

**A NUMERICAL INVESTIGATION OF THE SCALE-UP EFFECTS  
ON FLOW, HEAT TRANSFER, AND KINETICS PROCESSES OF FCC UNITS\***

S.L. Chang, C.Q. Zhou\*\*, S.A. Lottes, B. Golchert, and M. Petrick

Argonne National Laboratory  
9700 South Cass Avenue  
Argonne, IL 60439

\*\* Purdue University Calumet  
Hammond, IN 46323

RECEIVED  
SEP 28 1999  
OSTI

The submitted manuscript has been created by the University of Chicago as Operator of Argonne National Laboratory ("Argonne") under Contract No. W-31-109-ENG-38 with the U.S. Department of Energy. The U.S. Government retains for itself, and others acting on its behalf, a paid-up, nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.

Submitted to  
1998 International Mechanical Engineering Congress and Exposition,  
Nov. 15-20, 1998, Anaheim, CA  
sponsored by  
the K-11 committee of the Heat Transfer Division of ASME.

---

\* Work supported by U.S. Department of Energy, Assistant Secretary for Fossil Energy, under Contract W-31-109-ENG-38.

## **DISCLAIMER**

**This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, make any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.**

## **DISCLAIMER**

**Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.**

# A NUMERICAL INVESTIGATION OF THE SCALED-UP EFFECTS ON FLOW, HEAT TRANSFER, AND KINETICS PROCESSES OF FCC UNITS

S.L. Chang, C.Q. Zhou\*, S.A. Lottes, B. Golchert, and M. Petrick

Argonne National Laboratory  
9700 South Cass Avenue  
Argonne, Illinois 60439

\*Purdue University Calumet  
Hammond, Indiana 46323

## ABSTRACT

Fluid Catalytic Cracking (FCC) technology is the most important process used by the refinery industry to convert crude oil to valuable lighter products such as gasoline. Process development is generally very time consuming especially when a small pilot unit is being scaled-up to a large commercial unit because of the lack of information to aid in the design of scaled-up units. Such information can now be obtained by analysis based on the pilot scale measurements and computer simulation that includes controlling physics of the FCC system. A Computational fluid dynamic (CFD) code, ICRKFLO, has been developed at Argonne National Laboratory (ANL) and has been successfully applied to the simulation of catalytic petroleum cracking risers. It employs hybrid hydrodynamic-chemical kinetic coupling techniques, enabling the analysis of an FCC unit with complex chemical reaction sets containing tens or hundreds of subspecies. The code has been continuously validated based on pilot-scale experimental data. It is now being used to investigate the effects of scaled-up FCC units. Among FCC operating conditions, the feed injection conditions are found to have a strong impact on the product yields of scaled-up FCC units. The feed injection conditions appear to affect flow and heat transfer patterns and the interaction of hydrodynamics and cracking kinetics causes the product yields to change accordingly.

## NOMENCLATURE

a	stoichiometric coefficients for Reaction (a)
a <sub>c</sub>	stoichiometric coefficients for Reaction (c)
b	stoichiometric coefficients for Reaction (b)
C <sub>p</sub>	specific heat (J/kg/K)
E	activation energy (J/kmol)
f <sub>i</sub>	species concentration
h	enthalpy (J/kg)
k <sub>c</sub>	reaction rate constant

M	molecular weight (kg/kmol)
m <sub>ev</sub>	evaporation rate (kg/s)
n	particle/droplet number density
p	pressure (Pa)
R	universal gas constant (8315 J/kmol/K)
S	source term
T	temperature (K)
u	x-velocity (m/s)
v	y-velocity (m/s)
x	coordinate in the main flow direction (m)
y	coordinate in the cross-stream direction (m)

## Greek Symbols

$\alpha$	catalyst decay parameter
$\Gamma$	effective diffusivity (m <sup>2</sup> /s <sup>2</sup> )
$\theta$	gas volume fraction
$\rho$	density (kg/m <sup>3</sup> )
$\xi$	general flow property

## Subscripts

b	boiling point
d	droplet phase
i	gas species or droplet/particle size group
p	particle phase

## INTRODUCTION

Fluid Catalytic Cracking (FCC) technology was developed in the 1940's. Since then, it has become the most important process used by the refinery industry to convert crude oil to more valuable products such as gasoline. Today, the FCC units in U.S. refineries produce about 40% of the nation's gasoline pool. The FCC process has been greatly improved over the years by the refineries to compete in the global markets and meet more stringent environmental regulations. So

far, the development of catalysts has the most significant impact on the improvement of the FCC technology. In a modern FCC unit, it is essential to optimize product selectivity for each type of feed processed. Recently, the refineries have shown much interest in the advancement of the feed injection system and the development of short residence time riser units (Bienstock, et al., 1993). The 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 generally about 1 barrel per day (bpd) and the capacity of a commercial unit can be as high as 100,000 bpd. The process of scaling-up from a 1 bpd unit to a 100,000 bpd unit requires many intermediate steps for testing. These intermediate tests are expensive and time consuming. To facilitate and speed up the development of new and/or upgraded FCC systems, detailed knowledge of the relationships between process operating parameters and conditions within the system are needed. Such knowledge can be obtained by analysis of measurements from test units and computer simulation that includes the primary controlling physics of the FCC system.

Computer simulation of an FCC system began with a kinetic calculation based on an assumed or simplified flow field. Weekman and Nace (1970) used a three-lump cracking kinetic model to predict gasoline production in an FCC unit. The three lumps were feed oil, gasoline, and dry gas. Later, with the advancement of computational techniques and computer hardware, computational fluid dynamics (CFD) codes were used to simulate FCC flow. Theologos and Markatos (1993) incorporated Weekman and Nace's lumped kinetic model into a CFD code to simulate FCC riser reactors. The simulation included two-phase flow (gas and particle) and two cracking reactions of three lumped species: oil, gasoline, and dry gas. The code was used to predict engineering aspects of a riser reactor including pressure drop, particle slip velocity, and temperature distribution. A separate CFD code was developed at Argonne National Laboratory (ANL) for the simulation of FCC riser reactors (1996). The ANL code included three-phase (gas, liquid, and particle) flow and a four-lump kinetic model developed by Dave, et al. (1993). Later the code was expanded to include a general kinetic calculation for many product species (1997). This code has been validated with pilot-scale data and used to predict pressure drop, temperature, species, and catalyst distributions, and droplet evaporation rates of various FCC riser reactor designs.

