Why FCC Riser is Taller than Model Predictions?

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Introduction

Economy of refineries relies heavily on its fluid catalytic cracking unit (FCCU), since it converts low-market value heavier products into a more valuable lighter product (mostly gasoline). A typical industrial FCCU consists of mainly four parts—riser, separator, stripper and regenerator. Hydrocarbon feed (gas oil) is atomized and fed to a transport bed tubular riser reactor along with hot catalyst. Normally the height of an industrial scale riser is 30–35 m to provide a residence time of about 5 s. Feed droplets entering the riser are vaporized almost instantaneously, and hydrocarbon vapor cracks down to lighter molecules as it travels up with hot catalyst. Hot regenerated catalyst act as a heat source for vaporization of feed and for endothermic cracking reactions. During cracking, coke gets deposited on the catalyst and, thus, the catalyst loses its activity. Cracked hydrocarbon vapors are separated from deactivated catalyst in the separator and sent to fractionators for further separation. Deactivated catalyst flows into a regenerator (after passing through the stripper), where coke deposited on catalyst is burnt off and makes catalyst sufficiently hot. This hot-regenerated catalyst is recycled back in to the riser reactor.

Modeling Approaches

Considering the importance of FCC unit, a large number of investigators have attempted its modeling, but attained only limited success particularly in predicting riser behavior. Complexity of the riser lies in two facts (1) feed (like any other petroleum fractions) is composed of a mixture of extremely large numbers of unknown compounds, and (2) complex hydrodynamics due to presence of all three phases (solid, liquid and gas), with gas-phase volume expansion due to vaporization and cracking reaction. Hydrodynamics of the riser have been modeled by using widely different approaches ranging from simple plug-flow to three-dimensional (3-D) fluctuating velocities. On the other hand, all efforts to model cracking kinetics consider components of similar characteristics as a single lump of components, and each individual lump is treated as a single species. These lumping approaches can be broadly classified into three categories (1) parametric: considers gasoline, gas and coke as product lumps with feed (and feed fractions) as reacting specie.[1–3] Mostly, the number of lumps used in this approach varies from 3–19,[4] (2) pseudo-cracking: considers feed and product to be a mixture of few hypothetical/pseudo components,[5,6] for which all physicochemical properties are determined by using empirical equations. Number of lumps in this approach varies from 15–50, and (3) structure oriented lumping: originally proposed by Quann[7] in which a set of vectors of structural features are used to represent composition, reactions and properties of a mixture of hydrocarbons. This approach for specifying FCC feedstock may lead to a network of elementary chemical reactions as large as those containing more than 30,000 reaction steps.[8]

Comparison with Industrial Data

Several investigators have tried to model FCC reactor using the aforementioned approaches, but only few of them compared their results with an industrial scale unit (Figure 1). Most of them report that catalytic cracking of hydrocarbon reaction are very fast and conversion takes place within 10–15 m from the inlet of an industrial scale riser.[3,6,9–11] However, Derouin et al.[12] observed that actual plant conversion of gas oil and gasoline yield continues to increase significantly up to about 35 m. They correlated industrial data using axial dispersion model, but pointed out that several

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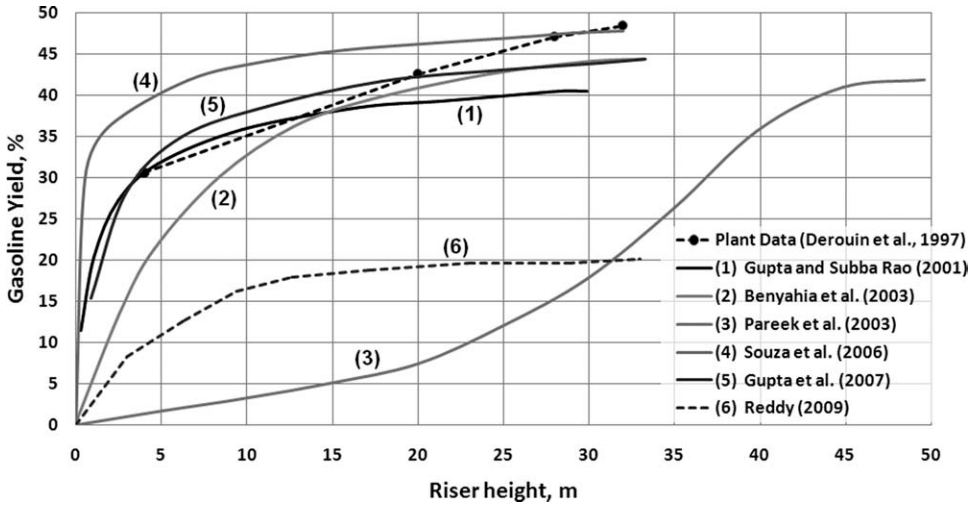

