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Computer Simulation of FCC Riser Reactors*

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DISCLAIMER

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Abstract

A three-dimensional computational fluid dynamics (CFD) code, ICRKFLO, was developed to simulate the multiphase reacting flow system in a fluid catalytic cracking (FCC) riser reactor. The code solves flow properties based on fundamental conservation laws of mass, momentum, and energy for gas, liquid, and solid phases. Useful phenomenological models were developed to represent the controlling FCC processes, including droplet dispersion and evaporation, particle-solid interactions, and interfacial heat transfer between gas, droplets, and particles. Techniques were also developed to facilitate numerical calculations. These techniques include a hybrid flow-kinetic treatment to include detailed kinetic calculations, a time-integral approach to overcome numerical stiffness problems of chemical reactions, and a sectional coupling and blocked-cell technique for handling complex geometry. The copyrighted ICRKFLO software has been validated with experimental data from pilot- and commercial-scale FCC units. The code can be used to evaluate the impacts of design and operating conditions on the production of gasoline and other oil products.

Introduction

Computational fluid dynamics (CFD) simulation has become a new and important tool to help develop advanced energy conversion/combustion systems. A typical example is the advancement of the fluid catalytic cracking (FCC) technology. The FCC technology that produces gasoline and other valuable oil products was first developed in the 1940s. Since then, it has become the most important process used by the refinery industry to produce gasoline. The process has been greatly improved over the years by the U.S. refineries to compete in global markets and meet more stringent environmental regulations. The FCC units in U.S. refineries today produce about 40% of the nation's gasoline supply. The advancement of catalysts has been the most significant reason for the advancement of FCC technology. Recently, refineries have shown much interest in improving feed injection systems and developing short-residence-time riser units [1]. Advanced FCC processes are usually tested in a small pilot-scale unit and gradually scaled up to a large commercial unit. The capacity of a pilot-scale unit is about 1 barrel per day (bpd), and the capacity of a commercial unit can be as high as 100,000 bpd. The scale-up process requires several intermediate steps for construction, tests, and adjustments. These tests are expensive and time-consuming. Detailed knowledge of the relationships between process operating parameters and flow conditions within the system can decrease the development time of new and/or upgraded FCC systems. Such knowledge can be obtained by analyses based on a computer simulation that includes the controlling processes of an FCC system and the testing results of pilot units.

Chemical kinetics and flow dynamics are two controlling processes of an FCC system. In older FCC riser units, the residence time is long and the flow is fully developed in the riser. Under this circumstance, the chemical kinetics is the only controlling process in an FCC riser, and kinetic calculations can be made based on assumed or simplified flow fields. Since there are thousands of oil species in the cracking processes, models of lumped species and reduced kinetic reactions are developed for a kinetic calculation. Weekman and Nace [2] first introduced a three-lump (feed oil, gasoline, and dry gas) cracking kinetic model to predict gasoline production in an FCC riser unit. Later, Jacob et al. [3] developed a ten-lump cracking kinetic model to predict more detailed distribution of oil species in an FCC riser system. Recently, Nigam and Klein [4] and Quann and Jaffee [5] have been developing ways to approach chemical kinetics computation and model building for cracking reaction systems with hundreds or thousands of oil species. These kinetic computations are usually based on simplified or assumed flow fields.

In recent years, the residence time of FCC units has been shortened significantly to improve their performance. Flow dynamics also becomes an important process for controlling the cracking processes. Computer simulation of a multiphase reacting flow system like an FCC riser flow is formidable because it requires a computer code to solve many coupled non-linear partial differential equations (PDEs) numerically. The numerical solution requires much computational power, both in speed and memory. The difficulty is magnified by the limited understanding of the physics of a multiphase flow. In the past decade, with the advancement of the understanding of multiphase flow, the numerical techniques required to solve the PDEs, and computer hardware, newer versions of CFD codes were found to be capable of modeling an FCC flow system. Theologos et al. [6] used a commercial CFD code to simulate an FCC riser reactor. The simulation was a two-phase flow (gas and particle) simulation with Weekman and Nace's three-lump kinetic model. The simulation was used to predict engineering aspects of a riser reactor, including pressure drop, particle slip velocity, and temperature distribution. However, the simulation does not include an important element of the riser flow - the feed oil spray, and the number of lumped species is limited.