The ANL code was used in a study to investigate the effects of riser size on the flow, heat transfer, and kinetics processes of FCC units. This paper reports the results of the study.

## THEORETICAL APPROACH

The ANL code, a multi-phase, multi-species, turbulent reacting flow simulation code, is called the Integral CraKing FLOW Simulation or ICRKFLO. A version of the code was specifically written for the FCC riser flow simulation. An FCC riser flow consists of numerous species from many reactions in the cracking process. To include all the reactions and species in a CFD computation is extremely difficult due to numerical stiffness problems. A hybrid technique is used to successfully compute both hydrodynamics and chemical kinetics of a large number of species lumps. The hybrid technique divides the whole FCC flow computation into two stages: (1) a reacting flow calculation and (2) a subspecies kinetics calculation. The reacting flow calculation is a typical hydrodynamic flow calculation with a small but sufficient number of lumped species to account for the

impact of density change due to reaction on the flow. The subspecies kinetics calculation calculates the transport of many subspecies (of order 10 to 100) based on the flow field calculated from the first reacting flow calculation.

## First-Step: Reacting Flow Calculation

An FCC flow consists of oil vapor, feed liquid droplets, and solid catalyst particles. The first-step reacting flow calculation solves for the flow properties of all three phases. An Eulerian approach is adopted to formulate the flow governing equations for all three phases. The gas phase formulation includes a simplified 4-lump kinetic model to account for the effects of density change due to reaction on the flow field.

### Gas Flow Formulation

The first-step calculation includes a simplified kinetic model. The kinetic model considers four lumped oil components in two cracking reactions. Oil species are grouped into four lumps: feed oil ( $P_o$ ), light oil ( $P_l$ ), dry gas ( $P_g$ ), and coke ( $C_k$ ). Feed oil consists of those oil species of a boiling point higher than 500 K. Light oil includes those species with a boiling point lower than 500 K and a carbon number higher than 5. Dry gas includes oil vapor of carbon number  $C_5$  and below. Coke a byproduct of the cracking reaction is mostly carbon. The cut-off boiling temperature between feed and light oil lumps may be 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. These reactions are denoted as follows:



where the stoichiometric coefficients,  $a_1$ ,  $a_2$ ,  $a_3$ ,  $b_1$ , and  $b_2$ , are expressed in mass fractions. Some inert/lift gas species, i.e., nitrogen and steam, can also be included in the gas flow calculation.

The gas flow is described by its properties, such as, pressure  $p$ , density  $\rho$ , temperature  $T$ , enthalpy  $h$ , species concentration  $f_i$ , and velocities ( $u$  and  $v$ ). Subscript  $i$  of the concentration variable  $f_i$  represents feed oil vapor, light oil vapor, dry gas, nitrogen, or steam. These properties can be determined from the state equations and the conservation equations. The state equations include the ideal gas equation (1) and the caloric equation (2).

$$p = \rho RT \sum_{i=\text{gas}} \left( \frac{f_i}{M_i} \right) \quad (1)$$

$$h = \sum_{i=\text{gas}} f_i C_{p_i} (T - T_r) \quad (2)$$

In equation (1),  $R$  is the universal gas constant and  $M_i$  is molecular weight of species  $i$ .

The conservation equations include the continuity, the  $x$ - and  $y$ -momentum, energy, and species equations. These equations can be expressed in a common form:

$$\frac{\partial}{\partial x} (\theta \rho u \xi - \Gamma_\xi \frac{\partial \xi}{\partial x}) + \frac{\partial}{\partial y} (\theta \rho v \xi - \Gamma_\xi \frac{\partial \xi}{\partial y}) = S_\xi \quad (3)$$

in which  $\xi$  is a general gas flow property,  $x$  and  $y$  are coordinates,  $\theta$  is gas volume fraction,  $\Gamma$  is effective diffusivity, and  $S_i$  is the sum of source terms. The general gas flow property is a constant 1 for the continuity equation,  $u$  for the  $x$ -momentum equation,  $v$  for the  $y$ -momentum equation,  $h$  for the energy equation, and  $f_i$  for the species equations. The effective diffusivity is calculated from both laminar and turbulent viscosities and turbulent viscosity is determined from a  $k$ - $\epsilon$  model modified for multiphase flow.

The continuity equation has a source term accounting for droplet evaporation. The evaporation rate is calculated in the droplet evaporation model. The momentum equations have source terms for the drag forces from droplets and particles and the enthalpy equation has source terms for the heat transfer to/from droplets and particles. The drag forces and heat transfer rates are calculated in the interfacial model. The species equations for the feed oil and dry gas have source terms to account for the consumption of feed oil and the generation of dry gas from the reactions (a) and (b). The species consumption/generation terms are calculated in a kinetic model. The governing transport equations for the inert gases have no source terms. The light oil concentration is obtained from the algebraic species conservation equation (4) after the feed oil, dry gas, and inert gas equations are solved.

$$\sum_{i=\text{gas}} f_i = 1 \quad (4)$$

The models used to determine the source terms are briefly described in the phenomenological models section.

