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MULTI-PHASE REACTING FLOW IN A BENT REACTOR*

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A SECTIONAL COUPLING APPROACH FOR THE SIMULATION OF MULTI-PHASE REACTING FLOW IN A BENT REACTOR*

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ABSTRACT

Multi-phase reacting flows of a bent fluidized catalytic cracking (FCC) reactor have been simulated using the ICRKFLO code. A new sectional coupling approach has been developed to handle the complex geometry, which divides the bent reactor into two sections and computations are performed for the two sections successively. The computational results show that the ICRKFLO incorporated with the new sectional coupling approach can predict product yields very well compared with experimental data and can be used to identify critical processes and parameters which may be modified to improve the quality and quantity of the FCC products.

INTRODUCTION

The use of computational fluid dynamics (CFD) to enhance the understanding of hydrodynamics, thermodynamics, and chemical kinetics of a reacting flow system is increasing. For the past 20 years, CFD codes highly evolved with the advancement in both numerical techniques and computer hardware. CFD applications were extended from simple laboratory-type to complex industrial-type flow systems. Computer simulation is regarded as an effective and cost-saving tool to further improve the performance of flow systems.

One of the CFD applications is the petroleum/catalyst flow in a fluidized catalytic cracking (FCC) reactor. The commercial-scale FCC system was first introduced in early 1940’s. Since

then, the FCC process has been constantly improved and become the key conversion process in
the modern refinery industry. Over the course of process improvement, cracking reaction time of
an FCC unit becomes much shorter and hydrodynamic effects on cracking processes becomes
more apparent. In reviewing the history of FCC process improvement (Bienstock et al. 1993),
Bienstock and et al. suggested that fundamental understanding of the hydrodynamics and heat
transfer in the injection zone and riser is critical to the development of a new high performance
FCC unit. The improvement of FCC performance increases the compatibility of the refinery
industry and also reduces pollutant emissions to the environment. A computer code based on
both hydrodynamics and kinetics can be a powerful tool to improve the FCC performance.

Weekman and Nace (1970) used a three-lump cracking kinetic model to predict gasoline
production in an FCC unit. The three lumps are the oil, the gasoline, and the dry gas. Later,
Dave et al. (1993) expanded the model and included an additional coke lump in the simulation to
predict the coking of the heavy oil cracking processes. Both models dealt with the kinetic
process only. Pita and Sundaresan (1991) developed a computer model to investigate the flow of
lumped kinetic model into a computational fluid dynamics (CFD) calculation for an FCC riser
reactor. The flow system included gas and particle phases, and the cracking reactions involved
three lumped species: oil, gasoline, and dry gas.

With extensive computational simulation experience, Argonne National Laboratory has
developed a new computer code for the simulation of a three-phase (gas, liquid, and solid) flow
in FCC riser reactors. The computer code referred to as ICRKFLO uses a sectional coupling,
time integral approach to handle cracking flows, including heat transfer between solid, liquid,
and gas; vaporization of the oil droplets; oil cracking; and coke formation. The time integral
approach couples hydrodynamic and kinetic processes in a numerical calculation and prevents
the calculation from becoming numerically unstable.

The ICRKFLO code was derived from an existing integral reacting flow computer code -
ICOMFLO (Lottes and Chang, 1993). ICOMFLO solves general conservation equations of
mass, momentum, and energy numerically for two-phase flows (gas/liquid or gas/solid). It has
been successfully used to predict characteristics of multiphase 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). When experimental data or test results were available, the predictions by the code generally showed good agreement with the measurements (Lottes and Chang, 1991; Chang et al., 1993). The new ICRKFLO code adds a few features to the ICOMFLO code. The new features include (1) calculation of three-phase (gas, liquid, and solid) flow, (2) an integral kinetic model for heavy oil cracking, and (3) formation and transportation of coke, (4) the capability to treat a complex geometry.

