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A Validation Process for Multi-Phase Reacting Flow CFD Code

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DISCLAIMER

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Abstract

Computational fluid dynamic (CFD) code calculates flow properties for the analysis of a flow system. Flow properties are computed based on conservation principles and various phenomenological models. The accuracy of the computed flow properties highly depends on the validity of the models and the degree of numerical convergence. Validation of a CFD code is essential for application of an engineering system. Multiphase reacting flows are common in industrial applications and few CFD code are available. A CFD code was developed for the simulation of multiphase reacting flows. A validation process was also developed for such a CFD code. The validation was performed for several cases.

Keywords: CFD, Multi-Phase Flow, Cracking Reactions, Code Validation

INTRODUCTION

Many industrial devices are multiphase reacting flow systems. Among them are fluid catalytic cracking (FCC) reactors, glass melting furnaces, coal-fired combustors, and diesel engines. These devices that consume energy to produce various gasoline and glass products and electric power, also produce pollutant emissions. Facing the increasing pressure from the public, advanced devices need to be developed to increase energy efficiency and decrease pollutant emissions. The improvement of the systems relies on the understanding of the detailed physics and interaction of parameters controlling the operation of these systems. In the past, experiments and tests were the primary sources of the information. Recently, the rapid development of computational fluid dynamic (CFD) applications makes it possible that the CFD codes can be used to help understand the controlling processes of the systems and improve the systems.

A multiphase reacting flow system generally includes gas, liquid, and/or solid phases. A diesel spray includes gas and liquid droplets; a coal-fired combustion includes gas and pulverized coal particles; a glass-melting furnace includes gas, liquid glass, and solid batch material; an FCC reactor includes gas, liquid oil droplets, and solid catalyst particles. A multiphase reacting flow CFD code faces two challenging problems: (1) development of adequate models for interfacial interactions and (2) resolution of reaction species. The interactions between phases, including vaporization, nucleation, deposition, collision, drag, and heat transfer, are all complicated. Adequate models are lacking for several interfacial interaction processes, e.g., the dispersion of particles in a pipe flow by particle/solid collisions. Chemical reactions in an industrial system are complex and can generate hundreds or thousands species. For example, the cracking of heavy oil can produce thousands of lighter oil products, including diesel, gasoline, and olefins. To include all these reactions in a CFD calculation takes too much computing time and can cause severe numerical instability problems. Methodologies need to be developed to select reactions and species for a reasonable CFD calculation.

A CFD code for the simulation of a multiphase reacting flow often needs to develop adequate interfacial interactions and chemical reaction models specific for the system. The accuracy of the CFD calculation relies on the validity of these models and the degree of numerical convergence. A CFD code ICRKFLO was developed to simulate the multiphase reacting flow of an FCC riser reactor system. This paper presents the validation process for the ICRKFLO code.

A MULTIPHASE REACTING FLOW CODE

A CFD code is developed in four major steps: (1) formulation and discretization of the governing equations, (2) the development of iteration routines for solving the governing equations, (3) the coding of the equations and iteration routines, and (4) debug and validation.

Formulation of Governing Equation

ICRKFLO uses the Eulerian approach to formulate the governing equations for the gas, liquid, and solid phases. The approach divides liquid droplets and solid particles into size groups and treats each group as a fluid continuum. The governing equations for a multiphase reacting flow can be derived from the conservation laws of mass, momentum, and energy. The gas phase conservation equations include the continuity, momentum, energy, and species equations. These equations can be expressed in a common form:

$$\sum_{i=1}^{3} \frac{\partial}{\partial x_i}(\theta \rho u_i \xi - \Gamma_\xi \frac{\partial \xi}{\partial x_i}) = S_\xi \tag{1}$$

in which ξ is a general gas flow property (1, velocity u_i, enthalpy h, or species concentration f), x_i are coordinates, θ is gas volume fraction, Γ is effective diffusivity, and S_ξ is the sum of source terms. The effective diffusivity including both laminar and turbulent viscosities and the source terms are discussed in the phenomenological models section.