### Liquid Flow Formulation

Feed oil is injected into the riser in sprays. Oil droplets in a spray generally have many sizes. The droplet size distribution is divided into various size groups. Droplets of a size group  $k$  are treated as a continuum flow. The droplet number density  $n_k$ , temperature  $T_k$ , and velocities ( $u_{d,k}$  and  $v_{d,k}$ ) of the size group are determined from the conservation equations of mass, momentum, and energy. These equations can be expressed in a common form:

$$\frac{\partial}{\partial x} (n_k u_{d,k} \xi - \Gamma \xi \frac{\partial n_k \xi}{\partial x}) + \frac{\partial}{\partial y} (n_k v_{d,k} \xi - \Gamma \xi \frac{\partial n_k \xi}{\partial y}) = S_\xi \quad (5)$$

in which  $\xi$  is a general droplet property,  $\Gamma$  is the droplet diffusivity resulting from interaction with turbulence in the gas phase, and  $S_\xi$  is the sum of source terms.

The droplet number density equation has a sink term for the evaporation rate of droplets. The evaporation rates of various size groups are calculated in the droplet evaporation model. The momentum equations have source terms for the drag force from gas and particles, and the energy equation has source terms for the heat transfer from gas and particles. The drag forces and heat transfer rates are calculated in the interfacial model.

### Particle Flow Governing Equations

Particles can also be divided into various size groups. Particles of each size group  $k$  are treated as a continuum flow. In this application, catalyst particles are a fairly uniform size (about 60 micron diameter), and therefore only one size group is used for catalyst particles. The particle number density  $n_k$ , temperature  $T_k$ , and velocities ( $u_{p,k}$  and  $v_{p,k}$ ) of the size group are solved from the conservation equations of mass, momentum, and energy. A special

particle property for the FCC flow simulation is the coke concentration  $C_k$ . Coke generated from the cracking reactions (a) and (b) precipitates on the surface of catalyst particles. A transport equation is needed for coke. The conservation and transport equations are all expressed in a common form similar to equation (5).

The particle number density equation has no source term. The particle momentum equations have source terms for the drag forces from gas and droplets and the energy equation has source terms for the heat transfer to/from gas and droplets. The drag forces and heat transfer rates are calculated in the interfacial model. The coke equation has a source term to account for the generation of coke from reactions (a) and (b). The coke generation rate is calculated in the kinetic model.

### Phenomenological Models

Phenomenological models include a time-integral lumped cracking model, a spray evaporation model, an interfacial interaction model, and a  $k$ - $\epsilon$  turbulence model. These models are briefly described as follows.

#### Time-Integral Lumped Cracking Model

The lumped cracking model was developed based on the lumped kinetics modeling works by Dave et al. (1993) and the integral reacting-flow time-scale-conversion method by Chang and Lottes (1993). Many reacting flow calculations experience 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 kinetic model is used to determine the consumption rate for the feed oil species, and the generation rates for light oil, dry gas, and coke. The species consumption/generation rates are used in the source terms of the gas species equations.

#### Spray Evaporation Model

Liquid feed oil needs to be vaporized so the oil vapor may be cracked into products. A droplet evaporation model was based on the fundamental physics of stationary single droplet evaporation and then modified for large groups of droplets in a connective environment. The model is used to calculate the local evaporation rate of the droplets. The evaporation rate is used in the source terms of the gas continuity and droplet number density equations.

#### Interfacial Interaction Models

Interfacial models were developed for the interactions between phases. The interactions include the exchanges of mass, momentum, and energy.

In the dilute flow region, oil droplets and catalyst particles are driven mainly by the drag force from the gas flow. An empirical Reynolds formula correlating the drag force with local flow properties and velocity difference is used to calculate the interfacial drag force. The drag force is used in the source terms of the gas, liquid, and solid momentum equations. Catalyst particles are the principal heat carriers, supplying energy to vaporize the oil droplets. An empirical Nusselt formula is used to calculate the heat transfer between particles and gas, and droplets and gas. The heat transfer rate is used in the source terms of the gas, liquid, and solid energy equations.

In a dense particle flow region, particle-particle and particle-wall collisions become significant. Particles can be moved from a high to a

low particle flux region. The particle diffusivity is a linear function of the gradient of local particle mass flux. The particle diffusivity is used in the particle momentum equation. Next to a wall, the collisions between particles and the wall cause the particle flow to lose its momentum. The solid shear stress is used as a boundary condition for the particle momentum equations.

If particles are packed, particles are directly in contact with the neighboring particles. A solid pressure is exerted on the particles. The solid pressure is generally assumed to be a function of local solid volume fraction when solid fraction exceeds a packed value. Lyczkowski et al. (1994) used local solid volume fraction to calculate solid pressure in a study of gas/particle flow in fluidized bed reactors. This approach is commonly used for the simulation of gas/particle flows, but when particle volume fraction is near the packed state, a small change in calculated solid volume fraction results in huge change in solid stress, which can easily cause numerical instability and divergence of the computation. An alternative approach that is much more numerically stable is to calculate solid volume fraction from an accumulated solid pressure. The solid pressure is used in the source terms of the particle momentum equations.

#### Multi-phase k-ε Turbulent Model

A turbulent flow consists of a spectrum of rotational eddies. The eddies, having a size ranging from a tiny, molecular sized rotation to one the size of the flow, can effectively transport and mix species, momentum, heat, and other transportable components or properties of the flow. The mixing rates of the turbulent motion are generally several orders of magnitude greater than those of the molecular diffusion. Patankar and Spalding (1972) developed a turbulence model employing the turbulent kinetic energy  $k$  and its dissipation rate  $\epsilon$  for single phase flows. Two additional transport equations, like Eq.(5), for these turbulent parameters were introduced. By solving these two transport equations, the turbulent diffusivity can be determined from the values of  $k$  and  $\epsilon$ . Among others, Zhou and Chiu (1983) later modified the turbulence model for multi-phase flows and an enhanced version of their model is used to model multiphase turbulence effects.

In the first-step reacting flow calculation, the governing equations of the flow field of an FCC riser are solved. In the riser, local flow properties such as velocity, temperature, catalyst particle number density, feed droplet number density, evaporation rate, and major species concentrations are calculated. These flow properties are then used to perform a detailed kinetics calculation.