A sectional coupling approach has been developed for the flow simulation of bent FCC reactors. The ICRKFLO code with the sectional coupling approach was used to predict flow characteristics and product yields of bent FCC riser reactors. This paper presents the development of the approach and results of the calculation.

THEORETICAL APPROACH

Figure 1 shows a generalized thermal cracker unit that includes three major components: a riser reactor, a stripper, and a regenerator. Oil is fed into the riser reactor, where it is mixed and heated by regenerated particles to induce cracking. The cracking processes produce various fuel products and coke. The coke and some oil products are deposited on particle surfaces. A steam stripper separates particles and oil products for further processing. The spent particles covered with coke are sent to the regenerator to burn off the coke with air. The hot regenerated particles are then recycled back to the riser reactor. For this study, only the riser reactor is modeled and analyzed.

A riser reactor can have a complex geometry. The oil injector arrangement of a riser is 3-dimensional in nature and its long tube usually has bends and/or area changes (expansion or reduction). Figure 2 shows a few examples: (a) inverse L bend, (b) inverse U bend, (c) J bend, and (d) area expansion with four oil injectors. ICRKFLO uses a sectional-coupling approach and a new triangular blocked-cell technique to handle the complex riser geometry.
Sectional Coupling Approach

A sectional coupling approach was developed for the flow simulation of bend reactors. The approach consists of 2 major steps: (1) straight tube sections are selected to represent a riser, and (2) flow field of each section is calculated using a CFD code, e.g., ICRKFLO, in a sequential order.

Figure 3 shows the sectional representation for those riser reactors shown in Fig. 2. Two straight tube sections A and B are used to represent the inverse L bend riser (Fig. 3a); four
sections for the inverse U bend riser (Fig. 3b); 2 sections for the J bend riser (Fig. 3c), and 2 sections for the riser of 4 injectors (Fig. 3d). A flow field calculation depends on the boundary conditions including inlet and exit. In most CFD calculations, the inlet conditions are specified while the exit conditions are assumed. An assumption of fully developed flow conditions at the exit has been adopted by many people. For the sectional coupling approach, the inlet flow conditions of a section are either the actual inlet flow conditions or the computed values of the previous section. But the popular fully developed flow conditions are generally unacceptable for the exit conditions. The exit flow conditions of a section are adjusted during the iteration routine of the flow field calculation so that global mass balances for all phases can be maintained.

Figure 3. Sectional Representation of Riser Reactors

Triangular Blocked Cell Technique

Not all grid cells have to be included in the CFD solution procedure, some can be marked as blocked. A blocked cell is impermeable to fluid flow and can be used to construct irregular boundary surface. Figure 4 shows an example of computational grid using both regular flow cells and rectangular blocked cells (shaded cells) to represent a flow field with a convergent passage. Rectangular blocked cells are easy to implement but can create stair step type of corner cells as shown in Fig. 4. Multi-phase flow calculations using this approach tend to show
unrealistic particle pile-up in the corner cells and sometimes the particle pile-up leads to severe numerical instability.

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Figure 4. Irregular Flow Field Represented by Rectangular Blocked-Cells

A new triangular blocked-cell approach was developed to alleviate the numerical instability problem by fitting a diagonal or curved boundary contour more smoothly. Formulation of a triangular blocked-cell is similar to that of a flow cell. The major difference is that the flow volume and the property diffusivity length of a triangular blocked-cell are only half of those of a regular flow cell. Slip or non-slip conditions are assumed for the liquid and solid phases on the contoured wall. Figure 5 shows the same convergent flow field as shown in Fig. 4 but it is represented by using flow cells, and both rectangular and triangular blocked-cells. Calculations were made for solving the convergent flow field using the new triangular blocked-cell approach and the traditional rectangular blocked-cell approach. Some calculations using the rectangular blocked-cell approach experienced severe numerical instability because the particles pile up in corner cells. However for the same problem, the triangular blocked-cell approach achieved a stable convergent solution.
Governing Equations

The ICRKFLO code solves conservation equations of general flow properties for three phases: gaseous species, liquid droplets, and solid particles. General conservation laws, expressed by elliptic-type partial differential equations, are used in conjunction with rate equations governing the mass, momentum, enthalpy, and species for a three-phase flow with gas species, liquid droplets, and solid particles.

