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INTERACTIONS OF MULTIPHASE HYDRODYNAMICS, DROPLET EVAPORATION, AND CHEMICAL KINETICS IN FCC RISER REACTORS*

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DISCLAIMER

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ABSTRACT

A computational fluid dynamics (CFD) computer code, ICRKFLO, has been developed for flow simulation of fluid catalytic cracking (FCC) riser reactors, which convert crude oil into gasoline and other valuable products. The FCC flow, especially in the entry region, is a three-phase reacting flow including hot catalyst particles, inert lift gas, and feed oil droplets. The impact of the hydrodynamics processes of heat transfer, droplet evaporation, and mixing on the chemical kinetics or riser performance can be significant. ICRKFLO was used to evaluate the impact of these processes on the performance of an advanced FCC unit. The code solves for major flow properties of all three phases in an FCC riser, with models governing the transport of catalyst particles and feed oil droplets, the vaporization of the feed oil droplets, the cracking of the oil vapor, and the formation and deposition of coke on particles. First, the code was validated against available test data of a pilot-scale FCC unit. Then, flow calculations for the FCC unit were performed. Computational results indicate that the heat transfer and droplet vaporization processes have a significant impact on the performance of a pilot-scale FCC unit. The impact is expected to be even greater on commercial scale units.

NOMENCLATURE

n_i	droplet or particle number density (number of droplets/m^3)
r	droplet or particle size (μm)
S	Source term of a governing equation
T	temperature (K)
t	time (s)
u	velocity component in the x-direction (m/s)
v	velocity component in the y-direction (m/s)

Greek Symbols

ε	turbulence dissipation rate (J/s)
Γ	effective diffusivity (pa-s)
κ	thermal conductivity (W/m/K)
μ	viscosity (pa-s)
θ	gas volume fraction
ρ	gas density (kg/m^3)
ξ	general variable for 1, u, v, h, f, k or ε

Subscripts

b	boiling point
d	droplet
k	size group k of droplets or particles
p	particle
s	solid
δ	slip property

INTRODUCTION

Many of the most important processes in energy production and utilization technologies and in the chemical industries involve the interactions of multi-phase hydrodynamics, droplet evaporation, and chemical kinetics. These interactions play key roles in controlling the process efficiency, pollutant production, and the degree to which the process meets its intended function, such as the production of optimum product yields in refining a variety of crude oils or the maximum production of useful energy with minimum generation of pollutants in a furnace or an engine. Advanced processes must be continually developed for industries to meet new environmental regulations and to

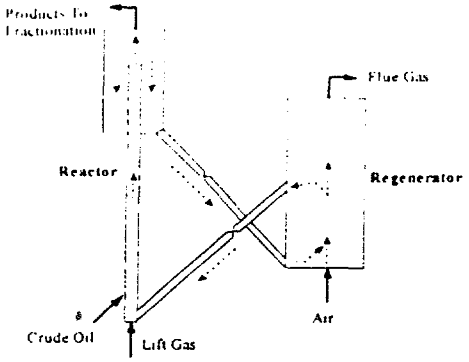


Figure 1 Schematic Diagram of A Typical FCC Unit

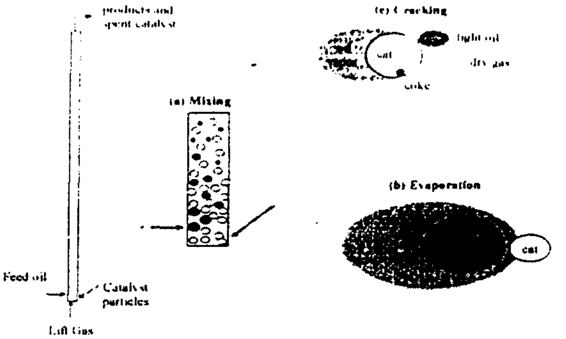


Figure 2 Mixing, Evaporation, and Cracking Processes in a Riser Reactor

stay competitive in their product markets. To decrease the development time of advanced multi-phase reacting flow systems, detailed knowledge of the relationships between process operating parameters for given system geometry and process progress within the system are necessary. Such knowledge can be obtained by the analysis based on the controlling physics of the system combined with the powerful tool of computer simulation. Computational fluid dynamics (CFD) based analysis is increasingly in use as a tool to investigate complex flow systems. During the past 20 years, CFD codes have evolved greatly with the advancement in both numerical techniques and computer hardware. CFD applications were extended from simple laboratory-type systems to much more complex industrial-type flow systems. Computer simulation is regarded as an effective and cost-saving tool to further improve the performance of flow systems.

Fluid Catalytic Cracking System

As one of the applications of multi-phase reacting flow systems, the fluid catalytic cracking (FCC) process is extensively used for the conversion of very heavy fractions of crude oil into valuable lighter products in modern refinery industry. The FCC units and their catalysts are in continuous evolution. The refining industry must adapt to market changes: gasoline yield and/or quality maximization, new petrochemical production, conversion of residues, and environmental requirements. Currently, FCC operating capacity is estimated at 12,800,00 barrels per day worldwide and 4,400,000 barrels per day in the US. It is also estimated that the US will need about 200,000 barrels per day of additional capacity in the next few years.