#### Second-Step: Subspecies Kinetics Calculation

The major gaseous species in the flow calculation may be grouped (lumped) into broad categories: feed oil, light oil, dry gas, and inert gas. However, within these species lumps exist a very large number of oil subspecies produced from numerous kinetic reactions in the riser. These subspecies are not included in the first-step flow calculation due to numerical stiffness problems. After the first-step calculation, the transport equations of these kinetic subspecies can be solved on the pre-determined flow field. Free from the interactions of the pressure and velocity fluctuations, the calculation of the partially de-coupled species transport equations becomes very stable numerically.

#### Subspecies Selection

The de-coupled kinetics calculation allows for a high degree of flexibility in the selection of subspecies and associated reactions. For convenience in discussion, a set of subspecies lumps is used. The set of subspecies lumps consists of  $n-1$  oil vapor lumps ( $P_i$ ,  $i=2, n$ ) and a by-product coke ( $C_k$ ). Some subspecies are defined by their average carbon number:  $P_2$ ,  $P_3$ , and  $P_4$  represent  $C_2$ ,  $C_3$ , and  $C_4$ , respectively. Other subspecies ( $P_3-P_n$ ) are defined by boiling point range. The subspecies  $P_3$  represents  $C_5$  and those oil species that have a boiling temperature between room temperature and  $T_{b3}$ .  $T_{b3}$  is an arbitrarily chosen temperature higher than room temperature. The other species  $P_i$  ( $i=6, n$ ) represent those oil species that have a boiling temperature between  $T_{b,i-1}$  and  $T_{bi}$ .  $T_{bi}$  is an arbitrarily chosen temperature higher than  $T_{b,i-1}$ . Figure 1 plots the average molecular weights ( $w$ ), hydrogen atom to carbon ratios ( $H/C$ ), and carbon numbers ( $C$ ) versus the boiling temperature  $T_{bi}$  of the subspecies lumps.

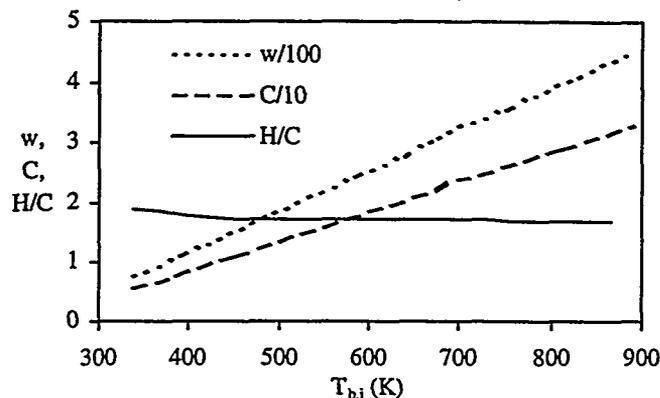
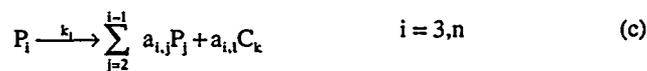


Figure 1 Fluid Properties of Hybrid Transport Species

#### Subspecies Reactions

The subspecies reaction model uses reaction set (c) in which a subspecies  $P_i$  is cracked into lighter species  $P_j$ ,  $j=2, i-1$ , and coke is a by-product.



In reaction set (c),  $a_{ij}$ 's are stoichiometric coefficients and  $k_i$ 's are the reaction rates. An Arrhenius type formula, Eq.(6), is used to express reaction rate of the  $i$ th cracking reaction.

$$k_i = k_{o,i} \exp[-E_i/R(\frac{1}{T} - \frac{1}{T_r})] \times \theta_i \exp(-\alpha_i f_{ck}) \quad i=3, n \quad (6)$$

in which,  $k_{o,i}$  is the rate constant,  $E_i$  is the activation energy, and  $\alpha_i$  is deactivation coefficient of the  $i$ th cracking reaction, and  $\theta_i$  is the catalyst volume fraction,  $T_r$  is the reference temperature, and  $f_{ck}$  is coke concentration. The catalyst volume fraction, temperature, and coke concentration are determined from the previous flow calculation step. The rate constants, activation energies, and deactivation coefficients need to be extracted from experimental data.

### Subspecies Transport Equations

A gas phase subspecies  $P_i$  is generated in the riser by the evaporation of oil droplets and/or the cracking reactions. The subspecies generated is transported by convection, diffusion, and turbulence in the flow and part of a subspecies is converted to lighter subspecies by the cracking reactions. The governing equation of the species concentration  $f_{P,i}$  can be derived as,

$$\frac{\partial}{\partial x}(\theta \rho u f_{P,i} - \Gamma_f \frac{\partial f_{P,i}}{\partial x}) + \frac{\partial}{\partial y}(\theta \rho v f_{P,i} - \Gamma_f \frac{\partial f_{P,i}}{\partial y}) \quad (7)$$

$$= f_{i,o} \dot{m}_{evp} + \sum_{j=i+1}^n a_{ji} k_j f_{P,j} - \sum_{j=2}^{i-1} a_{ij} k_i f_{P,i}$$

The density, velocity, temperature, evaporation rate, void fraction, catalyst volume fraction, and coke concentration determined from the previous flow calculation step are used in solving the species transport equation, Eq.(7).

### NUMERICAL SCHEME

From the previous sections, a set of governing equations are derived to solve for the velocity, pressure, density, temperature, and species concentration of an FCC riser flow. A control volume approach was used to convert the governing equations to algebraic equations on a discretized grid system. The grid system is staggered, consisting of three grids: an x-momentum grid for the gas phase x-momentum equation, a gas phase y-momentum grid, and a scalar grid for all the other equations. The algebraic equations are solved iteratively with proper boundary conditions. In the calculations, Patankar's SIMPLER computational scheme (1980) is used to solve the pressure linked momentum equations.

Grid sensitivity studies were conducted to choose a grid distribution which gave independent numerical results to three significant decimal places regardless of further grid refinement in order to conserve computational time and still provide adequately accurate results. Grids from 3000 to 5000 cells gave adequate grid independence for this study. An important feature of the control volume approach 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.