Since 1993, ANL has been working with several refining companies to develop CFD capabilities to support advanced FCC development. A CFD code called ICRKFLO was developed based on an existing multiphase reacting flow code. The code includes the formulation of a three-phase (gas, liquid, and particle) flow and a hybrid approach than can handle a large number of lumped oil species. It can predict oil product concentrations of a riser based on locally computed flow properties. The code has been validated with both pilot- and commercial-scale data. This paper presents the code, its unique models and numerical approaches, the validation, and some selected results.

FCC Riser Flow Characteristics

A typical FCC unit includes three major components: a riser reactor, a stripper/separator, and a regenerator. Figure 1 shows a simple sketch of the FCC unit. Catalyst particles are transported to the bottom of the riser reactor from a regenerator. A spray of feed oil is injected into the riser to mix with catalyst particles and be converted to lighter oil products. A small amount of inert gas is used to lift particles in the entrance region of the riser. Oil droplets are vaporized when heated to the boiling point. Then, the oil vapor is cracked into various lighter oil products by the catalyst and heat. Coke is a by-product of the cracking processes. The deposition of coke on catalyst surface lowers catalyst activity. The end of the riser is connected to a separator, in which oil products and spent catalyst particles (covered with coke) are separated. Oil products are sent to a distillation column for further processing, and the spent particles are transported to the regenerator to burn off the coke with air. After the coke deposit is burned off, the catalyst particles are hot and regenerated. Then, the catalyst is recycled back to the riser reactor for the next run of cracking. This study focuses on the riser flow.

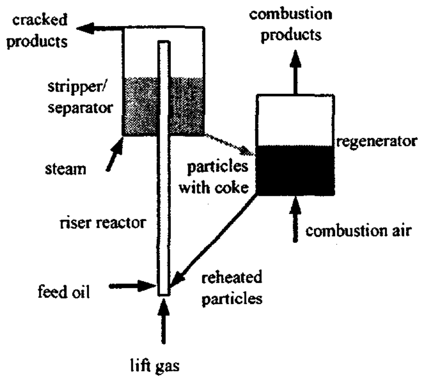

Figure 1 A Typical FCC Unit

There are three major processes in a riser flow: mixing, vaporization, and the cracking reaction, as shown in Figure 2. 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, and catalyst particles. During the mixing process, the heat carried by the catalyst particles is transferred to the gas and the oil droplets. Generally, the catalyst is heated up to a temperature much higher than the boiling point of the feed oil. Consequently, the vaporization process is dominated by boiling and controlled by the heat transfer rate to oil droplets.

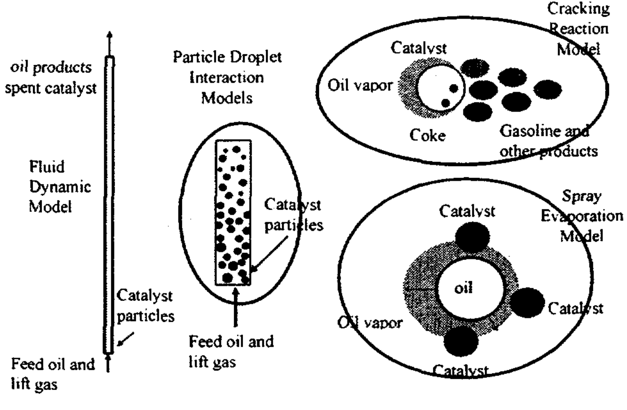

Figure 2 Major Processes in an FCC Riser Reactor

During the vaporization process, a liquid oil droplet is releasing oil vapor 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 contacts catalyst particles, and the cracking reactions on the catalyst surface convert the feed oil vapor to light oil vapor and dry gas. Coke is a by-product of the process. These processes all have an impact on the riser performance.