As shown in Figure 1, a typical FCC unit has two major components: a riser reactor and a catalyst regenerator. The riser is used to convert crude oil to lighter and more valuable products and the regenerator is used to regenerate the spent catalyst for recycle to the riser. Liquid crude oil is injected into the riser and mixed with regenerated hot catalyst particles to vaporize and to crack into gasoline, diesel fuel, jet fuel, and other products. Coke is a by-product of the cracking reactions. Its deposition on the surfaces of catalyst particles de-activates the catalyst. The spent catalyst is regenerated by burning off the coke deposit. The burning of coke in the regenerator also reheats the catalyst.

A typical pilot scale FCC riser and its mixing, evaporation, and cracking processes are illustrated in Figure 2. The catalyst stream consists of regenerated hot catalyst particles and a small amount of carrier gas, entering from the lower right side of the riser. The inert lift gas stream of nitrogen enters the riser from the bottom to lift the catalyst particles up the riser before the hot particles are mixed with the feed oil. The feed oil stream is injected from the lower left side of the riser, forming a spray of droplets in the riser.

The mixing process includes the combined effects of interfacial interactions (momentum and heat transfer between phases), flow convection and turbulent diffusion of gas, oil droplets (solid circles), and catalyst particles particles (hollow circles). During the mixing process, the heat carried by the catalyst particles is transferred to the gas and the oil droplets. Under the typical operating conditions of an FCC riser reactor, the catalyst temperature is much higher than the boiling point of the feed oil. Consequently, the vaporization process is dominated and characterized by the heat transfer rate to oil droplets.

During the vaporization process, a liquid oil droplet (dark colored circle) is releasing oil vapor (light colored ellipse) in the presence of a hot catalyst particle. Following the vaporization process, the cracking process takes place. Four lumps including feed oil, gasoline (or light oil), dry gas, and coke are shown in Figure 2. Feed oil vapor (larger ellipse) contacts a catalyst particle, and the cracking reactions on the catalyst surface convert the feed oil vapor to light oil vapor and dry gas (smaller ellipses). Coke (dark circle) is a by-product of the process. Interfacial drag, heat transfer, and droplet vaporization processes have an impact on the performance of a riser reactor. This impact becomes very large for short riser residence times and for commercial scale risers.

CFD Application to FCC Systems

Over the course of process improvement, cracking reaction time in an FCC unit has been reduced from minutes to seconds. The reduction of reaction time greatly improves the efficiency of the FCC units but the hydrodynamic effects of feed injection and mixing have a much greater impact on cracking processes and product yields when reactor residence time becomes small or the riser aspect ratio is relatively small as in commercial scale units when compared to pilot scale units. In reviewing the history of FCC process improvement, Bienstock et al. (1993) indicated that fundamental understanding of the hydrodynamics and heat transfer in the injection zone of a riser is critical to the development of a new high performance FCC unit. The refinery industry has identified the CFD capability as a critical area for the advancement of the FCC technology.

The simulation of the flow field in a FCC riser reactor is extremely complex. It involves three phases (gas, liquid, and solid), multiple gas species, turbulent mixing, heat transfer, mass transfer, and cracking reactions. Several computer codes have been developed in the past for modeling portions of the kinetics or hydrodynamic processes in riser reactors. Weekman and Nace (1970) developed a 3-lump (feed oil, gasoline, and dry gas) cracking kinetic model to predict gasoline production in an FCC unit. Dave and et al. (1993) expanded the model by introducing an additional coke lump in the simulation to predict the coking of the heavy oil cracking processes. Pita and Sundaresan (1991) first used a CFD code for a riser flow simulation. The simulation investigated the gas-particle flow patterns in a vertical riser. Later, Theologos and Markatos (1993) incorporated Weekman's 3-lump kinetic model in a commercial CFD code for their FCC flow simulation. The simulation includes cracking reactions in a two-phase (gas and particle) flow. In an attempt to simulate a more realistic FCC riser flow, Chang and et al. (1995) developed an ICRKFLO code that includes all three phases (gas, particle and droplet) of the FCC flow. The code also includes models that govern heat carrier particle transport, feed oil droplet transport, vaporization of the feed oil droplets, cracking of the feed oil, and coke formation and deposition on heat carrier particles.

The ICRKFLO code was developed at Angonne National laboratory by expanding and enhancing an existing two-phase reacting flow computer code. The computer code was originally a general computational fluid dynamics code for two-phase flows (gas/liquid or gas/solid). It had been successfully used to predict characteristics of two-phase reacting flows in coal-fired combustors (Chang and Lottes, 1993), air-breathing jet engines (Zhou and Chiu, 1983), and internal combustion engines (Chang and Wang, 1987). For simulating a thermal cracking riser flow, new features were added to the code to model the complex interactions in a three-phase flow field containing a carrier gas and droplet and particulate condensed phases. The newly developed computer code was used to predict flow characteristics of various risers. In particular, interactions of multi-phase hydrodynamics, droplet evaporation, and chemical kinetics was investigated and will be presented in the following sections in detail.

THEORETICAL APPROACH

ICRKFLO uses a combination of fundamental governing conservation equations of physics and models for interphase exchange that use both fundamental physics and engineering correlations to characterize the interphase exchange processes to simulate the riser flow.