The simulated riser flow includes five gas species, five droplet size groups (120 micron mean diameter), a single particle size group (60 micron diameter), 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 gas mass flow rate) for the gas phase and  $10^{-7}$  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 iterations. Each iteration includes 10 gas phase calculations and 3 liquid and solid phase calculations. On a Pentium™ 133 personal computer with 16 megabytes of random access memory, using a 32-bit FORTRAN compiler, this computation takes about 4 hours for a grid of about 3000 cells. The subspecies calculation is generally much faster than the flow calculation depending on the number of subspecies to be calculated.

### VALIDATION

The ICRKFLO code has been validated by comparing calculated flow properties against several sets of experimental and test data. The flow properties used for comparisons include velocities, residence time, pressure drop, temperature, particle volume fraction, and most importantly product yields.

Figure 2 shows a comparison of measured and computed yield data over several operating conditions. Agreement of computational results with measured results is excellent. Some other validation results can be found in previous works (Chang et al., 1996, and Chang et al., 1997).

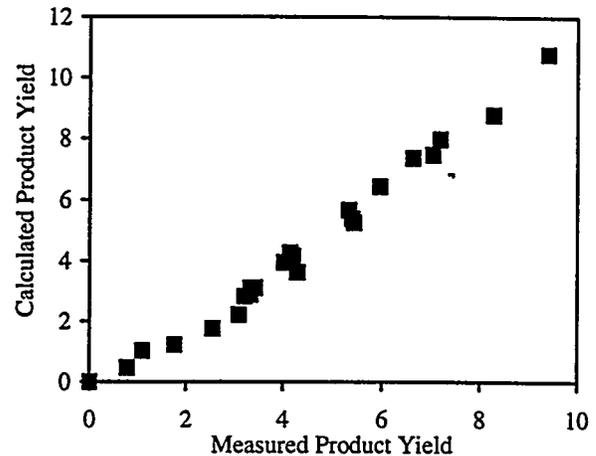


Figure 2 Comparison of Calculated and Measured FCC Riser Product Yields

### RESULTS AND DISCUSSION

To show the kinds of flow and process effects that occur when scale-up is done without preserving geometric or flow similarity a variety of simulations were performed. Some of the results are shown in Figures 3 to 8. These simulations were typical of the conditions used for scale-up in industrial FCC systems. In these cases many of the operating conditions remain the same, such as catalyst temperature at the inlet and feed oil droplet and catalyst size, while other parameters, such as inlet mass flow rates are scaled with the cross sectional area. The simulated risers were all the same height, about 20 meters. Riser diameters and injector configurations for five different cases are given in Table 1.

Table 1. Simulated Riser Diameter and Injector Configurations

Case/Riser Configuration	Riser Diameter (meters)	Feed Oil Inlet Location	Catalyst Inlet Location
i	0.01	bottom	right side
ii	0.1	bottom	right side
iii	1	bottom	right side
iv	1	bottom	left and right sides
v	1	left and right sides	bottom

Configuration (i) is a typical pilot scale FCC riser and configuration (v) is a typical commercial scale riser with the bottom modeled at about one to two meters above a typical Y-bend catalyst entry section. The other configurations are intermediate between the pilot scale and the commercial scale. Clearly the pilot scale and the commercial scale are very different. Residence times in the pilot and commercial scale risers tend to be about the same, in the range of one to two seconds, because riser heights and mass flow rates per unit cross section are about the same. By preserving residence time and scaling mass flow rates by the cross section area, industrial users hope that knowledge gained by pilot scale experiments about the process chemistry can be extrapolated to the commercial scale.

The simulations performed in this work are intended to show that the processes in a commercial scale riser are governed by a complex mixture of three phase mass, momentum, and heat transfer as well as the process chemistry. This complex mix of flow processes can and does change greatly when scale-up is limited to a simple capacity scale-up in number of barrels of oil processed per day. These FCC riser systems are so complex, however, with such a large number of non-dimensional scaling parameters, that preserving similarity in scaling up the process capacity of the system is just not feasible. Because preservation of similarity of system governing parameters is not feasible, gaining an understanding of the changes in flow field development that occur in capacity scale-up becomes important in the effort to optimize operation of the scaled up FCC unit.

### Flow Calculation

Due to space limitations only simulation results for one set of operating conditions and scaled mass flow rates are shown in Figures 3 to 8. A grayscale key is plotted on the right side of each figure indicating the corresponding shade for the property value. As shown in Figure 3, the velocity field is plotted as velocity vectors. The vector length is proportional to velocity magnitude. All the numbers are normalized. Results for other operating conditions do tend to show the same kind of trends, and the most important observation is that simple capacity scale-up yields very large differences in flow field patterns, including the distributions of gas velocity, particle number density, gas temperature, droplet number density, and feed oil, as shown in Figures 3 to 7. When capacity is scaled-up with an increase in diameter of the unit, cross section distributions tend to be much less uniform and this non-uniformity persists much farther up the riser, indicating that mixing rates are significantly slower in capacity scaled-up FCC units. This slower mixing rate and the non-uniform cross section distributions result in delayed vaporization and, in general, a delayed onset of crude oil cracking reactions. Light oil is the primary lumped cracking product, which includes gasoline. Slower mixing and vaporization delay onset of reaction and yield lower concentrations of the desired cracking product, light oil, as shown in Figure 8.

The gas velocity field is highly influenced by the mixing between catalyst and feed oil and the addition of new mass in the gas phase from vaporizing oil droplets, as shown in Figure 3. Clearly, for the pilot-scale inlet configuration flow development rapidly becomes uniform over the riser cross section. As the riser diameter is increased, the degree of the catalyst penetration to the center of the riser is decreased.

