dimensional predictions of fluidized bed reactors. Moreover, Gomez-Prado et al. (2007) observed an improvement on the product yields prediction when a catalyst profile computed though a 2-D gas-solid model was used, instead of using a constant solid profile, to simulate an FCC unit.

The work presented herein extends these contributions by considering a three-dimensional and three-phase flow model which takes into account vaporization of the liquid droplets, heterogeneous cracking reactions and catalyst deactivation to simulate an industrial FCC riser. The influence of using two-phase or three-phase flow model and the effect of different geometric configurations on the reactor performance were also studied.

2. Modeling And Simulation

An Eulerian-Eulerian-Lagrangian approach was applied to simulate the dynamic three-phase flow inside the riser. Heat transfer and vaporization of feedstock were accounted in this model. The catalytic cracking reactions, including the catalyst deactivation, were predicted using the 4-lump model. The Fluent CFD code was used to obtain the numerical data, and appropriate user-defined functions were implemented to model the heterogeneous kinetics and the catalyst deactivation. The models used and the setup of the simulations are described below.

2.1 Three-phase flow model

An Eulerian description was used to model the gas and the solid phases, while the Lagrangian approach described the liquid droplets. The movement of the gas and solid phases was determined by solving transport equations for velocity and applying closure equations to predict the exchange between the continuum phases. The momentum transfer was modeled using the Gidaspow drag model; the heat transfer was predicted using the Ranz-Marshall correlation for the Nusselt number; and the turbulence in the gas phase was modeled using the Reynolds stress model (RSM). Fluctuations in particle velocity were modeled using the kinetic theory of granular flow. The trajectory of the discrete phase droplets was predicted solving the forces acting on each particle: gravity and drag force. Heat balances were applied to predict the temperature of the droplets. The mass transfer from the liquid phase to the gas phase was estimated by the difference of the species concentration in the droplet surface and its concentration in the bulk of the gas. Details about the equations and models used to predict the three-phase flow can be found in Ansys Fluent 12.0 Theory Guide (2009).

2.2 Catalytic cracking reactions

The cracking reactions were predicted using a 4-lump model, in which the chemical species are grouped into four different lumps (gas oil, gasoline, gas and coke), classified according the number of carbon in its molecule. The representative reactions of this kinetic model and classification of each lump are shown in Figure 1.

The cracking of gas oil was considered as irreversible second-order reactions and the cracking of gasoline, as irreversible first-order reactions. The dependence of kinetic constants on temperature obeys the Arrhenius equation. As long as the cracking

reactions occur, coke is deposited on the catalyst surface, reducing its activity. In order to model this catalyst deactivation, a function related to the coke concentration in the system was used. The kinetic constants for the model and the deactivation parameters used in the present study were estimated for FCC10 catalyst (sample free of metal traps, nickel and vanadium) by Farag et al. (1994). Since the activation energies and heats of reaction were not estimated by them, those values reported by Juárez et al. (1997) and Han and Chung (2001) were used.
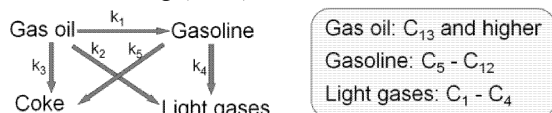

Figure 1: 4-lump model.

2.3 Simulations

The commercial code Ansys Fluent 12.0 was used to solve the model equations and appropriate user-defined functions were developed to implement heterogeneous kinetics and catalyst deactivation into the software. Three-dimensional predictions were carried out in order to evaluate the effects of geometry on the flow. Two configurations for the riser outlet were tested: a smooth L-shape exit and an abrupt T-shape exit. Studies about the influence of the riser outlet configuration on the gas-solids flow (Cheng et al., 1998; Gupta and Berruti, 2000) have shown that the smooth exits present less turbulence and no solids backmixing. However, because of the high wear by friction observed in this type of exit, the configuration most used in the FCC industrial units is the abrupt exits, since it requires less maintenance. Details of the geometry of simulated reactors are illustrated in Figure 2. The mesh used in this work consists of approximately one million hexahedrical volumes.
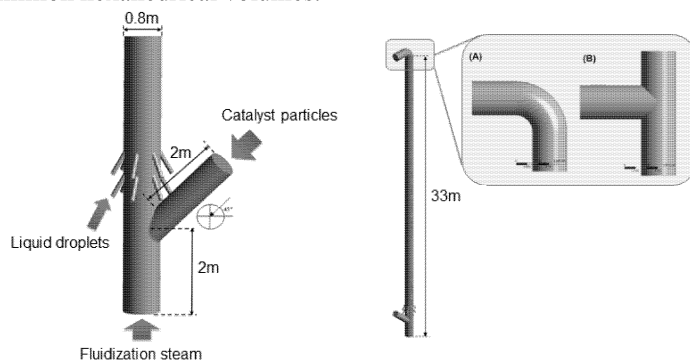

Figure 2: Geometry of riser - (A) smooth L-shape exit and (B) abrupt T-shape exit.

In addition to the three-phase simulations for the two exit types, a two-phase gas-solid case was performed in order to compare with the results of the three-phase simulation. The simulated cases were described in Table 1. The operating conditions used in the simulations are shown in Table 2. About 7 wt% of the total vapor is fed in with the catalyst at the lateral entrance, while the remaining vapor is injected into the base of the

reactor to help in the bed fluidization. Twelve ½ inch ducts at 30° angles to the main duct are used to feed in the liquid droplets. The physical properties of the reactive species and the catalyst were taken from the work of Martignoni and de Lasa (2001) and Landeghem et al. (1996).