Simulation Approach

ICRKFLO is a three-dimensional CFD code developed specifically for an FCC riser flow. The formulation of the code includes major hydrodynamic and cracking processes of the FCC riser flow. Oil vapor species produced in the FCC cracking process can number in the thousands. Solving for all species is frivolous and often causes severe numerical stiffness problems when it is coupled with the hydrodynamic calculation. But solving for only a few species may not be enough for the analysis of the product yields.

A hybrid approach is adopted to allow enough oil species to be included for a more realistic representation of the cracking process. In the two-step hybrid approach, a smaller number of major species are solved, coupled with the hydrodynamic calculation in the first step and a much larger number of minor subspecies are solved in the second step based on the flow field calculated in the first step.

Hydrodynamic Formulation with Reduced Reaction Mechanism

An FCC riser flow consists of gas, liquid, and solid phases. An FCC flow simulation should include all three phases. The gas species can be divided into two groups: major lumped species for the first-step calculation and minor subspecies for the second-step calculation. The major gas species

divided into a spectrum of size groups. The solid flow contains the catalyst particles. The particles can also be divided into various size groups.

The code calculates flow properties of all three phases. The gas flow properties to be calculated include pressure, density, temperature, velocity components, and species concentrations. The liquid properties include droplet number density, temperature, and velocity components for each size group. The solid properties include particle number density, temperature, velocity components, and coke fraction for each size group. An Eulerian approach is employed to formulate governing equations of these properties. The governing equations include the equations of state and those derived from the conservation laws of mass, momentum, and energy.

Gas Equations

The equations of state for the gas flow include the ideal gas, the caloric, and the species unity equations. The ideal gas law gives a functional relationship among pressure, temperature, and density. The caloric equation gives an expression of enthalpy in terms of temperature. The species unity equation says that the summation of all gas species mass fractions equals one.

The conservation equations derived for the gas flow include the continuity, momentum, enthalpy, and species equations. All the equations are elliptic-type partial differential equations. For convenience of numerical calculation, the equations are put in a common form,

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(\theta \rho u_i \xi - \frac{\mu + \mu_t}{\sigma_\xi} \frac{\partial \xi}{\partial x_i}\right) = S_\xi \tag{1}$$

in which ξ is a general flow property for the scalar 1, velocity components u_1, u_2, and u_3, enthalpy h, and species concentrations f_n, f_l, f_o, and f_g; x_1, x_2, and x_3 are coordinates; θ is gas volume fraction; μ and μ_t are laminar and turbulent viscosities; σ_ξ is a diffusivity coefficient for ξ; and S_ξ is the source term of the ξ equation. Turbulent viscosity is determined from a turbulence model (see Multiphase k-ε Section).

The source terms of the gas governing equations are mostly related to the interactions between phases and the cracking reactions. The source term of the continuity equation accounts for the mass generation from the droplet evaporation (see Spray Evaporation Section). The source terms of the momentum equations account for the interfacial drag forces from both droplets and particles (see Interfacial Interaction Section) and the momentum from the mass added by the evaporation process. The source terms of the enthalpy equation account for the droplet evaporation (see Spray Evaporation Section) and the interfacial heat transfer from both droplets and particles (see Interfacial Interaction Section). The source terms of the feed oil equation account for the species generation from the droplet evaporation (see Spray Evaporation Section) and the species consumption of the cracking reaction (see Time-Integral Lump Reaction Section). The source term of the dry gas equation accounts for the production of dry gas from the cracking reaction (see Time-Integral Lump Reaction Section). The governing equations of the inert gases have no source term.