Heat from the catalyst vaporizes the feed oil droplet spray, and gas phase expansion resulting from vaporization is primarily what

drives the flow up the riser. Consequently, when the catalyst particles do not penetrate to the centerline well (Figure 4), the mixing time is increased and non-uniformity over the riser cross-section is more severe and persists farther up the riser. The consequent temperature non-uniformity in larger capacity FCC units (Figure 6) causes a large cross section variation in vaporization rates, which leads to unvaporized feed droplets persisting a long distance up the riser (Figure 5). These trends that occur with capacity scale-up lead to a number of problems, already noted. Large non-uniformity in catalyst and feed oil vapor distribution leads to non-uniformity in the local catalyst to oil ratio. The large non-uniformity in local temperature and catalyst to oil ratio can lead to large variations in the course and extent of feed oil vapor cracking reactions that affect the product yields at the riser exit as shown in Figures 7 and 8.

Using simulation to see the effects on the flow field and mixing patterns when capacity scale-up is done can provide insights that lead to changing the operating conditions or riser configuration in a way that yields better mixing and consequently higher yields of desirable refined petroleum products from the FCC units. Such insights become particularly important when commercial riser residence times become shorter, which is the current trend. For shorter residence times the portion of the riser over which mixing occurs increases. Pilot scale experiments cannot show how to optimize FCC risers under these circumstances. FCC riser simulations that use chemistry process data obtained from pilot scale experiments can provide the insights necessary to significantly improve the operation of commercial scale risers.

### Subspecies Calculation

A typical result of subspecies calculation is shown in Figure 9, which gives product yield distributions at the exit of the riser for different cases. A set of kinetic constants was determined to give the good match between the computational results and experimental data for a pilot scale riser (Chang et al., 1997). The same set of kinetic constants was used for the scale-up analysis. As indicated in Figure 9, with the pilot scale inlet configuration (cases i, ii, and iii), as the riser diameter increases, less light oil lumps are produced. As discussed earlier, this is caused by reduced penetration of catalyst and poorer mixing between catalyst and oil vapor, resulting in less cracking. For the commercial scale riser with the inlet configuration close to the real operating condition (case v), more light oil lumps are produced in comparison to the pilot scale inlet configuration (case iii). To produce desired optimum product yields, further parametric studies are needed.

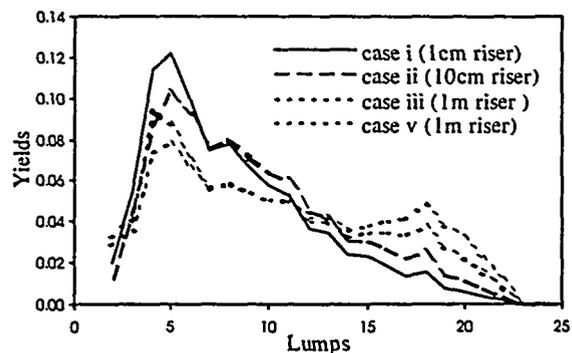


Figure 9 Yield distributions at the exit of risers

## CONCLUSION

The scale-up effects on the flow, heat transfer, and kinetics process of FCC riser reactors were investigated using a validated CFD code, ICRKFLO. A hybrid technique is used to couple the hydrodynamics and chemical kinetics in a way that can handle many species in the FCC cracking reactions. It has been found that the inlet configuration has a big impact on commercial scale risers. The feed injection conditions appear to affect flow and heat transfer patterns and the interaction of hydrodynamics and cracking kinetics cause the product yields to change accordingly.

## ACKNOWLEDGMENTS

This work was supported by U.S. Department of Energy, Assistant Secretary for Energy Efficiency and Renewable Energy, under Contract W-31-109-ENG-38 and managed by Erhping HuangFu of the Office of Industrial Technology.

## REFERENCES

- Bienstock, M.G., D.C. Draemel, P.K. Ladwig, R.D. Patel, and P.H. Maher, "A History of FCC Process Improvement Through Technology Development and Application," AIChE Spring National Meeting, Houston, TX, (1993).
- Chang, S.L., and S.A. Lottes, "Integral Combustion Simulation of a Turbulent Reacting Flow in a Channel with Cross-Stream Injection," Numerical Heat Transfer Part A, 24(1):25-43 (1993).
- Chang, S.L., S.A. Lottes, C.Q. Zhou, and M. Petrick, A Hybrid Technique for Coupling Chemical Kinetics and Hydrodynamics Computations in Multi-Phase Reacting Flow Systems, HTD-Vol. 352, Proceedings of the ASME Heat Transfer Division 2:149-158, the 1997 International Mechanical Engineering Congress and Exposition, Dallas, TX (November 16-21, 1997).
- Chang, S.L., S.A. Lottes, C.Q. Zhou, and M. Petrick, Evaluation of Multiphase Heat Transfer and Droplet Evaporation in Petroleum Cracking Flows, HTD-Vol. 335, Proceedings of the ASME Heat Transfer Division 4:17-27, International Mechanical Engineering Congress and Exposition, Atlanta, GA (November 17-22, 1996).
- Dave, N.C., G.J. Duffy, and P. Udaja, "A Four-Lump Kinetic Model for the Cracking/Coking of Recycled Heavy Oil," Fuel, 72(9):1331-1334, (1993).
- Lyczkowski, R.W., J.X. Bouillard, S.L. Chang and S.A. Lottes State-of-the-Art Review of Computational Fluid Dynamics Modeling for Fluid-Solids Systems, the International Symposium on Parallel Computing in Multiphase Flow Systems Simulations, 1994 ASME Winter Annual Meeting, Chicago, IL (November 6-11, 1994).
- Patankar, S.V. and D.B. Spalding, "A Calculation Procedure for Heat, Mass and Momentum Transfer in Three-dimensional Parabolic Flows", Int. J. Heat Mass Transfer, vol. 15, p.1787 (1972).
- Patankar, S.V., "Numerical Heat Transfer and Fluid Flow", Hemisphere, Washington, D.C. (1980).
- Theologos, K.N. and N.C. Markatos, "Advanced Modeling of Fluid Catalytic Cracking Riser-Type Reactors," AIChE Journal, 39(6):1007-1017, (1993).
- Weekman, V.W. and D.M. Nace, "Kinetics of Catalytic Cracking Selectivity in Fixed, Moving, and Fluid Bed Reactors," AIChE Journal, 16(3):397-404, (1970).
- Zhou, X.Q., and H.H. Chiu, "Spray Group Combustion Processes in Air Breathing Propulsion Combustors," AIAA/SAE/ASME 19th Joint Propulsion Conference, Seattle, Washington, AIAA-83-1323, (1983).