Governing Equations

The ICRKFLO code solves the governing equations for a flow system containing three phases: gaseous species, liquid droplets, and solid particles. The governing conservation equations for mass, momentum, enthalpy, and species are expressed as elliptic-type partial differential equations. For convenience in numerical formulation, the governing transport/conservation equations for the gas phase are put in a common form for the thermal cracking riser flow environment., Eq.(1):

$$\frac{\partial}{\partial x}\left(\theta\rho u\xi - \Gamma_\xi \frac{\partial \xi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\theta\rho v\xi - \Gamma_\xi \frac{\partial \xi}{\partial y}\right) = S_\xi \qquad (1)$$

in which ξ is a general flow property, x and y are coordinates, θ is gas volume fraction, u, v are velocity components, Γ is effective diffusivity, and S_ξ is the sum of source terms.

The liquid and particle phase formulations are based on an Eulerian model. In this formulation, the liquid or particle-phase state of the flow is governed by the elliptic partial differential transport equations of fluid mechanics. Liquid droplets in a spray have a spectrum of droplet sizes. To compute droplet properties in a droplet size distribution, droplets need to be divided into size groups, and the governing equations are solved for each size group.

Experiments show that droplets have a non-uniform size distribution in a spray. For a typical spray, a droplet number density distribution function $g_c(r)$ is defined as Eq.(2).

$$g_c(r) = br^c \exp(-ar^d) \qquad (2)$$

The droplet number density distribution function employs 4 parameters a, b, c, and d. Once empirical parameters c and d are set, parameters a and b can be expressed in terms of the total droplet number density n_o and the volume mean radius r_m. The droplet number density distribution function usually used in the ICRKFLO code is expressed in a dimensionless form, Eq. (3).

$$\frac{g_c r_m}{n_o} = 5.2(r/r_m)^4 \exp[-1.14(r/r_m)^4] \qquad (3)$$

Figure 3 shows the droplet number density distribution function represented by a solid line. It is a typical bell-shaped distribution. As the droplet radius increases, the number density function increases from zero at zero radius to a peak ($g = 1.66\, n_o/r_m$) at a radius $r = 0.97\, r_m$ and decreases afterward. Empirical constants c and d are used to adjust the width of the distribution for matching experimental data, when data is available.

In numerical calculations, the droplet size distribution function is simplified by lumping droplets into size groups. A 5-lump droplet number density distribution is shown in Figure 3, represented by the dashed line rectangles. The arrows indicate the effects of the vaporization process. Vaporization causes droplets to shift from larger to smaller size groups at a computed rate and also results in deposition of vapor from the droplets into the gas phase.

Similar to the gas phase formulation, the governing transport equations for the liquid and particle phases are put in a common form, Eq.(4).

$$\frac{\partial}{\partial x}\left(n_k u_{c,k}\xi - \Gamma_\xi \frac{\partial n_k \xi}{\partial x}\right) + \frac{\partial}{\partial y}\left(n_k v_{c,k}\xi - \Gamma_\xi \frac{\partial n_k \xi}{\partial y}\right) = S_\xi \qquad (4)$$

in which n_k is the droplet or particle number density of k^{th} size group, $u_{c,k}$ and $v_{c,k}$ are droplet or particle velocity components of k^{th} size

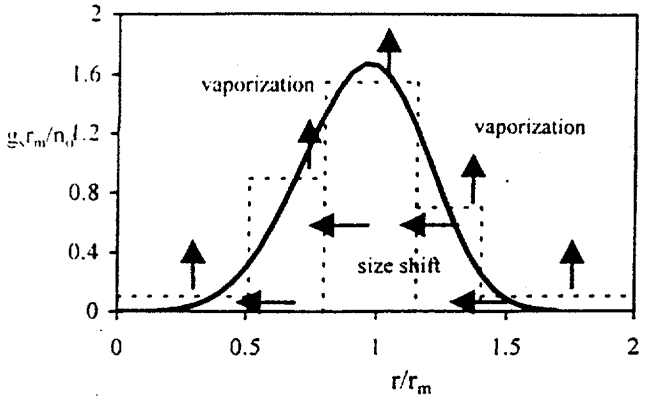


Figure 3 Droplet Number Density Distribution Function

group in the x and y direction respectively, Γ is droplet or particle diffusivity, and S_ξ is the sum of source terms. The formulation and computer code allow for a size spectrum of both droplets and particles, however, in this study only one size of group of particles was used although a size spectrum of five droplet size groups was used. The decision to use mono-sized particles was made to conserve computer resources, and it is considered a reasonable first step in developing a three-phase reacting flow model with heat, momentum, and mass transfer between all three phases. A size spectrum of five droplet size groups was used because a droplet size spectrum is a required component of the vaporization model, which shifts the spectrum toward the smaller droplet sizes in order to balance mass in the vaporization mass transfer between the droplet and gas phase.

Phenomenological Models

Phenomenological models are used to define the diffusivity and source terms of the governing equations. ICRKFLO uses 6 major phenomenological models: a lumped integral (as opposed to differential) reaction model, a coke interphase transfer and transport model, a two-parameter turbulence model modified for multiphase flows, an interfacial drag and heat transfer model, a droplet/particle turbulent dispersion model, and a droplet evaporation model. The primary interfacial transfer models for momentum, heat, and mass that greatly influence development of flow patterns and cracking processes in an FCC riser are presented in the following sections.