For k^{th} size group of the droplet/particle phase, the conservation equations of mass, momentum, and energy are expressed in a common form:

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

in which ξ is a general droplet/particle property (1, velocity $u_{k,j}$, temperature T_k,), Γ is the droplet/particle diffusivity resulting from interaction with turbulence in the gas phase, and S_ξ is the sum of source terms. The particle equations have an additional coke transport equation. Coke generated from the cracking reactions precipitates on the surface of catalyst particles.

The effective diffusivity in the conservation equations is calculated from both laminar and turbulent viscosities. Laminar viscosity is a fluid property and turbulent viscosity needs to be determined from a multi-phase k-ε turbulence model. The source terms of the governing equations are derived from various phenomenological models. The continuity equation has a source term accounting for droplet evaporation. The evaporation rate is calculated from a spray evaporation model. The species equations include source terms for species consumption/generation. The species consumption/generation rates can be derived using a time-integral lumped kinetic model. The momentum equations include source terms for the remaining viscous stress terms, drag forces between phases and momentum added or removed due to mass transfer between phases. The energy equations include source terms for the heat transfer between phases and heat of reaction in the gas phase. The drag forces and heat transfer rates are calculated from an interfacial interactions model. The particle flow is one of the most interesting and difficult to model because particle collisions are frequent and they tend to redistribute the particles in the flow. A particle-solid (particle-particle and particle-wall) interaction model was required to properly characterize the dense particle flow. More details of these models can be found in previous publications [1,2].

The CFD code uses a control volume approach to convert the governing equations to algebraic equations on a discretized grid system. The grid system is staggered and consists 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 converted algebraic equations can be expressed as:

$$a_p \xi(i,j,k) + \sum_{\alpha=\pm 1} \sum_{\beta=\pm 1} \sum_{\gamma=\pm 1} a_{\alpha\beta\gamma} \xi(i+\alpha, j+\beta, k+\gamma) = S_\xi(i,j,k) \qquad (3)$$

in which ξ is a variable to be solved, a_p and $a_{\alpha\beta\gamma}$ are constants derived from the conversion process, S is the source/sink term, and i, j, and k are indices of the grid location.

Iterative Solution Routine

The algebraic equations, Eq.(3), are solved iteratively with applicable boundary conditions. There are several layers of iteration routines in solving the algebraic equations. The first is the iteration for each flow property, the second is the iteration for the calculation of each phase flow, and the third is the global iteration for the calculation from one phase flow to the next. 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^{-8} for both the liquid and solid phases.

In order to conserve computational time and still provide adequately accurate results, grid sensitivity studies were conducted to choose final grids that gave grid-independent numerical results. For the current study, little would be gained from attempting to refine the grid to make results grid independent to more than three or four significant digits.

The simulated FCC reactor flow includes four gas species, five droplet size groups, a single particle size group, and a coke species carried by particles. A converged solution can be obtained in about 2000 iterations. Each iteration typically includes ten gas phase, three liquid, and three solid phase flow iterations. On a Pentium™ III 600 personal computer with 128 megabytes of random access memory, using a 32-bit FORTRAN compiler, this computation takes about four hours.

VALIDATION PROCESS

Due to the complexity of a multiphase reacting flow system, a CFD code often needs to include new models specifically developed for the flow system. Validation of these models and the code is essential for this CFD application.