Figure 5. Irregular Flow Field Represented by Rectangular and Triangular Blocked-Cells

The gas-phase governing equations include conservation of momentum, energy, and mass, and transport of turbulence parameters, with separate equations for the state of an ideal gas and gaseous species conservation. The liquid-phase formulation is based on an Eulerian model. Liquid droplets of a spray plume have a spectrum of sizes. To compute properties of liquid droplets with a size spectrum, the droplets are divided into size groups, which is just a discretization of the droplet size spectrum. For each size group, droplet properties are determined by solving the governing equations. The governing equations include conservation of droplet number density, momentum, and energy. The solid-phase state of the flow is also based on the Eulerian model and therefore governed by the equations of conservation of particle number density, momentum, and energy for each size group. An additional equation for coke
transport and deposition on particles is also included. The governing equations contain source terms for interphase and intraphase property exchange rates.

All the governing transport and conservation equations for three phases are elliptic-type partial differential equations. For convenience in numerical formulation, they are arranged in a common form. For gas phase, this formulation is given as:

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

(1)

in which $\xi$ is a general flow property, $x$ and $y$ are coordinates, $\theta$ is gas volume fraction, $u$ and $v$ are velocity components, $\Gamma$ is effective diffusivity (calculated from both laminar and turbulent viscosities and an appropriate nondimensional scaling factor), and $S_\xi$ is the sum of source terms.

For droplet and solid phases, the formulation is given as:

$$\frac{\partial}{\partial x} \left( n_k u_{d,k} \xi - \Gamma \frac{\partial n_k \xi}{\partial x} \right) + \frac{\partial}{\partial y} \left( n_k v_{d,k} \xi - \Gamma \frac{\partial n_k \xi}{\partial y} \right) = S_\xi$$

(2)

in which $n_k$ is droplet or particle number density of kth size group, $u_{d,k}$ and $v_{d,k}$ are droplet or particle velocity components of kth size group in the $x$ and $y$ direction respectively, $\Gamma$ is droplet or particle diffusivity resulting from interaction with turbulence in the gas phase, and $S_\xi$ is the sum of source terms.

**Phenomenological Models**

Phenomenological models are used to characterize multi-phase cracking flow in the FCC unit, including interfacial drag and heat transfer, droplet dispersion and evaporation, coke formation and transport, two-parameter multi-phase turbulence, and lumped integral reaction models. Oil is injected in a spray into the FCC reactor for cracking. The droplet dispersion and evaporation model divides the size distribution of oil droplets into a number of size groups, calculates the evaporation rates of the droplets, and translates the evaporation rates into a droplet size distribution shift. Hot catalyst particles transfer heat to oil droplets for vaporization. An interfacial model uses empirical correlations to calculate interfacial momentum and energy transfer. Coke is a by-product of the FCC cracking processes. It is formed during the cracking reactions when the heavier oil is converted to lighter products and deposited on the surface of
catalyst particles. A coke transport model was developed to characterize the formation of the coke and its transportation in the flow. The commonly used k-e turbulence model was modified to include the effects of interaction of both the droplet and particle phases with the gas phase turbulence.