Interfacial Drag Model. Empirical equations are commonly used to correlate the drag force with the slip velocity (the velocity difference between the gas and solid phases, with components u_δ, v_δ). Drag force is a vector defined by two orthogonal components in x and y directions, which have the similar formulation. For a single droplet or particle in the gas, the x-direction drag force ($F_{d,x}$) of gas exerted on the droplet or particle can be expressed as Eq.(5).

$$F_{d,x} = \frac{1}{2}\rho\,|\,u_\delta\,|\,u_\delta \pi r^2 C_d \tag{5}$$

The empirical drag coefficient, C_d, is given in Eq.(6). It includes two major effects, one is viscous, based on a correlation using a Reynolds number Re_δ, Eq.(7), and the other is the evaporation effect represented by a transfer number B, Eq.(8). In Eq.(8), L is the latent heat of a droplet and T_b is the phase change temperature of a droplet.

$$C_d = \frac{24}{Re_\delta}\frac{(1+0.15\,Re_\delta^{0.687})}{1+B} \tag{6}$$

$$Re_\delta = \frac{2\rho\,|\,u_\delta\,|}{\mu} \tag{7}$$

$$B = \begin{cases} C_p(T-T_b)/L & \text{evaporation} \\ 0 & \text{otherwise} \end{cases} \tag{8}$$

Interfacial Heat Transfer Model. Empirical equations are also used to correlate the interfacial heat transfer with the slip velocity. For a single particle or droplet in the gas, the heat transfer between the gas and the particle or droplet, when droplets are not vaporizing, is expressed as,

$$q_c = 2\pi r Nu_\delta (T - T_c)\delta(T_b) \tag{9}$$

in which, λ is thermal conductivity of the gas, Nu_δ is an empirical Nusselt formula, Eq.(10), and $\delta(T_b)$ is a step function, which changes from one to zero when a droplet or particle reaches its phase change temperature. In Eq.(11), Sc is the Schmidt number, and D is the mass diffusivity of a species. After the droplet temperature reaches the boiling temperature, further heat transfer from the gas to particles goes into droplet evaporation. In this case, the step function $\delta(T_b)$ makes q_c zero for T_c equal to T_b.

$$Nu_\delta = \begin{cases} 1+0.276\,Re_\delta^{1/2}\,Sc^{1/3} & \text{evaporation} \\ 2+0.654\,Re_\delta^{1/2}\,Sc^{1/2} & \text{otherwise} \end{cases} \tag{10}$$

$$Sc = \frac{\mu}{\rho D} \tag{11}$$

Droplet Evaporation Model. The source term in the gas continuity equation is the evaporation rate of the droplets per unit volume. In ICRKFLO code, the droplet evaporation model is based on the fundamental physics of stationary single droplet evaporation and then modified for large groups of droplets in a convective environment using correlations. Direct interactions between droplets (collisions) are ignored, however, droplets do interact with each other indirectly through their effects on the gas phase. Because gas phase properties, such as specific heat, heat transfer coefficients, etc. may be functions of local gas phase properties, different size droplets will respond differently to varying local conditions. The evaporation model is characterized briefly as follows. The classical solution giving the droplet evaporation rate for a single stationary droplet is (Williams, 1985).

$$\left(\frac{dm}{dt}\right)_{stat} = 4\pi r(\lambda / C_p)\ln(1 + B) \qquad (12)$$

A correction for the convection effect, sometimes referred to as the Ranz-Marshall model (Aggarwal, et al., 1984) can be applied to the stationary solution Eq.(12) to yield an empirical correlation for vaporization in a flow. The correction adds a Nusselt number Nu_δ to the stationary solution.

$$\left(\frac{dm}{dt}\right)_{conv} = 4\pi r(\lambda / C_p)\ln(1 + B)Nu_\delta \qquad (13)$$

The total evaporation rate at a point per unit volume of physical space is determined by integrating the product of single droplet evaporation rate and the spray distribution function over the droplet size spectrum.

Lumped Integral Reaction Model. ICRKFLO uses a lumped cracking reaction model, based on lumped kinetics modeling works by Weekman and Nace (1970) and by Dave et al. (1993) and a new integral reacting-flow time-scale-conversion method (Chang and Lottes, 1993), for the simulation of FCC riser flows. The 4-lump kinetic model considers four lumped oil components in two cracking reactions. The four lumps include feed oil with higher boiling point, light oil with lower boiling point, dry gas including oil vapor of carbon number C_5 and below, and coke as a byproduct of the cracking reaction. The cut-off boiling temperature between feed and light oil lumps is chosen according to the feed stock and riser operating conditions. Two cracking reactions include: (a) one that converts feed oil to light oil, dry gas, and coke; and (b) another that converts light oil to dry gas and coke. Reaction rates of these reactions are expressed respectively in Arrhenius formula.