Figure 1. Actual plant data and predicted values of gasoline yield by various authors.

other factors like feedstock injection at the riser bottom, core-annulus flow behavior, thermal effects, etc., are yet to be considered. After looking at works of various other investigators, it appears that there are two factors—number of lumps and hydrodynamics—that need to be modeled concurrently in greater detail. On the other hand, allowing for larger number of lumps and three-phase turbulent flow simultaneously leads to excessive computational load which is difficult to handle. In lieu of this, various authors have blamed different factors to be the main culprit behind poor predictability, and modeled FCC riser with greater emphasis on the particular factors at the cost of the other.

Conciliation Attempts

Several authors felt that the assumption of instantaneous vaporization of feed in the inlet zone could be the reason for poor prediction of riser height. Considering this, Theologos et al.[13] looked at feed atomization and vaporization in greater detail using three-lump model of Weekman and Nace[1] and reported that feed gets completely evaporated between 0.25–1.65 m for droplet size ranging from 30 μm–500 μm. This indicates that assumption of instantaneous feed vaporization is not a main source of error in predicting riser height. Similarly, some felt that the interphase film coefficient for heat and mass transfer could be the reason behind poor predictability. Considering this Pareek et al.[14] introduced heat-transfer coefficient across vapor film surrounding catalyst particle, along with increased number of lumps (10-lump), assuming plug-flow condition, however, predicted gasoline yield deviated considerably from the reality (Figure1).

Gupta and Subba Rao[9] concentrated their research on slip velocity between catalyst and hydrocarbon vapor in plug-flow condition. They used kinetic parameters of the four-lump model obtained by Pitault et al.[15] An excellent agreement between predicted and observed values is observed in the inlet zone, but large under prediction in the upper section of the riser is clearly seen in Figure 1. Predictions of Benyahia et al.[10] improved considerably between 10–25 m of riser height. However, deviation was quite prominent in the inlet and exit regions. They used more rigorous fluid dynamic equations based on particulate phase fluctuating energy explained by Gidaspow,[16] but took the simplest three-lump model proposed in a twin article by Weekman et al.[17,18]

Applying a conservative approach, Souza et al.[11] considered 2-D flow with six lumps. However, the continuity and