**Lumped Integral Reaction Model**

A lumped integral reaction model was developed for the oil cracking processes in the FCC unit using a time integral approach. The time integral approach bridges the large time scale difference between flow time and reaction time that may occur in some local regions of the flow field where wide variation in process time scales can lead to numerical instabilities or poor convergence of the computation. The kinetic portion of the model is developed based on the works of Dave et al. (1993): 2 cracking reactions and 4 lumped species. The 4 lumped species are (1) the feed oil A₁ for oil species with boiling point ranging from 344°C (650°F) and above, (2) the light oil A₂ for those ranging from C₅-344°C (650°F), (3) dry gas A₃ for C₄-, and (4) coke A₄. The 2 cracking reactions are (a) conversion from feed oil to light oil, dry gas, and coke and (b) conversion from light oil to dry gas and coke. Coke produced in the cracking process deposits on particle surfaces and is transported by carrier particles. These reactions are denoted as follows:

\[
\begin{align*}
A_1 & \rightarrow a_1 A_2 + a_2 A_3 + a_3 A_4 \\
A_2 & \rightarrow b_1 A_3 + b_2 A_4
\end{align*}
\]  

in which stoichiometric coefficients are expressed in mass fractions.

The feed oil and light oil cracking reactions are assumed to be a second-order and a first-order reactions, respectively (Dave et al, 1993). Eq.(3) shows a reaction rate expression for both the feed oil cracking reaction R₁ and the light oil conversion reaction R₂.

\[
R_i = k_i \phi_i f_i^{n_i}, \quad i = 1(heavy \ oil), \ or \ 2(light \ oil)
\]  

in which \( f_i \) is the mass concentration, \( n_1 \) is 2, \( n_2 \) is 1, and

\[
k_i = k_{o,i} \exp(-E_i / RT)
\]
In the reaction rate expression, $k$ is the rate constant, $\phi$ is catalyst decay function, $f$ is the mass fraction of the reactant (feed oil or light oil), and $n$ is the order of the reaction. The rate constant $k$ is determined by an Arrhenius formula Eq.(4), in which the activation energy $E$ and the constant $k_0$ need to be determined experimentally, $R$ is the universal gas constant, and $T$ is the gas temperature. As gas oil and gasoline are cracked, coke is formed on the catalyst surface. The coke adheres to the surface and blocks active sites of catalyst. Therefore, catalyst activity declines as the cracking reactions proceed. Voorhies (1945) showed that catalyst activity is a function of catalyst residence time $t_c$, the cumulative contact time of catalyst with gas oil vapor. Weekman and Nace (1970) proposed an exponential function Eq.(5) to account for the decay of the catalyst activity for both cracking reactions in a reactor. The catalyst deactivation constant in the catalyst decay function is expressed in general Arrhenius formula Eq.(6).

The source term of a species conservation equation accounts for the formation and consumption of a species. Rates of species formation and consumption are calculated from the reaction rates, Eq.(3). A time integral approach converts the reaction time scale to the flow time scale by integrating the reaction rate over the flow field. This approach has shown great improvement in numerical convergence and stability (Chang and Lottes, 1993).
A J-bent riser was selected for the numerical simulation. The grid employed in the computations is a staggered system. A momentum cell is used to solve for gas velocity components and a scalar cell is used to solve for other flow properties. Two two-dimensional grids were chosen for the flow field of the riser: one grid of 65 by 15 scalar cells for section-A and the other 63 by 15 grid for section-B. Figure 6 shows the grids. Since a more complex flow pattern is expected in the mixing zone where oil is injected, a finer grained grid cell structure is defined in this zone. Rectangular and triangular blocked cells can be used to construct the entrance region of section-A where tube diameter changes and the inlet elbow region of section-B where the riser tube turns an angle.

The grids were chosen to be the coarsest which gave stable numerical results to approximate three decimal digits upon further grid refinement in order to conserve computational time and still provide adequately accurate results. An important feature of the control volume approach used by the ICRKFLO code is that it is conservative in terms of mass, energy, species, and all variables solved for via the transport equations, both locally and globally to a very high degree regardless of grid size. This feature helps to ensure that results are physically realistic regardless of grid size and that trends in parametric studies are relatively independent of grid size even for relatively coarse grids. Little would be gained therefore in attempting to refine the grid to make results grid independent to more than 3 or 4 decimal digits.

