COMPARISON OF ASYMMETRIC WITH SYMMETRIC FEED OIL INJECTION PARAMETERS IN A RISER REACTOR

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Comparison of Asymmetric with Symmetric Feed Oil Injection Parameters in a Riser Reactor

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Abstract
A computational fluid dynamic (CFD) computer code was used to determine the effects of product yields of three feed injection parameters in a fluidized catalytic cracking (FCC) riser reactor. This study includes the effects of both symmetrical and non-symmetrical injection parameters. All these parameters have significant effects on the feed oil spray distribution, vaporization rates and the resulting product yields. This study also indicates that optimum parameter ranges exist for the investigated parameters.

Introduction
A computational fluid dynamic (CFD) computer code was used to determine the effects of asymmetry on product yields in two feed injection parameters in a fluidized catalytic cracking (FCC) riser reactor. FCC reactors are used in the petroleum refining industry to convert heavy oil into lighter molecular weight hydrocarbon products. The oil industry has recently recognized that feed injector design has a significant impact on multiphase mixing in the riser, and thus on the product yields. Due to the geometry and nature of these risers, however, the effects have been extremely difficult to measure and characterize directly. Experimental results obtained from pilot scales are not good indicators of commercial-scale unit performance due to differences in aspect ratio and other similarity discrepancies between the pilot and commercial scales. The use of a computer simulation can provide the necessary data to analyze the flow at all points of the riser. The ability to characterize the flow behavior through the riser as a function of individual parameters enables the existence of optimum operating condition windows to be identified. Previous work on the modeling of flow through FCC units was done as early as 1970. Weekman and Nace proposed a 3-lump cracking kinetic model to predict gasoline yields [1]. This model was expanded over the past three decades to include additional lumped models with multi-phase flow capability [2,3]. Recent work done at Argonne National Laboratory has resulted in a three-phase, four-lump integral kinetic cracking computer code, ICRKFLO [4]. The riser was modeled by using a two-dimensional approach with the ICRKFLO code.

Theoretical Formulation
A schematic of a typical FCC riser is shown in Figure 1. The flow through the riser is made up of gas and droplet liquid phases, as well as a solid catalyst particle phase. After the liquid droplets are heated by the surrounding gas, they vaporize and react in the presence of the catalyst particles and crack into smaller molecular weight hydrocarbons. The heat of vaporization and heat of reaction is supplied from the catalyst particles, which are heated to a high temperature in the process of burning.
off coke deposits in the regenerator before entering the riser. Therefore, the computer model must accurately represent this type of three-phase reacting flow. The code

uses an Eulerian approach for the liquid/solid phase, as well as for the gas phase. Separate transport equations are written for all three phases of the flow, and the conservation equations (mass, momentum, and energy) are solved for each phase. These equations can be represented by elliptical partial differential equations. Put into general form, the equation for the gas phase is:

\[ \frac{\partial}{\partial x} \left( \rho u \xi - \Gamma_{\xi} \frac{\partial \xi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \rho v \xi - \Gamma_{\xi} \frac{\partial \xi}{\partial y} \right) = S_{\xi} \]

\( \xi = 1, u, v, h, Y_b, k, \) or \( \varepsilon \)

and for the liquid/solid phase is:

\[ \frac{\partial}{\partial x} \left( n_k u_k \xi - \Gamma_{n_k} \frac{\partial n_k \xi}{\partial x} \right) + \frac{\partial}{\partial y} \left( n_k v_k \xi - \Gamma_{n_k} \frac{\partial n_k \xi}{\partial y} \right) = S_{n_k} \]