Droplet Equations

The liquid-phase formulation is based on an Eulerian approach, which treats liquid droplets as a continuous fluid. A spray of liquid oil is injected into an FCC riser. The spray consists of droplets of a size spectrum. To compute liquid properties, the droplets are divided into various size groups, k=1,K. For the kth size group, governing equations are derived to solve for droplet number density $n_{d,k}$; velocity components $u_{d,k,i}$, where i=1,3; and temperature $T_{d,k}$. A common formulation of these equations for the droplets of the kth size group is given as:

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i}\left(n_{d,k} u_{d,k,i}\xi - \Gamma_\xi \frac{\partial n_{d,k}\xi}{\partial x_i}\right) = S_\xi \qquad (2)$$

in which ξ is a general droplet property for number density, velocity components, or temperature; Γ is droplet diffusivity resulting from interaction with turbulence in the gas phase (See Turbulence Section), and S_ξ is the sum of source terms.

The source terms of the droplet conservation equations are mostly related to the interactions between phases. The source terms of the droplet number density equation account for the size shift of droplet number density due to the evaporation process (see Spray Evaporation Section). The source term of the droplet momentum equations accounts for the interfacial drag forces from gas flow (see Interfacial Interaction Section). The source terms of the temperature equation account for the interfacial heat transfer from both gas flow and particles (see Interfacial Interaction Section).

Particle Equations

The solid-phase formulation is also based on an Eulerian approach, treating solid particles as a continuous fluid. Particles are also divided into various size groups. For each size group k, governing equations are derived to solve for particle number density $n_{p,k}$, velocity components $u_{p,k,i}$, i=1,3, and temperature $T_{p,k}$, and coke fraction, C_k. Coke has a strong impact on the cracking reaction because it can deactivate the catalyst. A common formulation similar to Eq.(2) can be derived for the governing equations of the kth particle size group.

The particle number density equation has no source term. The source terms of the particle momentum equations account for the drag force from the gas flow and the shear stress and solid pressure through particle-solid interactions (see Interfacial Interaction Section). The source terms of the particle temperature equation account for the heat transfer to/from gas and droplets (see Interfacial Interaction Section). The source term of the coke equation accounts for the production of coke from cracking reactions (see Time-Integral Lump Reaction Section).

Phenomenological Models

Phenomenological models are used to determine turbulent diffusivity and the source/sink terms of the above-mentioned governing equations. A time-integral lumped reaction model is used to calculate the generation and consumption rates of the oil species and coke as the source terms of the species and coke equations. A spray evaporation model is used to calculate the droplet evaporation rates and translates the evaporation rates into a droplet size distribution shift. The evaporation rate is used in the source term of the gas continuity equation and the sink term of the gas enthalpy equation. The shift of the droplet size distribution is used to formulate the source/sink terms of the droplet number density equations. A mutli-phase k-ε turbulence model is used to calculate turbulent viscosities and diffusivities of species and heat. Models of interfacial interactions are used to calculate the rates of interfacial momentum and heat transfer for the momentum and energy equations of all three phases.

Time-Integral Lump Reaction Model

The reaction model was developed based on a four-lump kinetic model developed by Dave et al. [7]. The four-lump kinetic model considers four lumped oil components in two cracking reactions. The four oil lumps are feed oil, light oil, dry gas, and coke. Feed oil is the heavier oil components and the light oil is the lighter oil components, based on the boiling point. The cutoff boiling point is arbitrarily chosen, e.g., 494 K. Dry gas is the oil vapor components of carbon number lower than C_5. Coke is a byproduct of the cracking reactions.

Two cracking reactions used here are reaction (a), the feed oil cracking reaction that converts feed oil to light oil, dry gas, and coke, and reaction (b) the light oil cracking reaction that converts light oil to dry gas and coke.

$$P_o \xrightarrow{k_1} a_1 P_l + a_2 P_g + a_3 C_k \qquad (a)$$

$$P_l \xrightarrow{k_b} b_1 P_g + b_2 C_k \qquad (b)$$

where P_o, P_l, P_g, C_k represent feed oil, light oil, dry gas, and coke, respectively; a_1, a_2, a_3, b_1, and b_2 are mass stoichiometric coefficients; and k_1 and k_2 are reaction rates. Reaction rates are generally expressed in Arrhenius formulae, and the associated rate constants can be extracted from pilot-scale test data. A methodology of extracting these kinetic constants will be briefly described in the Extraction of Kinetic Constants Section.