Table 1: Description of simulated cases

	Case 1	Case 2	Case 3
Exit geometry	smooth L-shape	smooth L-shape	abrupt T-shape
Number of phases	three-phase	two-phase	three-phase

Table 2: Operating conditions used in the simulations

Mass flow of feed oil	20 kg/s
Catalyst-to-oil ratio	7 kg_{cat}/kg_{oil}
Steam	7 wt%
Feed temperature	500 K
Catalyst inlet temperature	960 K
Droplet inlet diameter	100 μm

3. Results And Discussion

The results presented in this section were obtained by the transient simulation of the cases. After 10 seconds of simulation the time-averaged values of the estimated variables were calculated by simulating the cases by additional 5 seconds.

The average cross-section values for the gas-phase density, gas-phase velocity and catalyst volume fraction along the reactor height are shown in Figure 3. It can be seen an increase in the gas-phase density after vaporization of the heavy oil and then a decrease due to the formation of lighter products by the cracking reactions. The gas-phase velocity was increased because of both the vaporization of feedstock and the volumetric expansion due to the reactions. The drag force between the phases also accelerates the catalyst particles, decreasing their volume fraction and separating the bed into a dense region close to the bottom and a dilute region in the rest of the riser.
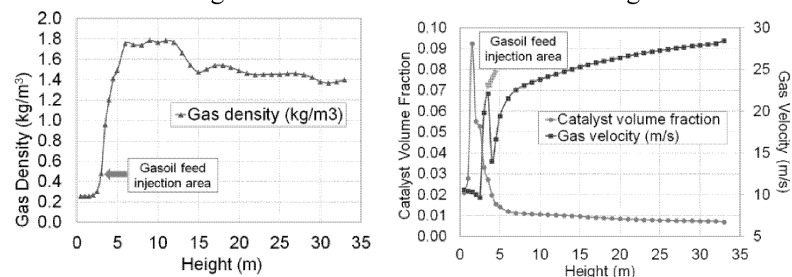

Figure 3: Radial average gas density, gas velocity and catalyst volume fraction.

The solids velocity profiles, for the Cases 1 and 3, are represented as streamlines in Figure 4. Swirl areas can be observed in the outlet region of the T-shape exit riser

(Figure 4, B), indicating the presence of fluid backmixing there. These vortices are not present in the smooth L-shape exit riser (Figure 4, A), in which the solids directly flow to the outlet without reverse flow. The catalyst volume fraction in axial planes located at 32m height for both cases are also shown in Figure 4. Because of the recirculation observed in Case 3 (T-shape exit), part of the catalyst flows through the wall countercurrent to the main flux, and a more pronounced core-annulus pattern, with a higher concentration of solids on the walls, is seen in this case.
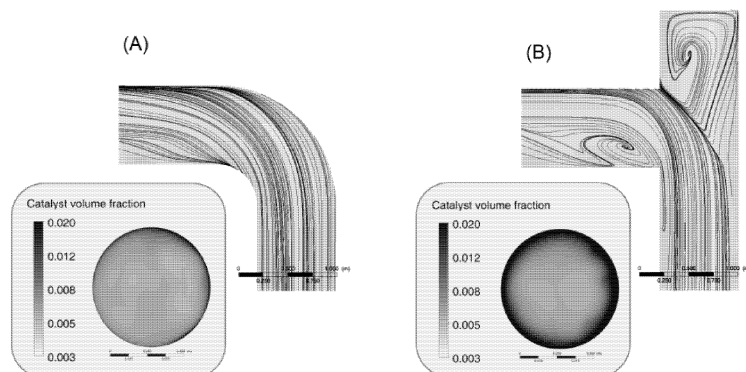

Figure 4: Solids velocity streamlines and catalyst volume fraction of Cases 1 and 3.

The model are verified by comparing the simulated results with the data reported by Ali et al. (1997), obtained for an industrial riser with similar scale of simulated geometries and operating under same conditions used in the simulations. Values for gasoline and coke yields at the reactor outlet are shown in Table 3. Comparing the products yields obtained for Cases 1 and 2 each other, it can be seen that the yields are lower in the three-phase simulation. Because of the instantaneous vaporization hypothesis, assumed in Case 2, the cracking reactions initiate as long as the gas-phase found the catalyst, proportioning a higher conversion in this case. However, when the T-shape exit riser is used in the prediction of the three-phase flow, the product yields are even higher than that obtained for the two-phase model. The flow backmixing observed in Case 3, provides a higher residence time and more contact between the gas and the solid phases, increasing the species yields, with gasoline yield very close to that obtained in the industrial plant.

Table 3: Comparison of model results with the plant data of Ali et al. (1997)

	Plant	Case 1	Case 2	Case 3
Gasoline yield (wt%)	43.9	39.4	41.7	43.0
Coke yield (wt%)	5.8	6.0	6.2	6.5

4. Conclusions

The fluid dynamic results obtained in this work revealed non-uniform flow patterns both axially and radially inside FCC reactors, reinforcing the importance of using three-

dimensional models to predict the flow. The adoption of the hypothesis of instantaneous vaporization, through the use of the two-phase flow model, provided results significantly different than those obtained for the three-phase flow model with feedstock vaporization. The test of different geometric configurations for the riser exit in the three-phase flow predictions showed relevant changes in the characteristics of the flow and, consequently, in the reactions yields. In conclusion, the study presented here showed the importance of using three-phase and three-dimensional models with the application of detailed geometries in order to correctly predict the reaction yields in industrial FCC reactors.

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