Figure 6 Grid System for the Selected Riser
The simulated riser flow includes four gas species, five droplet size groups, a single particle size group, and a coke species carried by particles. In this computer code, a calculation is considered to have converged if the local and global mass balances of the three phases are smaller than a set of predetermined criteria. For this simulation, convergence criteria, defined by average mass residual of all computational cells, are $10^{-10}$ (in dimensionless form, normalized by the inlet mass flow rate) for the gas phase and $10^{-9}$ for both the liquid and solid phases. Generally in this application, with reasonable boundary conditions (inlet flow rates etc.), a converged solution can be obtained in about 700 numerical iterations. A numerical iteration includes 10 gas-phase calculations and 3 liquid- and solid-phase calculations. 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

The ICRKFLO computer code was verified by comparing the results of numerical simulation with experimental data for several cases. In a previous study, a vertical riser reactor was simulated at different operating conditions. The predicted product yields and exit temperatures were well agreed with the experimental data (Chang et al. 1995). For a J-bent reactor, the product yields and temperature at different axial locations were also compared between predictions and experimental data with good agreement. However, the detailed information is proprietary and can not be presented here. This section will present general results of numerical simulations of the bent riser reactor using the ICRKFLO incorporated with the newly developed sectional coupling approach. A baseline case and parametric studies including effects of oil injection location, oil injection velocity, oil injection angle, and inlet particle distribution on the flow pattern and the cracking performance will be discussed.

Baseline Case

A baseline case is used to demonstrate that: (1) sectional coupling approach is applicable for the bend riser flow, and (2) a lumped cracking reaction model can be integrated with the hydrodynamic calculation. The grids chosen for sections (A) and (B) of the selected riser are
shown in Fig. 6. The inlet flow conditions were assumed uniformed and symmetric. Separate calculations were made for sections (A) and (B) of the selected riser.

The gas pressure, density, temperature, velocities, species concentrations, and droplet and particle number densities in the entire flow field of the riser reactor were calculated using ICRKFLO. The flow simulation included the processes of mixing, heat transfer, vaporization, and cracking (including coke formation and deposition on carrier particles). The fluid constituents of the simulation include 4 gas species (feed oil vapor, light oil vapor, dry gas, and carrier gas), 5 size groups of liquid droplets, a single particle size group, and a coke species in the solid phase. A set of empirical kinetic parameters for heavy oil cracking reactions were determined by matching calculated product yields with the experimental data. A sensitivity study and a trial-and-error procedure were implemented in selecting the empirical kinetic constants. The final results showed very good agreement between the calculated and measured values.

Typical computational results are shown in Figs. 7 and 8 for section A and B respectively. Figure 7 includes 15 subplots: (a) gas velocity vectors, (b) pressure drop, (c) gas temperature, (d) gas density, (e) particle number density, (f)-(j) droplet number density of size groups 57, 171, 285, 400, 513 μm, respectively, (k) feed oil concentration, (l) light oil concentration, (m) dry gas concentration, (n) coke concentration, and (o) carrier gas concentration. Gray-scale color are plotted in each property figure. A gray-scale color key is plotted on the left side of the property figure. The key shows the corresponding shade for the property value; the darker the shade the higher the property value. The upper and lower bound values are also shown with the key. SI units are used for these flow properties: velocity (m/s), temperature (K), pressure drop (kPa), density (kg/m³), number density (#/mm³), and species concentration (kg/kg).