The reaction time scale is generally much shorter than the flow time scale. A flow calculation may suffer severe numerical instability or stiffness problems due to the large difference between the flow and the reaction time scales (see Numerical Convergence Section). A time-integral approach was developed to improve numerical convergence and stability. The approach converts the reaction time scale to the flow time scale by integrating the reaction rate over a computational cell of the flow field. This approach [8] has been shown to yield a great improvement in numerical convergence and stability of computations. In the integral reaction model, reaction rate as a function of computational cell residence time is derived, taking into account the reaction rate changes induced by changing species concentration as the flow proceeds through the cell. With this model, the reaction rate cannot be grossly overpredicted, and all of the feed oil vapor in a cell cannot be consumed in an iteration step. Thus, the oscillatory behavior of the differential reaction model is eliminated, and the reaction portion of the CFD code is numerically stabilized.

Spray Evaporation Model

The spray evaporation model provides (1) a droplet size distribution for the injection spray, (2) spray evaporation rate as the source term for the continuity and feed oil species equations, and (3) the droplet size shifting rate as the source term for the droplet number density equations.

Experiments show that droplets have a bell-shaped size distribution in a spray. As the droplet radius increases, the number density function increases from zero at zero radius to a peak and decreases afterward. Based on the distribution function, droplet size groups can be defined. The droplet number density of the size group k is defined as the number of droplets of a radius between r_{k-1} and r_k.

Vaporization causes droplets to shift from larger to smaller size groups at a computed rate and also results in transfer of vapor from the droplets into the gas phase. The source term in the gas continuity equation is the evaporation rate of the droplets per unit volume. In the 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. For each droplet size group, the number density decreases due to the evaporation of the size group, but increases due to the evaporation of the next larger size group. The rate of number density change becomes a source term for the droplet number density equation of the droplet size group k. More details of the spray model are given in Reference 9.

Interfacial Interaction Models

FCC riser flow is a three-phase flow, including gas, oil droplets, and catalyst particles. In such a flow, there are numerous interactions between phases. The interactions could be exchanges of mass, such as evaporation and coke deposition and transport, or exchanges of momentum and energy. The code includes three interfacial interaction models: a particle-solid interaction model, an interfacial drag model, and an interfacial heat transfer model.

Particle-Solid Interaction Model: The model has the capability to predict a unique U-shaped particle distribution in a riser flow. In a riser flow, catalyst particles frequently collide with each other, and some particles settle near the wall to form a U-shaped distribution. The collision effect is neglected in most CFD codes. This model derives a diffusive term by solid collision based on the gradient of the local particle mass flux. Solid diffusive terms are added to the particle momentum equations.

Solid Pressure Model: Particles can be packed in a riser where the velocity is low or flow direction changes. When packed, particles are directly in contact with the neighboring particles and exert a solid pressure on other particles. The solid pressure is assumed to be a function of local solid volume fraction when solid volume fraction exceeds a packed value, e.g., 0.6. The solid pressure is used in the source terms of the particle momentum equations.

Interfacial Heat Transfer Model: The model handles the heat transfer between (1) gas and droplets, (2) gas and particles, and (3) droplets and particles. The gas/droplet and gas/particle heat transfer models use conventional Nusselt formulae with the slip velocity to calculate the heat transfer rate. The slip velocity is the velocity difference between gas and droplet or particle. The droplet or particle heat transfer model is new. It accounts for the conduction heat transfer between a particle and droplet. This heat transfer is significant when droplets are much larger than particles or vice versa. The new model assumes particles collide with a droplet in the flow and conduction heat transfer occurs for each collision. The number of collisions between particles and a droplet can be calculated based on an effective collision volume. The effective collision volume is the sphere of a radius equal to the sum of the particle and droplet radii. The collision between a particle and a droplet results in conductive heat transfer from the hot particle to the cold droplet. The heat transfer rate is calculated using the Fourier Law of heat conduction. The conduction heat flux is added to the source terms of the droplet energy equation, and an equal amount of heat flux is subtracted from the source terms of the particle energy equation.