\( \xi = 1, u_{ck}, v_{ck}, \) or \( T_{ck} \)

where, \( \xi \) is a general flow property, \( \theta \) is gas volume fraction, \( \rho \) is density, \( n_k \) is droplet or particle number density for the \( k^{th} \) size group, \( \Gamma \) is effective diffusivity (laminar and turbulent), \( x \) and \( y \) are coordinates, \( u \) and \( v \) are gas velocity components, \( u_{ck} \) and \( v_{ck} \) are droplet or particle velocity components of the \( k^{th} \) size group, and \( S_{\xi} \) is the sum of all source terms for the variable \( \xi \). The source terms account for interfacial heat, mass, and momentum exchanges. Phenomenological models include droplet vaporization, turbulence, lumped integral reaction, coke formation and transport, interfacial drag and heat transfer, and reaction and subspecies flow models [4]. The vaporization rate of the feed oil droplets is based on a single stationary droplet [5], with modifications to include a Ranz-Marshall correction [6] for the convection effect. The droplet vaporization rate then becomes:

\[ \frac{\partial n}{\partial t} \text{conv} = 4\pi r \left( \frac{\lambda}{C_p} \right) \ln(1 + B) \text{Nu}_\varepsilon \]

where,

\[ B = \frac{C_p(T_c - T_b)}{q_t} \]

and,

\[ \text{Nu}_\varepsilon = 1 + 0.276 \text{Re}^{1/2} \text{Sc}^{1/3} \]

in which \( \lambda \) is the gas conductivity, \( r \) is droplet radius, \( C_p \) is the specific heat, and \( q_t \) is the latent heat. The computer code also accounts for transportable properties due to an evolving size spectrum of droplets that are a function of droplet size. Collisions between droplets are not modeled because droplets enter the system as a formed spray that is spreading out. Droplet collisions under these circumstances are assumed to be no more than a second or third order effect. Three related particle/wall and particle/collision models are included, however, because particle loading in the system is much higher than that of droplets, and these models are needed to account for observed phenomena in particle/gas flows. Once vaporization occurs, cracking reactions occur. ICRKFLO uses a two-equation, four-lump model [7] for these reactions. The reactions are:

\[ A_1 \rightarrow a_1 A_2 + a_2 A_3 + a_3 A_4 \]

\[ A_2 \rightarrow b_1 A_3 + b_2 A_4 \]

in which \( A_1 \) is feed oil, \( A_2 \) is light oil (gasoline), \( A_3 \) is dry gas (C_1-C_5), and \( A_4 \) is coke. The stoichiometric coefficients are expressed in mass fractions. The stoichiometric coefficients and related kinetic constants of the reactions can be determined empirically.

**Numerical Scheme**

The equations are discretized by using a control volume approach for the computational grid. The grid is an adaptive, rectilinear grid with staggered momentum cells. A modified form of the SIMPLER algorithm [8] adapted for multiphase flow is used to solve for the flow field. The convergence criteria for normalized mass residuals in the liquid/solid phase is of the order \( 10^{-8} \), and of the order \( 10^{-10} \) for the gas phase. A grid sensitivity study was performed to determine the optimum number of cells in
both directions. A 30 x 212 grid was used in this study. Many features of the code were validated from a comparison with published data and proprietary data supplied by industry partners [4].

Results and Discussion

The results of the study show that feed oil injection parameters do have significant effects on mixing, vaporization, and gasoline yields in a commercial-scale FCC riser. The feed oil injection parameters studied included mean droplet size, feed injection velocity, and feed injection angle. The two-dimensional riser simulation had opposing feed oil injection ports on opposite sides of the two-dimensional slice of grid cells going up the riser. For the first set of simulations, boundary conditions of the two sides of the riser equal (symmetric conditions). A second set of simulations was performed to assess the effects of asymmetry. In an FCC riser with four feed oil injection nozzles, for example, significant asymmetries can occur if one of the nozzles becomes plugged or even partially plugged. Small asymmetries occur if there are small differences in pressure in the feed oil lines to the nozzles. Each parameter was studied individually; that is, only one parameter was varied for each simulation in a set of simulations. A set of simulations was performed over a parameter range for each of the feed injection parameters. For the simulations to assess asymmetric effects, a near optimum (for gasoline product yield) case of droplet size and feed injection velocity was chosen. The feed spray velocity and angle on the right side were held constant through two series of simulations: one varying left-side injection angle to produce injection angle asymmetries, and one varying left-side injection velocity to produce injection velocity asymmetries.