Figure 7a shows gas velocity distribution. Gas appears to accelerate from the entrance region to the end of section A. The acceleration is due to the vaporization of feed oil. Small stagnation zones found in the corners of tube-expansion juncture are caused mainly by the injection of oil. Since particle size is small (60 μm), local slip velocity between gas and particle is small. Particle velocity shows similar distribution as the gas. Figure 7b shows the distribution
of pressure drop. The pressure drop reflects the energy used to overcome the friction and the gravity (potential energy gained by the solid particles). Figure 7c shows the distribution of gas temperature. Again, particle temperature shows a very similar distribution. The temperature distribution is non-uniform and asymmetric. The temperature is cooler near the wall and hotter in the center because heat is transferred from particles through gas to droplets for vaporization. The asymmetry is due to the gravity effect on the droplet vaporization patterns as shown in Figs. 7i and 7j.

Figure 7d shows the distribution of gas density. In the entrance region, the density is low because only carrier gas is present and it is light. Downstream the oil injection, density rises due to the heavy feed oil vapor resulted from evaporation. In the oil vaporization region, the density is asymmetric with a higher density to the right side. This is another indication of the gravity effect on the evaporation pattern. Similar asymmetric distribution is shown in Fig. 7k of the distribution of feed oil concentration. After the evaporation region, the density decreases because the cracking reaction produces light products. Figure 7e shows the distribution of particle number density. Particle number density is very high (particle void fraction is about 25%) in the entrance region. As particles enter the evaporation region, the velocity picks up and particle number density drops. The asymmetric distribution of the particles indicates that more oil vaporizes in the right side of the tube and the vapor pushes particles to the left side.

Figures 7f-7j show the distribution of droplet number density for size groups 57, 171, 285, 400, 513 μm, respectively. The distributions of droplets define a region of oil evaporation from oil injection location to about 1/3 of the section A. In this region, over 90% of oil droplets are vaporized. Smaller droplets do not penetrate well into the main flow and are vaporized near the walls. Larger droplets penetrate into the main flow and are vaporized in the tube center. Gravity has a significant effect on larger droplets, therefore, more droplets remains in the right half of the tube as shown in Figs. 7i and 7j.
Figure 7. Results of the Baseline Flow Calculation in Section A of the Riser
Figures 7k, 7l, 7m, and 7n show the distributions of feed oil, light oil, dry gas, and coke concentration. Oil vapor is produced in the evaporation region and after that it is cracked into light oil, dry gas and coke. Figure 7o shows the distribution of carrier gas. The distribution indicates that the carrier gas is diluted by the oil vapor.

Figure 7. Results of the Baseline Flow Calculation in Section A of the Riser (cont’d.)

In section A, most liquid oil is vaporized; a great portion of the oil vapor is converted to light oil; and some light oil starts to be converted to dry gas and coke. A flow of oil vapor, catalyst particles, and residual oil droplets (about 3%) from section A enters the section-B of the riser from lower left corner as indicated by the arrow in Fig. 8a. The flow is turned a 50° angle in the inlet area of the section B. The turn of the flow causes large pressure drop in this region as shown in Fig. 8b. Particles are small (60 μm) enough to be carried by the gas flow and most of them turn to the upward direction before reaching the opposite wall as shown in Fig. 8c. Some oil droplets are large (400 μm) and have enough momentum to reach the opposite wall as shown in Fig. 8d. In this region, the oil droplets continue to be vaporized and produce oil vapor as indicated in Fig. 8c. Light oil is produced by the cracking of the feed oil and at the same time,
the cracking reactions convert the light oil to other products, e.g., dry gas and coke. In section-B, the light oil appears to be overcracked and the light oil concentration drops slightly as shown in Fig. 8f. Dry gas and coke do not convert to other product so their concentrations increase along the tube as displayed in Figs. 8g and 8h. The asymmetric distributions of the oil vapor and product concentrations are caused by the flow turn at the inlet of section B.

A similar calculation was made for the section B of the riser. Some results are shown in Fig. 10, including the following subplots: (a) gas velocity, (b) pressure drop, (c) particle number density, (d) droplet number density (400-μm size group), (e) feed oil concentration, (f) light oil concentration, (g) dry gas concentration, and (h) coke concentration.