Interfacial Drag Model: Oil droplets and catalyst particles are driven by the drag force from the gas flow. The drag force is used in the source terms of the gas, liquid, and solid momentum equations. Empirical equations are commonly used to correlate the drag force with the slip velocity. The empirical drag coefficient is expressed as a function of Reynolds and transfer numbers.

Multiphase k-ε Turbulent Model

A turbulent flow consists of a spectrum of rotational eddies. The eddies, having a size ranging from a tiny, techniques are employed to construct regions of complex geometry in the mesh or mesh sections.

Grid Selection

The grid employed in the computation 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. For each FCC flow simulation, a grid sensitivity study is conducted to select the final grid system, which gives independent numerical results to three significant decimal digits upon further grid refinement. This approach conserves computational time while still providing 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.

Blocked-Cell Technique

Grid nodes can be excluded from a CFD calculation by marking them as blocked cells. A blocked cell is impermeable to fluid flow and can be used to construct irregular boundary surfaces. Rectangular blocked cells can be easily implemented. However, a sloped contour is hard to fit smoothly with these cells, and stair-step corner cells are generated. Multiphase flow calculations using this approach tend to show unrealistic particle pileup in the corner cells, and sometimes the particle pileup leads to severe numerical instability.

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 an open 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. A sloped contour can be well fitted by triangular blocked cells. Calculations were done by solving the converging 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 piled up in corner cells. For the same problem, the triangular blocked-cell approach achieved a stable, highly converged solution. Triangular blocked cells become wedges in a three-dimensional grid.

Sectional Coupling Technique

A sectional coupling approach was developed for the flow simulation of long riser reactors with bends. The approach consists of two major steps: (1) riser is represented by several straight tube sections, and (2) the flow field in each section is calculated using a CFD code, e.g., ICRKFLO, in sequence, with the exit flow conditions of the previous section are used as the inlet flow conditions for the next section. More detailed discussion can be found in Reference 13.

Numerical Convergence

A riser flow simulated by the authors generally includes four gas species, five to ten droplet size groups, a single particle size group, and a coke species carried by particles. An FCC riser flow 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. A convergence study was conducted to determine convergence criteria, defined by the average mass residual of all computational cells. To have a reasonably converged solution, the criteria need to be 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 2000 global iterations. Each global iteration includes ten gas phase iterations and three liquid and solid phase iterations. On a Pentium™ II 300 personal computer with 64 megabytes of random access memory, using a 32-bit FORTRAN compiler, a flow computation of about 10,000 nodes takes about 6 hours. The computational time increases with increased nodes. If a numerical instability is encountered, a computation never converges.

Numerical Instabilities

Numerical instabilities are often encountered in a flow calculation. Many of them are due to programming errors; some are a consequence of the non-linearity of the equations; some are caused by singularities in the flow system; and some arise from the discretized number system on the computer. The programming errors, as long as one can find them are easy to correct. As for the other two types of numerical problems, to find them is one thing and to resolve them is another. The resolution of these numerical problems usually requires the development of new formulations and/or new numerical routines.

Programming Errors: The authors found two very effective procedures to find and correct programming errors. One procedure concerning the flow symmetry includes the following steps: (1) run a full symmetric flow calculation, (2) compare the computed flow property numbers at two corresponding locations, and

(3) if the results are asymmetric, trace the computational steps back to the initial occurrence of the asymmetry. The other procedure concerning the mass and energy balances includes the following steps: (1) check global mass and energy balances, and (2) if mass or energy does not balance, isolate the source of the imbalance and fix it.