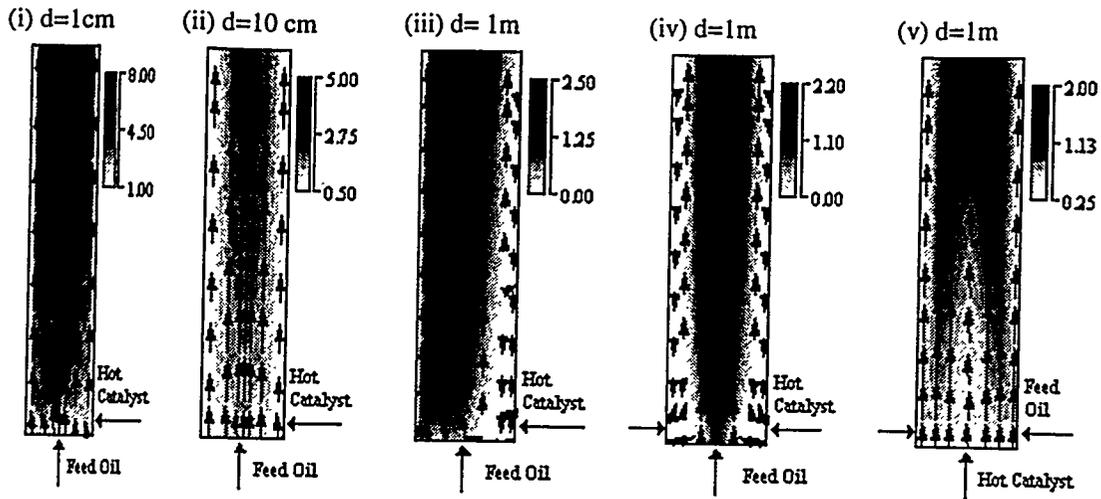


Figure 3 Gas Velocity Distribution (from the left to right: case i, ii, iii, iv, and v)

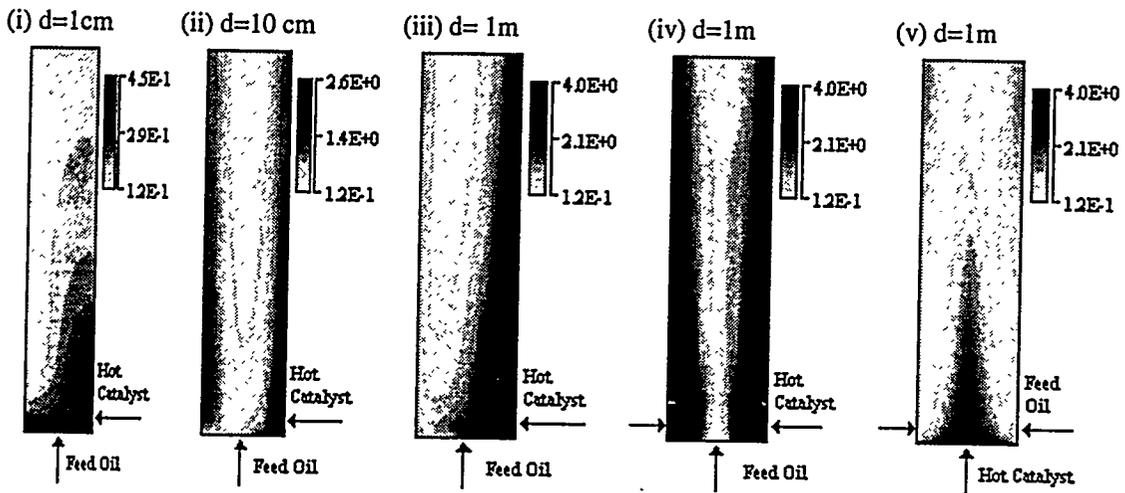


Figure 4 Particle Number Distribution (from the left to right: case i, ii, iii, iv, and v)

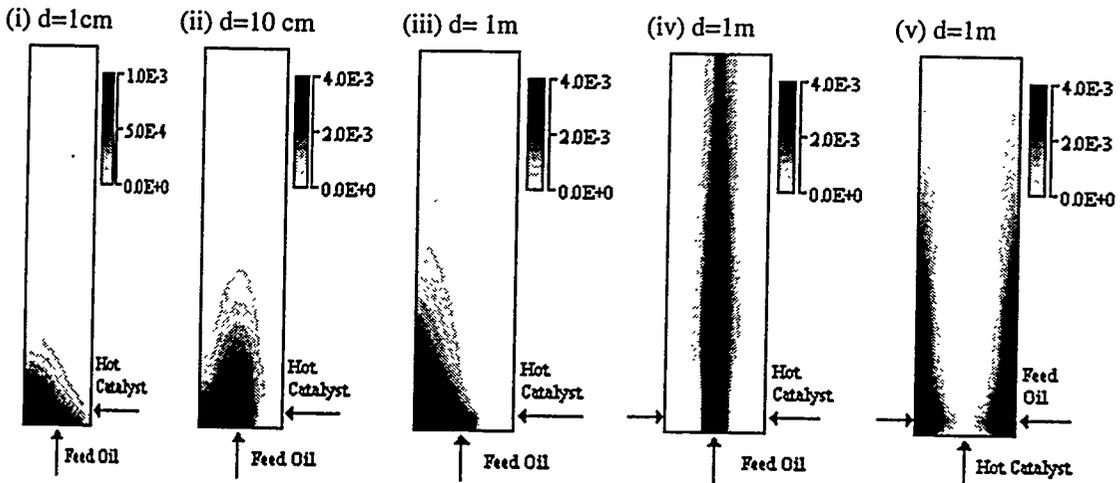


Figure 5 Medium Size Droplet Number Density Distribution (from the left to right: case i, ii, iii, iv, and v)