Feed Injection Velocity and Mean Droplet Size

Many measures of the effectiveness or ideality of the spray injection process may be defined. A good overall measure of the effectiveness or quality of the spray injection process is one that would be of primary interest to refiners, for example, the yields of desirable products such as gasoline. Two measures of the effectiveness of spray injection that are closely related to the physics that ultimately result in to optimum product yields are (1) the uniformity of droplet mass distributed over the cross section by the spray nozzles and (2) the distance the spray must travel downstream to reach 99% vaporization. Many interacting phenomena occur in the mixing zone, including those affecting the feed oil mass distribution, droplet heating, onset of vaporization, and subsequent cracking reactions. Understanding these complex local interactions as they relate to reactor performance is a very difficult undertaking. Therefore, the spray effectiveness measures defined above can provide quantitative measures that yield some insight into the cause and effect relationship between spray parameters and performance. However, due to the complexity of the phenomena, optimizing these measures does not necessarily result in to optimum performance.

Simulation provides a tool that can generate an enormous amount of data on conditions and system-state evolution as a multiphase mixture flows through the riser reactor. Space and effort limitations allow only some of the more basic and significant insights that can be obtained from simulation to be presented in this discussion.

Figure 2 shows relative gasoline yield for symmetric injection with varying spray injection velocity for various mean droplet sizes. High gasoline yields would, in general, be considered desirable. However, a similar study could be used to look for optimums in yields of diesel fuel or heating oil, if those or other products were considered to be of prime importance. Yield curves are shown over a wide spray injection velocity range for three mean droplet sizes. The spray injection velocities cannot be related directly to flow velocities in a nozzle because the spray injection velocity is a device-level simulation parameter that specifies a mean spray velocity after the spray has already formed. In a real device, this velocity would vary greatly depending on the measurement point in relation to the nozzle outlet. Thus, these velocities are in the range that would be encountered in actual equipment, but are not nozzle exit velocities, and their significance is to show trends. The trends shown in the gasoline yield curves reveal a number of characteristic relationships that are both important and physically reasonable.

![Figure 2 Effects of Droplet Velocity and Mean Droplet Size on Gasoline Yields](image)

First, there is an injection velocity that is optimal for gasoline yield for each mean droplet size. Basically, the optima exist because droplets do not penetrate to the reactor center if the injection velocity is too low. In this case, turbulent and diffusive mixing is too slow in a relatively short residence time commercial scale riser for the entire cross section of the riser to be effectively utilized in the cracking reactions over a substantial
portion of the riser length. Thus, insufficient injection velocity leads to performance degradation. Injection velocities that are too high can lead to over-penetration of the spray beyond the centerline with a similar mal-distribution of feed oil over the cross section, which also leads to performance degradation. The optimum spray injection velocity increases with decreasing mean droplet size. Optimal performance should reasonably be expected to require that the spray penetrate to the center of the reactor and be fairly evenly distributed over the reactor cross section. Droplet drag reduces cross-stream droplet velocities more rapidly for smaller droplets than for larger ones, thus requiring higher velocities for smaller droplets to reach the reactor center. Finally, the breadth of the optimum increases as the mean droplet size for the droplet size spectrum decreases within the range of droplet sizes tested. A combination of reasons may account for this characteristic. Because the spray consists of a size spectrum, larger droplets, which can carry a substantial percent of the total droplet mass of the spray, do exist in sprays with the smaller mean droplet sizes. Therefore, each spray will have a range of penetration depths into the cross section based on its size spectrum. Because small droplets carry much less mass (order $r^3$), the size distribution must consist of a much larger portion of droplets that are small or have relatively low velocities. This type of size distribution prevents the droplets from penetrating too far into the reactor and results in fairly even coverage of feed oil vapor over the cross section during the vaporization process.