Numerical Stiffness due to Fast Reactions: Reaction and flow time scales are often different by one or more orders of magnitude. The difference of time scales can cause severe numerical stiffness problems. If the differential Arrhenius rate formulation is directly used in the source term of a lumped species equation during the flow field computation, a numerical calculation often diverges or becomes unstable. The numerical problem can be explained as follows. If a computational cell has a high concentration of feed oil vapor and a high temperature in the early stages of an iteration routine, then a very high reaction rate is predicted from the differential rate equation. This procedure, predicting only an initial reaction rate for the cell, may lead to a greatly overpredicted reaction rate. This overprediction may occur even when an upper bound is placed on the reaction rate via the eddy breakup model. The overprediction is often great enough to cause all the feed oil vapor to be consumed in that cell for that iteration. So, in the next iteration, the cell will contain oil products only, and the predicted reaction rate for that next iteration step will be zero because of the zero reactant concentration. During that next iteration with predicted zero reaction rate, the flow may bring in a large concentration of feed oil vapor, which will remain to yield a high reactant concentration in the third iteration of this sequence. Clearly, this sequence of computational events may repeat endlessly, causing either divergence of the computation or a continuing oscillation. A time-integral approach was developed to improve numerical convergence and stability (see Time-Integral Lumped Reaction Model Section).

Exit Boundary Flow Conditions: The free flow boundary condition is often used as a reasonable approximation at the outflow exit for a non-reacting flow calculation because the computation is or can be structured so that the flow is nearly fully developed at the exit boundary. However, the free flow boundary condition for a multiphase reacting flow calculation is not as successful. In the simulation of reacting flows, reaction often continues up to or very close to the exit plane (if it did not, the reactor would be larger than necessary), and consequently the flow is often never adequately developed to the point where the free flow boundary condition can be applied. In these cases, the calculation generally converges poorly and sometimes diverges. In calculating an FCC riser flow with the free flow boundary condition, the authors found that the calculation was not converged and the average mass residual was only 10^{-6}. Instead of using the free flow conditions, a velocity gradient was assumed at the outflow exit. The gradient was calculated by balancing global mass flow after every solution iteration. By using the new boundary treatment, the FCC flow calculation converged with an average mass residual less than 10^{-10}. For multiphase reacting flow systems, outflow boundary treatments need to be examined carefully, and appropriate treatments need to be developed.

Other Numerical Instabilities: Other numerical instability problems that the authors have experienced in a CFD calculation are listed here without discussion: (1) flow reversal point where a velocity component changes sign, (2) stagnation point where zero velocity is calculated, (3) high heat transfer rate between phases, (4) the onset of droplet vaporization, (5) the time scale difference between the flow of different phases, and (6) the difference between a continuous function used in the formulation and a discretized function used in the computation. Due to the length limit on this paper, the discussion of these problems will be deferred to future publications.

Code Validation

A CFD code solves approximate algebraic equations with iteration routines. Even when a numerical computation converges, the result may still be different from the true solution of the governing equations. Validation with experimental data is needed to justify confidence in a numerical simulation.

ICRKFLO has been validated with experimental data obtained from pilot- and commercial-scale FCC units. Good agreement was found between computed results and experimental data.

An FCC riser flow exhibits a U-shaped radial solid volume fraction profile. Many CFD codes have difficulty in predicting such a profile. By using the new particle-solid interaction model, ICRKFLO can predict the U-shaped profile very well. The pressure drops predicted by ICRKFLO also are found to be in good agreement with the measured values [14].

In a study of a thermal cracking process, ICRKFLO demonstrated its capability to predict product yields of four major lumps, pressure drop, and temperatures [15]. In a recent study of FCC riser flows, an experimental test matrix was selected and experiments were run. The predicted subspecies concentrations showed good agreement with experimental data (see Results and Discussion).

Results and Discussion

A CFD code for FCC riser reactor can be used for several purposes: (1) to provide detailed flow information that is related to the performance of the system; (2) to evaluate the impact of operating conditions, e.g., temperature, catalyst to oil ratio, etc., on the performance of the system; (3) to determine optimal operating conditions of the system; and (4) to explore innovative concepts to improve the performance of the system.