Many reacting flow calculations suffer severe numerical stiffness problems due to the difference of the flow and the reaction time scales. A time scale bridging integral as opposed to differential approach was developed to overcome these numerical problems. The integral approach converts the reaction time scale used in the above derivation to the flow time scale of the hydrodynamic calculations (Chang et al., 1996).

Subspecies Formation And Transport Computation

The governing equations with incorporated phenomenological models developed in the previous sections are solved to obtain the flow properties and pattern of an FCC riser flow field. The local flow properties such as velocity, temperature, catalyst particle volume fraction, oil evaporation rate, and major species concentrations are calculated. The major gaseous species in the flow calculation include feed oil, light oil, dry gas, and inert gas. However, within these species lumps exist a very large number of oil species produced from numerous kinetic reactions in the riser. These species are not included in the flow calculation because of numerical stiffness problems. The formation and transport of the oil species have a strong impact on the flow field because of the significant density changes between feed oil and products. This density change effect is represented by the 4-lump model in the flow calculation. Assuming the 4-lump flow field solution as adequate to account for the density change effect, one can de-couple the solution routines of the transport equations of individual species or large numbers of groups of lumped species from the flow calculation and solve the transport equations on a pre-determined flow field. This second stage of reaction and transport computation is referred to as a subspecies computation. Free from the interactions of the pressure and velocity fluctuations, the calculation of the de-coupled species transport equations becomes very stable numerically. This technique is the essence of the hybrid approach to solving governing equations for a complex multi-phase reacting flow field along with solving for the local reaction kinetics and transport equations of a large number of subspecies or lumped subspecies groups, simply called lumps. The details are described in Chang et al. (1997)

NUMERICAL SCHEME

Computational Grid and Numerical Convergence

ICRKFLO was used to investigate flow characteristics in an FCC riser. In order to conserve computational time and still provide adequately accurate results, a grid sensitivity study was conducted to choose a grid system that uses as few cells as possible (approximately 1000 scalar cells) while yielding stable numerical results to approximately three significant decimal digits upon further grid refinement.

Obtaining a converged solution of a set of non-linear particle differential equations is always difficult. In the ICRKFLO computer code, a calculation is considered a converged solution if the local and global mass balances of the three phases are smaller than a set of pre-determined criteria. For these simulations, convergence criteria defined by average mass residual of all computational cells are 10^{-10} for gas phase and 10^{-8} for both liquid and solid phases. Generally in this application, with reasonable boundary conditions, a converged solution can be obtained in about 3000 numerical iterations. On a Pentium 90 personal computer with 16 megabytes of random access memory, using a 32-bit FORTRAN compiler, this computation takes about 4 hours.

RESULTS AND DISCUSSION

Code Validation

The developed ICRKFLO computer code has been validated by comparison between computational results and experimental data obtained by an industrial member of a cooperative research agreement. Comparison of ICRKFLO computational results with data in the open literature have also been done whenever possible. The predicted product yields, pressure, temperature, and other flow properties showed good agreement with experimental data (Chang et al. 1995, 1996, 1997).

Riser Flow Patterns

Numerical simulations were performed for various FCC riser flows. Typical flow patterns in the mixing zone for a pilot scale riser are displayed in Figures 4 (a), (b), and (c). A grayscale key is plotted on the left side of the property figure indicating the corresponding shade for the property value. Riser dimensions are proprietary shade for the property value. Riser dimensions are proprietary information of a petroleum company and will not be discussed here. All the numbers are normalized. The gas velocity, temperature, density, pressure, and particle number density are shown in Figure 4(a). The velocity field is plotted as velocity vectors. The vector length is proportional to velocity magnitude. The gas velocity field in the mixing zone of the riser is highly influenced by the addition of new mass in the gas phase from vaporizing oil droplets. The vaporizing droplets cause expansion of the gas and therefore an increase in gas velocity. The patterns of gas temperature and density distributions correspond to the patterns of droplet and particle number distributions in the mixing zone. In the locations where particle number density is higher, the gas temperature is higher due to heat transfer between the hot particles and gas. In the locations where droplet number density is higher, the gas temperature is lower due to vaporization. The catalyst particles are injected from the right side near the bottom of the riser. Some of them are accumulated in the left corner and some of them are pushed by the oil vapor to the right side along the riser.

Figure 4(b) shows the droplet number density with five different droplet sizes. It is clear that almost all the droplets are vaporized in the mixing zone. The droplets with smaller size react more quickly to drag effects and tend to follow the gas flow. They are also dispersed more rapidly by turbulence in the gas phase therefore spread more across the riser while the larger droplets are pushed to the left side of the riser through interaction with the catalyst/gas mixture flow near its inlet. As shown in Figure 4(c), a large amount of evaporation occurs in the left corner because of large droplet number density. Once the feed oil is vaporized, cracking reactions take place to convert feed oil into light oil and dry gas. Coke is produced during cracking. All these figures show that the flow pattern is strongly affected by the interactions of multi-phase hydrodynamics, droplet evaporation, and chemical kinetics in FCC riser reactors.