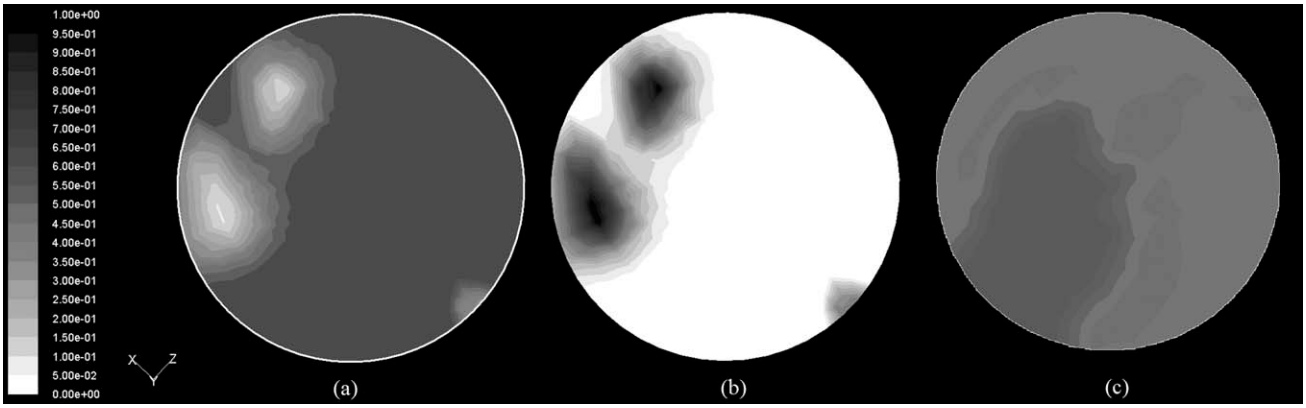

Figure 2. Concentration profile at the riser exit (a) mole-fraction of heavier component number 9, (b) mole-fraction of lighter component number 6, and (c) solids-volume fraction.

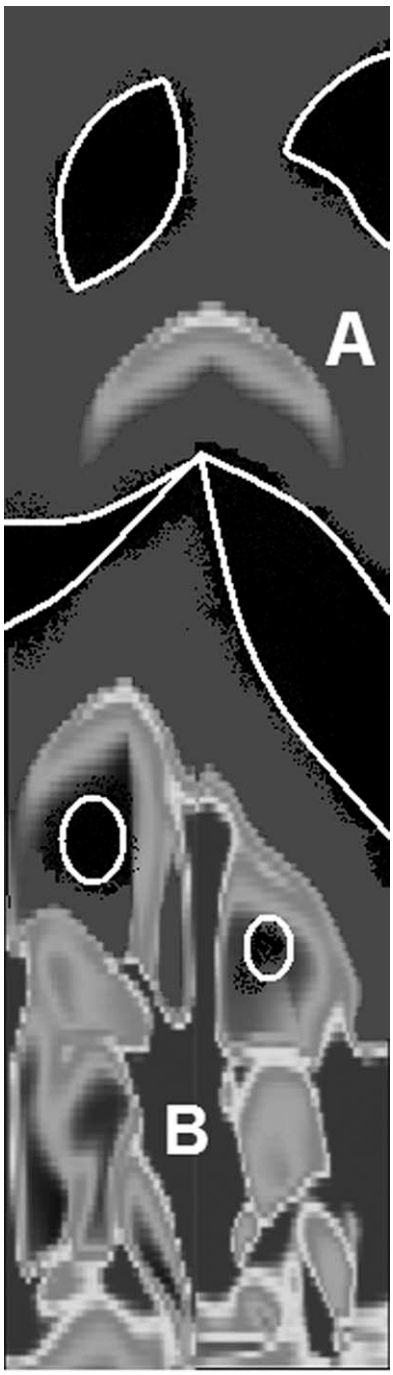

Figure 3. Schematic representation of localized reaction bubbles within emulsion phase.

momentum equations were greatly simplified due to assumptions of incompressible homogeneous mixture with laminar flow. Conversion and gasoline yield at riser exit could be predicted more accurately, but most of the conversion took place within 10 m from the inlet. Gupta et al.[6] introduced a new concept of cracking mechanism using 50 components (seven pure-components, and 43 pseudo-components), with more than 10,000 feasible parallel reaction steps. However, they compromise by assumed plug-flow with slip velocity between catalyst and vapor in the riser reactor as suggested by Gupta and Subba Rao.[9] Predictions were further improved and comparison was very good up to about 20 m of riser height, but beyond that no appreciable change in gasoline yield was observed.