In the tested cases, the broadening of the gasoline yield and feed conversion optima for smaller mean droplet sizes in the tested cases is very significant. This finding indicates that a droplet size spectrum with the smallest mean droplet size that still allows sufficient numbers of droplets to reach the centerline of the reactor under normal operating conditions will be the least sensitive to yield or conversion reductions when operating at off-optimum conditions. A note of caution, however, is in order regarding the apparent relation between the breadth of the injection velocity optimum and the mean droplet size. This particular characteristic has been tested only for a normal size distribution of droplets in the spray. Further study is required for a variety of size distributions to determine the effect of the size distribution on the breadth of the injection velocity optimum in relation to mean droplet size.

Another way of evaluating the effectiveness of the spray operating conditions is to determine the distance from the spray injectors for a given percentage of the spray mass to vaporize. In a simulation, the amount of unvaporized droplet mass crossing a plane of grid cells at any downstream location is easy to calculate. The downstream distances traveled by the droplets from the injector entry to a point where 99% of the spray mass is vaporized is shown in Figure 3, which depicts curves plotted as a function of droplet injection velocity. For the larger droplet sizes, these curves correlate very well (in the inverse) with the curves for feed oil conversion and gasoline yield. This correspondence for the larger droplet sizes means that those factors relating to the spray distribution over the cross section of the reactor that prolong the vaporization process (such as the local high concentrations of droplet number density in some regions that rapidly use up the locally available heat from near-field hot catalyst particles) are apparently the primary factors that limit the extent of the feed oil cracking reactions, which are endothermic.

![Figure 3 Effects of Droplet Velocity and Mean Droplet Diameter on Vaporization Distance](image)

This observation does not hold for the smallest mean droplet diameter spray. For the smallest mean droplet diameter spray, the 99% vaporization distance is nearly constant over the velocity injection range. Smaller droplets reach vaporization temperature faster and vaporize faster (the spray mass has a much higher surface to volume ratio for small droplets). Vertically conveyed heat carrier catalyst particles tend to form a slight characteristic U-shaped number density distribution, which means that somewhat more heat sources are available at shallow penetration depths. This heat is sufficient for vaporization in a fairly short and uniform distance. However, this heat is not sufficient to drive the endothermic cracking reactions to the same level of completeness for the shallower penetration depths of the bulk of the droplet mass at lower injection velocities. As seen in Figure 2, gasoline yields drop off at lower injection velocities for the smallest mean droplet size, even though the 99% vaporization distance is nearly constant over this range. This characteristic is also a consequence of the relatively slow cross-stream turbulent mixing process relative to initial spray penetration and the short reactor residence time (on the order of 1 second with a travel distance on the order of 10 diameters downstream, which is insufficient to achieve a well developed flow even for single phase non-reacting conditions).
Asymmetry in the velocity of the feed oil injection is illustrated in Figures 4 – 6. As the relative amount of asymmetry increases, the desirable yields at the riser exit decrease. Due to the two-dimensional nature of the riser (i.e., two injection locations instead of the actual number of nozzles) the asymmetry effects are quite significant. Figures 4 and 5, however, do represent the trends for the actual asymmetry. A 1% change in the velocity between nozzles translates into about a 1% decrease in the gasoline yields. The effects of velocity asymmetry on relative gasoline yields are shown in Figure 4. This figure shows that this relation is nearly linear. The velocity asymmetry causes a delay in the vaporization, as shown in Figure 5 where \( C/CO \) represents the fraction of feed oil vapor left unvaporized at the riser exit, normalized by the maximum amount of unvaporized feed oil. Figure 6 shows the difference in evaporation rate around the mixing zone for a substantial difference (about 40%) in injection velocity and mass flow rate, thus simulating a partially plugged nozzle. The evaporation rate is shown as a grayscale contour plot with the darkest regions having the highest vaporization rates. In the asymmetric case, vaporization rates remain high on the left side considerably farther downstream than for the symmetric case. This pattern indicates a substantial vaporization delay in the asymmetric case due to higher droplet loading on the left side. The vaporization delay causes a delay in the onset of cracking reactions and a consequent reduction in gasoline yield for the asymmetric case.