Figure 9 shows predicted cross-sectional species concentrations (f_i) along the normalized axial distance (x/L) including both section A and section B. It clearly shows that heavy oil vapor concentration rapidly increases in the mixing zone, while oil droplets are vaporized by the heat carrier particles, and gradually decreases in the reacting zone, where heavy oil vapor is converted to products. Up the riser, concentrations of dry gas, and coke steadily increase. However, light oil concentration increases along the axial position in the section A and slightly decreases in the section B due to the over cracking.

Parametric Studies

Effect of Injection Location

In the baseline case, the oil was injected at the tube-expansion juncture. When the injection location was moved to a distance further downstream, the major effect was on the flow pattern in the mixing zone as shown in Fig. 10. It should be noticed that this injection location was used for all the other cases in the parametric studies. Figure 10 includes (a) gas velocity distribution, (b) particle number density distribution, (c) the droplet number density distribution (400-μm size group), and (d) feed oil distribution.
Figure 8. Results of the Baseline Flow Calculation in Section B of the Riser
Figure 9. Axial Distribution of Species Concentrations

Figure 10. Results of the Injection Location Effect in Section-A of the Riser

Similar to the baseline case, the gas accelerates from the entrance region to the end of section A due to the vaporization of feed oil. However, a small stagnation zone is located at the
center of the tube which is caused by the cross injection of the oil as shown in Fig. 10a. Because of this stagnation zone, the particles tend to be pushed away from the center of the tube and accumulated near the two sides of the wall as shown in Fig. 10b. Figure 10c shows that the large droplets penetrate into the main flow and are vaporized in the center of the tube. The feed oil distribution displayed in Fig. 10d corresponds to the distributions of the particles and droplets. Similar to the baseline case, due to the gravity effect, more oil vaporizes in the right side of the tube as shown in Fig. 10d and the vapor pushes particles to the left side, causing asymmetric distribution of particles as indicated in Fig. 10b.

**Effect of Oil Injection Angle**

Two oil injection angles were simulated. One was 45° and the other was 90° to the wall. The results showed that the major effect was on the droplet penetration. When the oil was injected vertically to the wall (90°), the droplets penetrated more to the center of the tube. Consequently, the distributions of feed oil, light oil, dry gas, and coke were affected.

**Effect of Asymmetric Oil Injection**

The oil injection was symmetric to the center of the tube in the cases discussed above. The asymmetric oil injection was also simulated to investigate its effect on the flow pattern and the cracking performance. A calculation was made assuming that the oil injection velocity in the right side injection was 1.67 times larger than that in the left side with the injection angle of 45°. The results indicate that the stagnation zone is shifted to the left side slightly. Due to the larger momentum of the droplets in the right side, which overcomes the gravity effect, more droplets are induced to the left side and vaporized there. The large amount of oil vapor in the left side pushes the particles to the right side in the mixing zone.

**Effect of Inlet Particle Distribution**

The effects of inlet particle distribution was investigated for three cases. As shown in Fig. 11, these cases include uniform distribution (Case I), linear distribution with small gradient (Case II), and linear distribution with large gradient (Case III). Figure 12 shows the particle number density along the radius of the tube at a cross section in the mixing zone. Case I with
uniform inlet particle distribution gives two peaks near the wall due to the stagnation zone discussed earlier. In both case II and Case III, the particles pile up in the right side of the tube.

![Graph 1](image1.png)

**Figure 11.** Radial particle number density distribution at the inlet

![Graph 2](image2.png)

**Figure 12.** Radial particle number density distribution at the mixing zone
In Case II, the inlet particle number density at the right side is approximately three times higher than that at the left side. This nonuniformity reduces along the tube height. There is still a stagnation zone near the center of the tube in the mixing zone. However, more vaporization occurs in the right side because of the high particle number density, providing more heat for vaporization.