Effects Of Droplet Vaporization On Flow Patterns

The flow patterns in Figure 4 indicated strong effects of the droplet distribution. These effects are further demonstrated in Figures 5 and 6 including the distributions of mid-size droplet number density, particle number density, and gas temperatures. The riser dimension and input conditions are the same, and there is no cracking reaction for both figures. The only difference is that droplets are not vaporized in Figure 5 but vaporized in Figure 6. The droplet number density, particle number density, and gas temperature field are significantly different with droplet vaporization from the case without vaporization. Consequently, cold flow parametric mixing studies with no vaporization (no mass transfer from liquid to gas phase) cannot be used as a basis to predict efficiency of FCC cracking reactions and their products.

Some aspects of the interaction of the vaporization process with the general flow hydrodynamics and heat transfer can be seen more clearly when a computational experiment is run where only mono-sized droplets of the largest size are injected at the droplet/lift gas inlet. In this case smaller droplets do not enter the system at the inlet, but exist in the system only as a result of droplet shrinkage during the vaporization process. Some of the primary results of such a computation for reacting flow in a pilot scale riser are shown in Figure 7. The lower 1/5 of the riser is shown in the figure. Several observations can be made about the interrelations between the feed oil droplet and catalyst flow and the vaporization process. The initial catalyst distribution is asymmetric over the cross section because catalyst particles come in from one side only. However in a pilot scale system the cross section distribution of catalyst tends to even out fairly quickly due to dispersion of particles through interaction with gas phase turbulence as indicated in Figure 7 (a). Large droplets are less affected by drag than either smaller droplets or the smaller catalyst particles, and therefore once the cross section distribution of large droplets is established, it tends to persist as large droplets travel up the riser as shown in Figure 7 (b). Momentum exchange between large numbers of catalyst particles and lift gas and feed oil vapor induces a gas flow to the left, which is also transferred to large droplets and causes a high concentration of large droplets on the left side of the tube. Nearly all large droplets are gone due to vaporization by the time they have traveled about 1/7 the tube length. As seen in Figure 7 (c) no droplets of the smallest size group exist at the bottom of the riser tube. First, there is a preheating delay before the large droplets injected at the droplet inlet begin to vaporize, then there is a delay time while large droplets vaporize and shrink into the smallest size group before any significant number of small droplets appear on the number density plot. The smallest droplets are much more affected by drag and turbulent dispersion through interaction with the gas phase. Therefore, although there is a higher concentration of small droplets on the left side of the riser as expected from the distribution of larger droplets from which they come, turbulent dispersion makes their cross section distribution much more uniform than that of the largest droplets. It is worth noting that the smallest droplet group has a number density maximum located about at 1/10 the distance up the riser. Two factors cause number densities in the smallest group to drop after this region of maximum number density. First, the smallest droplets disappear because they vaporize completely. Second, as feed oil vapor is deposited into the gas phase due to vaporization, the acceleration caused by this expansion also accelerates and spreads out the droplets, causing the number density to drop. Finally it should be noted that a few percent of the original feed oil mass injected still exists in the presence of small droplets as far as 2/3 up the length of the riser tube (not shown in the Figure). Therefore, clearly reaction models for the feed oil vapor must either explicitly or implicitly take into account the vaporization delay of the feed oil.

Parametric Effects On FCC Product Yields

The FCC process is used to convert feed oil into more valuable light products. The product yields are affected by operating conditions including feed oil droplet size, catalyst to oil ratio, and riser exit temperature, and others. To demonstrate such parametric effects, gasoline yield, which is a very important product, will be used as one of the examples.

Figure 8 shows the effects of mean droplet size, catalyst to oil ratio, and the riser exit temperature on the Gasoline yield. All the numbers are normalized. As shown in the figure, the gasoline yield increases when droplet size decreases in the range tested. There is an optimum condition for gasoline product when varying the catalyst to oil ratio or the riser exit temperature. These results indicate that a desired product can be produced by selecting proper operating conditions. It is expected that CFD can be a useful tool to help achieving this goal.