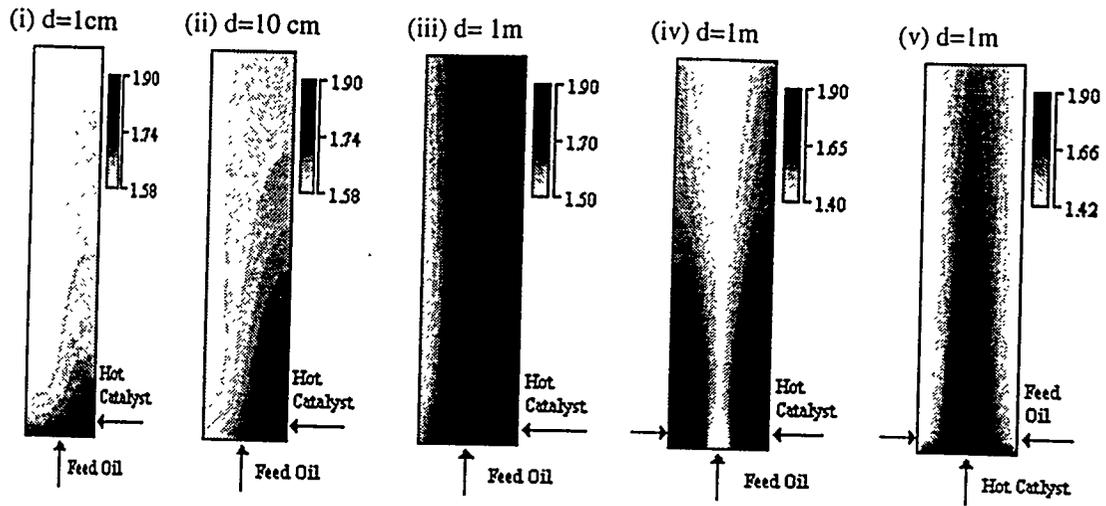


Figure 6 Gas Temperature Distribution (from the left to right: case i, ii, iii, iv, and v)

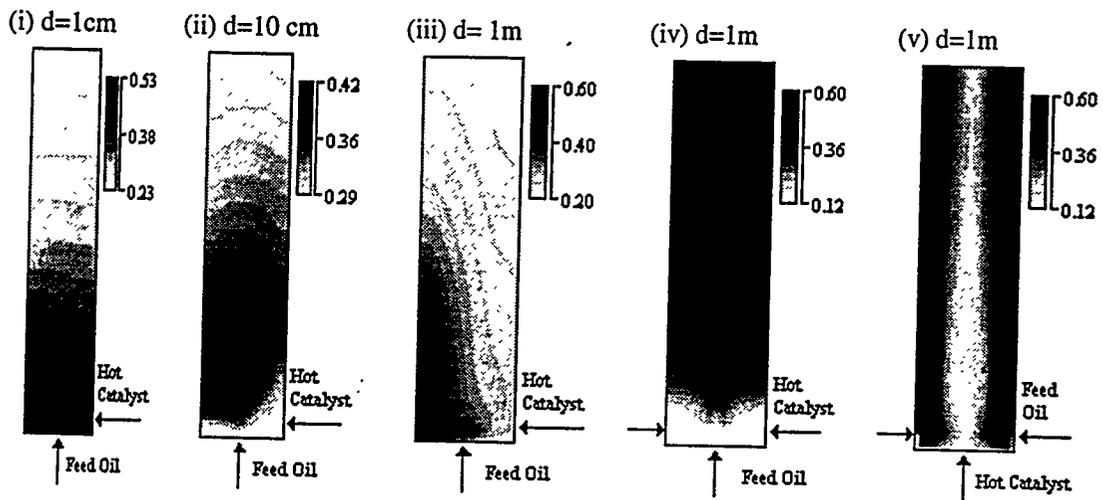


Figure 7 Feed Oil Distribution (from the left to right: case i, ii, iii, iv, and v)

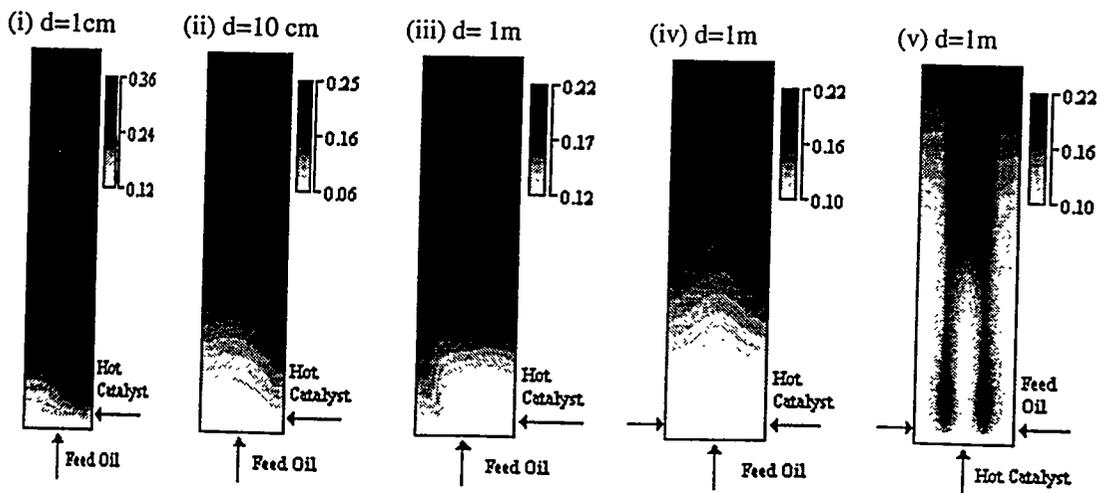


Figure 8 Light Oil Distribution (from the left to right: case i, ii, iii, iv, and v)