A major function of the ICRKFLO code is to predict product yields of a FCC riser reactor. Figure 3 shows the computed and measured product yields at various operating temperatures and catalyst-to-oil (C/O) ratios of an FCC riser. In the figure, the yields are plotted against various products, i.e., gasoline, diesel, liquid petroleum gas (LPG), and heavy oil. Product yields of two operating conditions are compared. At the higher temperature and C/O ratio, there is more LPG and gasoline and less diesel and feed oil. The dotted lines in Figure 3 represent the experimental measurements. The predicted product yields show good agreement with the experimental data.

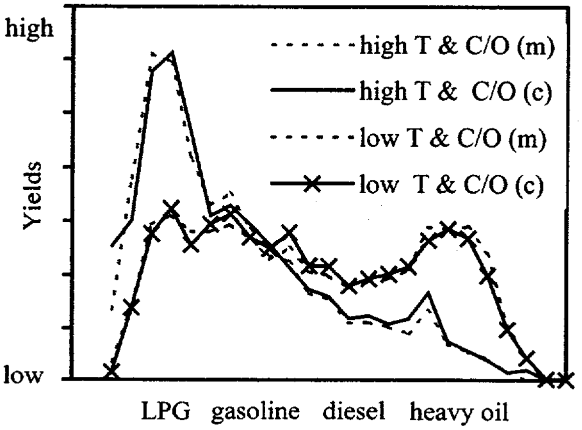

Figure 3 Comparison of Computed and Measured Product Yields at Various Operating Conditions

ICRKFLO has been used for various optimization studies. Figure 4 shows an example of the investigation of the impact of feed oil injection conditions on the product yields. Calculated yields of feed oil and gasoline are plotted versus spray injection Reynolds number. In the figure, the diamond and square points represent computed feed and light oil concentrations, respectively. These points appear to be very well correlated and can be represented by two simple curves as shown in the figure, a solid line for light oil concentration and a dotted line for feed oil concentration. A minimum and a maximum are found on the feed oil and the light oil curves, respectively. Since the oil conversion rate of an FCC unit is generally defined as one minus the feed oil concentration, the minimal feed oil yield is also the maximal oil conversion rate. This computational result suggests that maximum oil conversion rate and gasoline yield can be achieved by adjusting the feed injection Reynolds number.

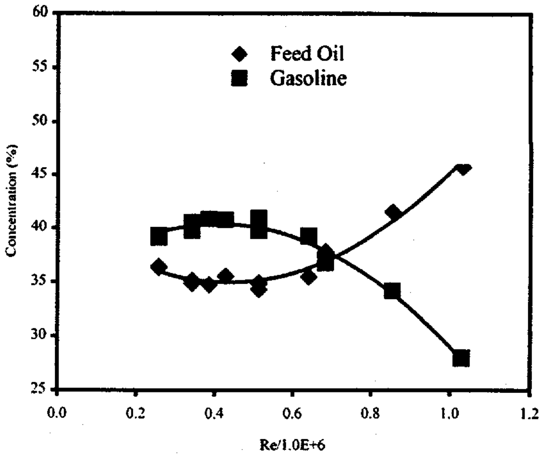

Figure 4 Product Yields vs. Injection Reynolds Number

ICRKFLO can also be used for the investigation of innovative FCC concepts, e.g., short-contact-time reactors and multistage reactors. Computational results [16] show that hydrodynamic processes, i.e., mixing and evaporation, have a strong impact on the product yields in a short-contact-time FCC riser unit.

Summary

Argonne National Laboratory has developed a copyrighted code, ICRKFLO, for the development of advanced multiphase reacting flow systems. It employs a hybrid hydrodynamic-chemical kinetic coupling technique and has been successfully applied to the simulation of FCC riser flows. 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 impacts of operating and design conditions on the product yields of an FCC riser reactor. 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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