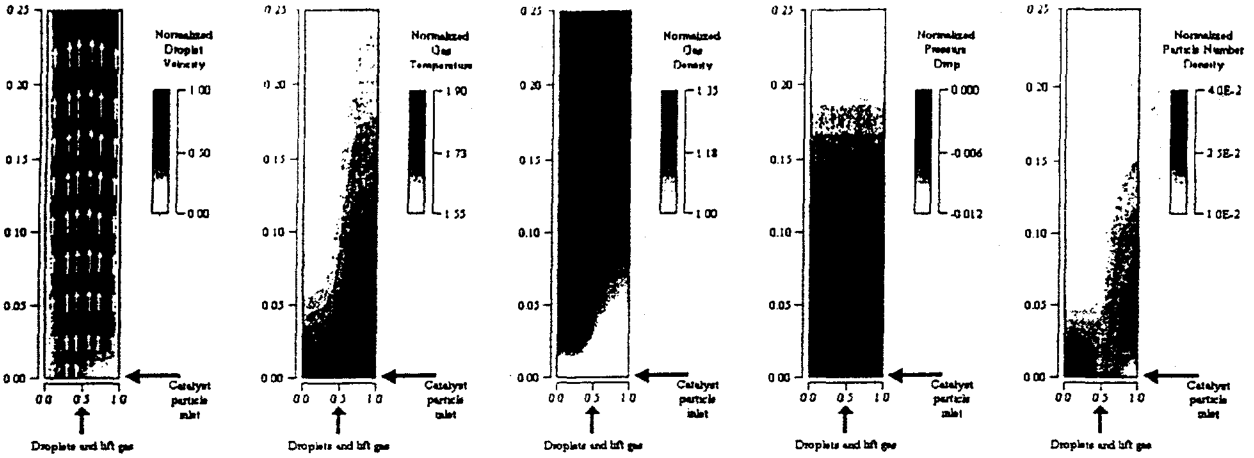


Fig. 4 (a) FCC Riser Flow Pattern

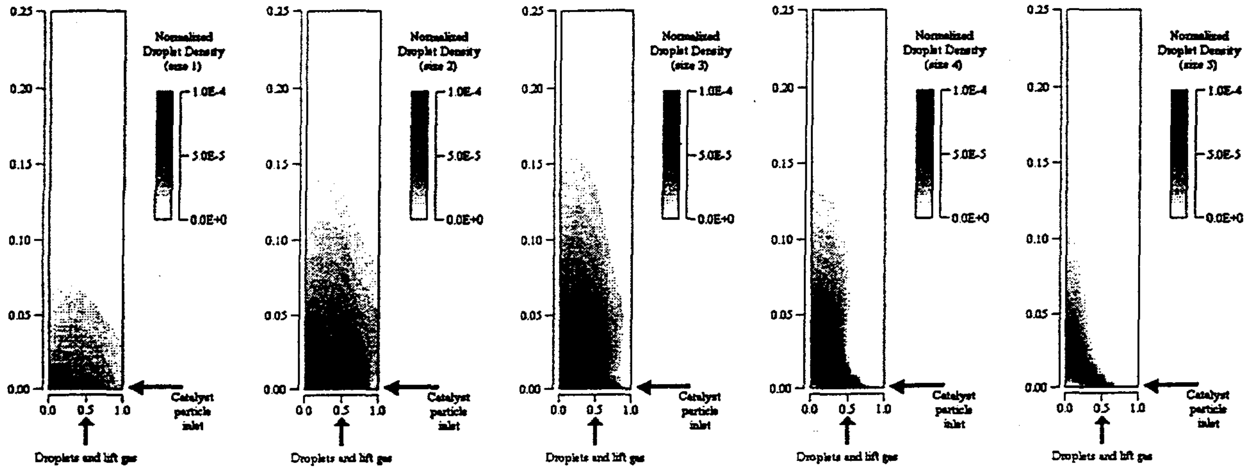


Fig. 4 (b) FCC Riser Flow Pattern

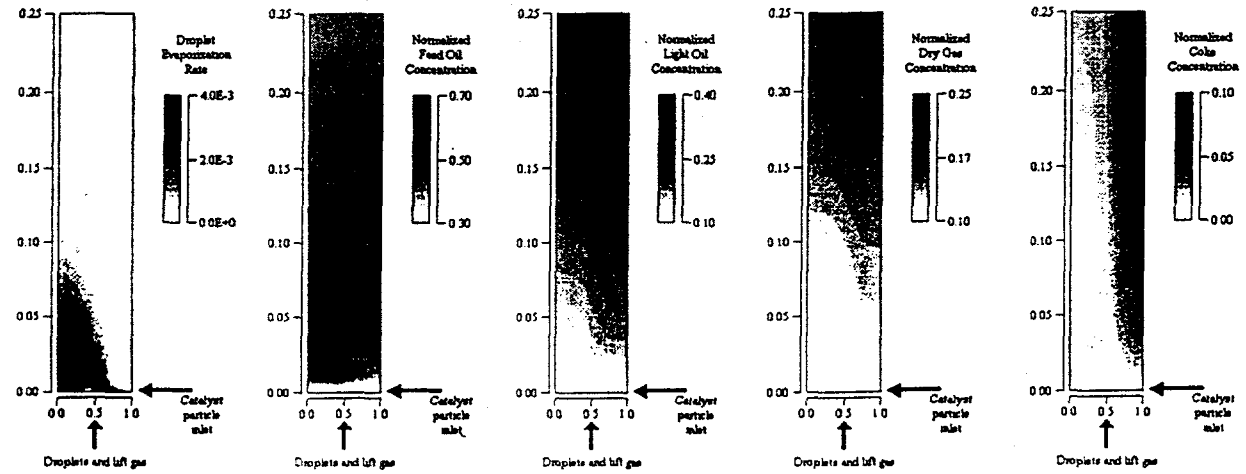


Fig. 4 (c) FCC Riser Flow Pattern

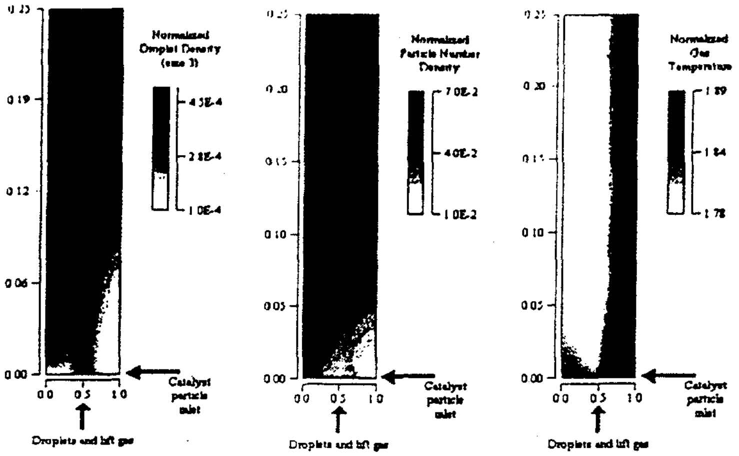


Fig. 5 FCC Riser Flow without Droplet Evaporation

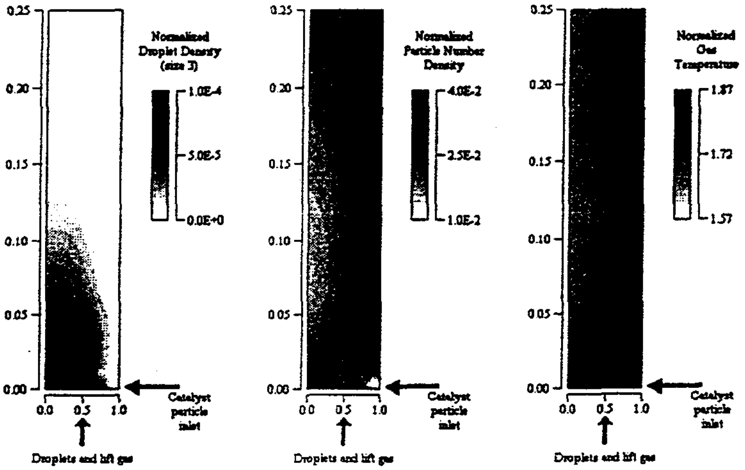
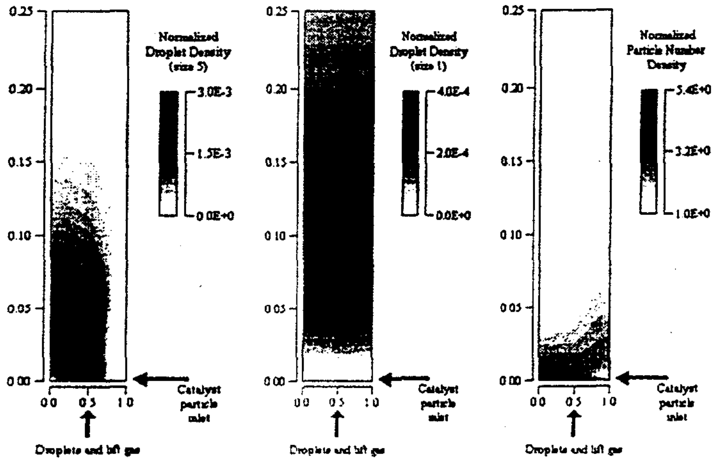


Fig 6 FCC Riser Flow with Droplet Evaporation



(a) Catalyst (b) Largest droplets (c) Smallest droplets

Figure 7 Catalyst particle and droplet distributions for mono-sized large droplet injection

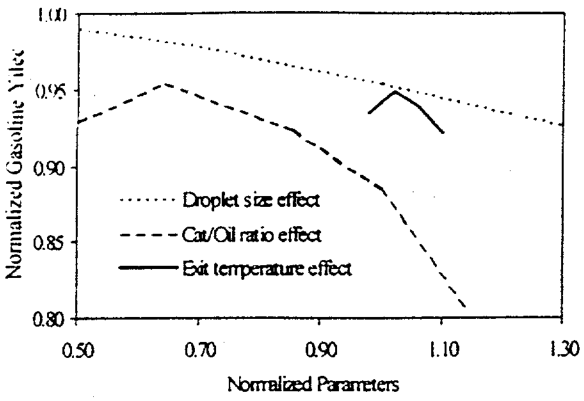


Figure 8 Parametric Effects on Gasoline Yields

CONCLUSIONS

Argonne National Laboratory has developed a copyrighted code ICRKFLO for the development of advanced multi-phase reacting flow systems. It employs a hybrid hydrodynamic-chemical kinetic coupling technique and has been successfully applied to the simulation of petroleum fluid catalytic cracking (FCC) risers. ICRKFLO solves for flow properties of all three phases (gas, liquid, and solid) locally in an FCC riser flow, with models governing the transport of catalyst particles and feed oil droplets, the vaporization of the feed oil droplets, the cracking of the oil vapor, and the formation and deposition of coke on particles. The code was validated by comparing computational results with experimental data for various cases.

The validated code was used to study the interactions of multi-phase hydrodynamics, droplet evaporation, and chemical kinetics in a pilot-scale FCC riser reactor. Results of this study showed that the hydrodynamics of mixing among the phases and interphase exchange rates in the entry region (or mixing zone) of the riser play an important role in the initial development of the flow and cracking processes within the riser. The mixing zone performance becomes even more important on commercial scale units because of the change in aspect ratio of the riser with consequent large change in internal flow patterns. Decreasing the residence time in a riser also magnifies the effects of mixing on performance. The ICRKFLO computer code can be a very useful tool to use in optimizing riser performance for specific operating conditions and performance goals, such as maximizing valuable product yields.

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