![Figure 13. Results of the Inlet Particle Distribution Effect in Section-A of the Riser](image)

This effect is shown more considerably in Case III, in which the inlet particle number density at the right side is approximately 20 times higher than that at the left side. The distributions of gas velocity, particles, droplets, and feed oil for Case III are shown in Fig. 13. As shown in Fig. 13a, the stagnation zone no longer exists and the gas velocity vectors are directed to the right side at the beginning of the tube and then turn to the left side in the mixing zone due to the large vaporization in the right side. In Fig. 13b, the radial particle number density distribution is nonuniform along the whole tube. The vaporization mainly occurs in the right side of the mixing zone as shown in Fig. 13d, and the large amount of vapor even pushes droplets to the left side. This changes the cracking performance dramatically.
CONCLUSION

A sectional-coupling approach is developed to simulate multi-phase reacting flows in a bent riser reactor of an FCC unit. It divides the bent reactor into two sections, which provides a simple and effective approach for handling a complex geometry. It can be extended to a reactor of many sections. The approach is incorporated into the ICRKFLO computer code that couples hydrodynamics and cracking kinetics including an integral lumped species reaction model. The numerical simulation predicts characteristics of the riser flow, including gas, liquid, and solid phases of the flow, vaporization of the feed oil, and subsequent cracking of the feed oil. The predictions compared very well with experimental results. The parametric studies indicate that the inlet particle distribution has strong effects on the flow field and product yields. The oil injection location and the oil injection velocity and angle mainly change the flow pattern in the mixing zone. Consequently, the product yields are also affected. The computational results are expected to lead to a better understanding of the internal processes in the riser and the effect of riser geometry and operating parameters on riser performance.

ACKNOWLEDGMENTS

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### NOMENCLATURE

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<td>$n_i$</td>
<td>droplet or particle number density</td>
<td></td>
</tr>
<tr>
<td>p</td>
<td>pressure (Pa)</td>
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</tr>
<tr>
<td>r</td>
<td>droplet or particle size (μm)</td>
<td></td>
</tr>
<tr>
<td>R</td>
<td>gas constant (J/kmol-K)</td>
<td></td>
</tr>
<tr>
<td>$R_i$</td>
<td>reaction rate (1/s)</td>
<td></td>
</tr>
<tr>
<td>S</td>
<td>Source term in governing equations</td>
<td></td>
</tr>
<tr>
<td>T</td>
<td>temperature (K)</td>
<td></td>
</tr>
<tr>
<td>t</td>
<td>time (s)</td>
<td></td>
</tr>
<tr>
<td>u</td>
<td>velocity component in the x-direction (m/s)</td>
<td></td>
</tr>
<tr>
<td>v</td>
<td>velocity component in the y-direction (m/s)</td>
<td></td>
</tr>
<tr>
<td>x</td>
<td>x coordinate (m)</td>
<td></td>
</tr>
<tr>
<td>y</td>
<td>y coordinate (m)</td>
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### Greek Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tr>
<td>$\alpha$</td>
<td>catalyst decay parameter</td>
</tr>
<tr>
<td>$\Gamma$</td>
<td>effective diffusivity (pa-s)</td>
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<tr>
<td>$\phi$</td>
<td>catalyst decay function</td>
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<tr>
<td>$\theta$</td>
<td>void fraction</td>
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<tr>
<td>$\rho$</td>
<td>density (kg/m³)</td>
</tr>
<tr>
<td>$\xi$</td>
<td>general variable for 1, u, v, h, f, k or $\varepsilon$</td>
</tr>
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</table>

### Subscripts

<table>
<thead>
<tr>
<th>Symbol</th>
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<tr>
<td>d</td>
<td>droplet</td>
</tr>
<tr>
<td>k</td>
<td>droplet size group k</td>
</tr>
<tr>
<td>$\xi$</td>
<td>general variable for 1, u, v, h, f, k or $\varepsilon$</td>
</tr>
</tbody>
</table>
REFERENCES