**Injection Angle**

For a constant spray mass flow rate, the injection angle measured from the vertical essentially changes the path length and consequent travel time to the center of the reactor. Effects of injection angle were tested only for sprays of 50 micron mean diameter at the optimum injection velocity. Figure 7 indicates a small but steady decrease in the vaporization distance as the injection angle is increased to 90 degrees (perpendicular to the streamwise direction). Figure 8 indicates that there is a consequent small but steady increase in gasoline yield as the injection angle is increased to 90 degrees. The difference over the entire injection angle range of 30 to 90 degrees is less than 3% in gasoline yield. Such an increase, though small, may be considered significant when large quantities of feed oil are processed. However, realizing such an increase in an actual unit, rather than in a tightly controlled simulation, could require tighter controls than would be feasible on the operating conditions of the real unit to keep it near optimum yield. This possible control difficulty arises because the angled injection, with longer path lengths to the reactor center, allows higher velocity injection (more mass flow from a given nozzle type) with a smaller cross-stream velocity component. In this case, more overall production per day may possibly be obtained from the unit without significant loss in gasoline yield as a result of over-penetration of the sprays. Therefore, the optimum operating conditions for spray angle may depend on whether the goal is to optimize the production rate of the FCC unit or to optimize the percentage of gasoline or other product yields.
The effect of a large asymmetry in injection angle, which could also result from a partially plugged nozzle, is illustrated in a gray-scale droplet number density plot in Figure 9. In this case, the spray distribution quickly becomes very uniform over the cross section for the symmetric case. For the highly asymmetric case, however, droplets from the left injector overshoot the centerline. Insufficient residence time for turbulent mixing to redistribute the droplets causes a concentrated region of high droplet number density far into the downstream of the mixing zone. Vaporization is delayed in this zone due to larger amounts of heat extracted from the gas in the zone, thus lowering the temperature and consequent heat transfer rate to droplets for vaporization. In addition, large amounts of feed oil vapor are also deposited in this cooler zone of high droplet concentration. The cracking reactions are therefore slowed down and delayed because feed oil must diffuse or turbulent mix out into the region where the hotter catalyst exists—a rather slow process compared to riser residence time. Consequently, gasoline product yield is much less in the highly asymmetric case. A quantitative measure of the mal-distribution of feed oil droplet mass can be seen in Figure 10, which shows a mean droplet mass deviation from the mean over a cross section in the mixing zone where most of the vaporization takes place. The difference between these two grows steadily as droplets in the symmetric case spread out fairly evenly over the riser cross section, while those from the highly asymmetric case do not. In the asymmetric case, the droplet mass deviation from the mean over the cross section is about 8% higher through much of the mixing zone.

In Figure 11 the vaporization distance is plotted against the injection angle ratio for the two sides (a value of one represents symmetric injection). As this ratio decreases (injection angle becoming more asymmetric), the vaporization distance is seen to increase by about 25%. This increase in vaporization distance delays the onset of cracking reactions. Even if the vaporized feed oil were evenly distributed over the riser cross section, which is not the case, the vaporization delay would decrease gasoline yield. The actual decrease in gasoline yield shown in Figure 12 is nearly linear as the injection angles become more asymmetric.
Conclusion

Effects of feed oil injection parameters on gasoline yields were studied by using a three-phase, reacting flow, computational fluid dynamics code. The parameters studied included injection velocity, mean droplet size, and injection angle, as well as asymmetries in these operating parameters in a two-injector system. As seen in this study, changes in feed oil injection parameters can produce dramatically different results on the flow of gas, droplets, and particles in a FCC riser. Injection velocity variations result in a change in penetration depth of the droplets into the catalyst flow. The average droplet size affects the evaporation rate of the droplets, and the feed injection angle has an impact on the mixing patterns in the riser. Asymmetry of these injection parameters also produces detrimental changes in the yields at the exit of the riser. All three of the studied parameters have a range with a significant optimum in gasoline yield. This indicates that optimum operating conditions exist for these parameters, and improvements in nozzle design and control of feed injection may improve the gasoline yield of FCC risers by a small but significant percent.

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