On the aforementioned basis, it appears that hydrodynamics and reaction mechanism, particularly the number of reacting species, are the two key parameters to be considered in greater detail for FCC modeling. However, no work could be performed so far to account for both parameters simultaneously, due to limitations of computational efficiency. Recently, we tried to apply 50-component reaction mechanism proposed by Gupta et al.[6] using FLUENT™, a more rigorous commercially available CFD package.[19] A riser reactor of 0.8 m dia. and 33 m height was modeled using hexahedral mesh (size 0.05). Total 143,226 volume elements were formed to apply 3-D k-ϵ model based on Eulerian-Lagrangian approach. Species transport model and particle surface reactions were enabled to model catalytic cracking reaction. To model cracking reactions, Arrhenius type rate constants were specified for each reaction step. Although original work of Gupta et al.[6] used 50 components with over 10,000 parallel reactions, we could only take 14 components, with 266 feasible reactions, as the number of feasible reaction steps increase several fold by increasing one pseudo-component. The software used requires that each reaction step be specified on separate forms manually,[20] which restricted us to consider only 14 components. (List of components considered and associated reaction rates used for this simulation are given as online supplementary document).

Reaction Bubble

Although reaction mechanism used in this work was the same as that of Gupta et al.[6] predicted values of gasoline yield was much below the actual value (Figure 1), perhaps due to a less number of pseudo-components, however, results revealed that consideration of at least 3-D two-phase turbulent flow is unavoidable for FCC simulation, as reactions are not taking place uniformly even within the emulsion phase of the bubbling fluidized bed of the catalyst. This fact is evident from Figure 2 showing mole fractions of two components (Figure 2a and 2b), and void fraction of solid catalyst at the riser exit (Figure 2c) at a particular instant of time. In Figure 2a it is observed that pseudo-component number 9 (a hypothetical component of gasoline range having average boiling point 378.6 K), is almost uniformly distributed over the entire cross section except at two small pockets where its concentration has decreased significantly. On the other hand, from Figure 2b, it can be noted that component number 6 (n-pentane, boiling point 303.11 K) is present only at those points where component number 9 is depleted (similar patterns, with different concentration values, were observed for all other components lighter than component number 9). These indicate that reactions are taking place only in small pockets of the fluidized bed. At first sight, it appeared that this may be due to bubbling fluidized bed, in which catalysts are present in the localized region. However, concentration of catalyst was observed to be almost uniform throughout the cross section forming an emulsion phase (void fraction 0.4–0.6), whereas cracking reaction was in the localized pocket. These figures indicate

that apart from gas bubbles in the fluidized bed, there exist bubbles of reaction within the dense region of the bubbling fluidized bed.

Feasibility of such reaction bubbles can be explained using Figure 3, where nonuniform distribution of catalysts in a fluidized bed is shown schematically. It is expected that catalytic cracking is possible only at those places where concentrations of both catalyst and cracking species are high, e.g., bubble boundaries (wake and cloud) in a fluidized bed. Second, activity of catalyst at these bubble boundaries is also important in deciding the rate of cracking reaction. On the other hand, activity of catalyst depends on the amount of carbon deposited, which in turn depends on the history of catalyst. Thus, it can easily be visualized that a favorable condition at the bubble boundary initiates cracking reaction which, almost instantaneously, deactivates the catalyst and reaction front moves deeper into the emulsion phase forming a reaction bubble marked as "A" in Figure 3. In this figure, dark patches surrounded by white lines represent familiar bubble phase of the fluidized bed, and the dark gray background shows the emulsion phase. Patterns of different shades signify intensity of the reaction of the particular species (or lump). As discussed earlier, maximum intensity of reaction should be at the bubble boundaries, however, since reaction rates are very fast, intense zone of reaction move deep into the emulsion phase faster than the bubble rise velocity, leading to formation of reaction bubbles inside the emulsion phase. It can be easily visualized that size of these reaction bubbles can be in some cases even larger than the vapor bubbles of the fluidized bed (marked as "B" in the same figure). Thus, available volume, where cracking reaction takes place, is much lower than the actual reactor volume. Therefore, actual reactor volume must be much larger than that predicted by conventional packed reaction zone approach in which it is normally considered that reaction is taking place uniformly throughout the emulsion phase.

Conclusion

Thus, it can be concluded from the aforementioned discussion that under-prediction of riser height by various models, is partially due to the lack of visualization of real processes occurring inside riser reactor, and partially due to the lack of a computational tool that can simultaneously handle both larger numbers of lumped component and robust hydrodynamic model to simulate turbulent three-phase flow.

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