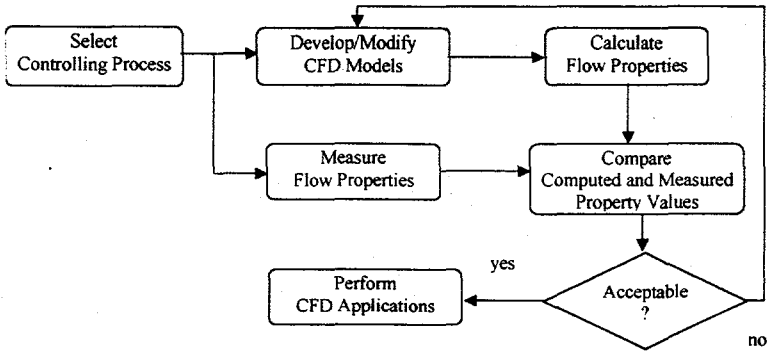


Figure 1 A Validation Process for CFD Model Development

Figure 1 shows a typical validation process for the development of CFD models. The process starts with the selection of a controlling process for the flow system. Next, a phenomenological model is developed based the understanding of the process and the model is used to calculate the relevant flow properties of the process. In parallel, tests or experiments are set up to measure the same flow properties. Then, the computed and measured property values are compared. If the comparison is not acceptable, the model is modified based the new information provided by the data and the entire process repeats. If the comparison is favorable, the model is used to perform CFD analysis of the multiphase reacting flow.

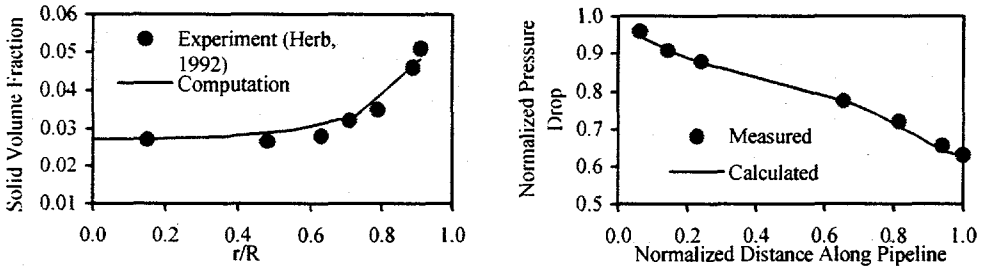
Several new interfacial interaction and cracking reaction models were developed for the simulation of an FCC riser flow. The models and the CFD code were validated with test/ experiment data. The results of the validation process are given in the following sections.

Multiphase Flow Characteristics

Interfacial interactions in an FCC riser include the exchanges of mass, momentum, and heat between phases. A multiphase CFD code usually uses empirical Reynolds and Nusselt formula to calculate the drag force and the heat transfer between particles and gases, and between droplets and gas, respectively. The vaporization rate of liquid spray is derived from the modified single droplet vaporization theory. The models appeared to be sufficient to calculate flow properties in pilot-scale risers (0.01-0.02m in diameter). Two pilot-scale riser units were setup in refinery sites for measurements of pressure drop, temperature, and flow residence time for various operating conditions. The computed flow properties were compared favorably with the test data [3].

However, the CFD code became inadequate when it was used to simulate larger-scale risers (0.1-2m in diameter). The catalyst distribution in a cross-section of these risers was found to be a U-shape as shown by the solid squares in Figure 2a. Conventional multiphase CFD codes with the above-mentioned interfacial interactions models calculated a complete different distribution, mostly flat. Clearly, these models are not adequate to simulate such a catalyst distribution. Since catalyst has the most dominant effect on the cracking process of a riser, new and improved models are certainly needed. A test program was setup by Particle Solid Research Institute (PSRI) for measurements of particle distributions and pressure drops in a 0.2m diameter riser for comparison with computed results of CFD simulations.

A new particle/solid interaction model was developed at Argonne National Lab (ANL) by adding particle diffusivity, shear stress and pressure terms to the flow calculation . Particle diffusivity is derived from the collision frequency among the particles; shear stress from the gradient of particle mass flux; and particle pressure from the direct particle contact in packed locations. With the new particle/solid interaction model, ICRKFLO calculated particle distribution and pressure drops for various riser/pipe flows to be compared with the PRSI data, a published data set in the literature, and several other industrial measurements. The comparisons were all favorable.



(a) Particle Number Density (b) Pressure Drop

Figure 2 Comparison of Calculated and Measured Flow Properties

Figure 2a shows a comparison of the computed and the measured solid volume fraction distributions in an FCC riser (Herb, 1992). The U-shape radial solid volume fraction profile is correctly predicted by the modified ICRKFLO code. In a separate study, pressure comparisons were made with measurements from a pulverized coal pipeline as shown in Figure 2b.

Reaction Models

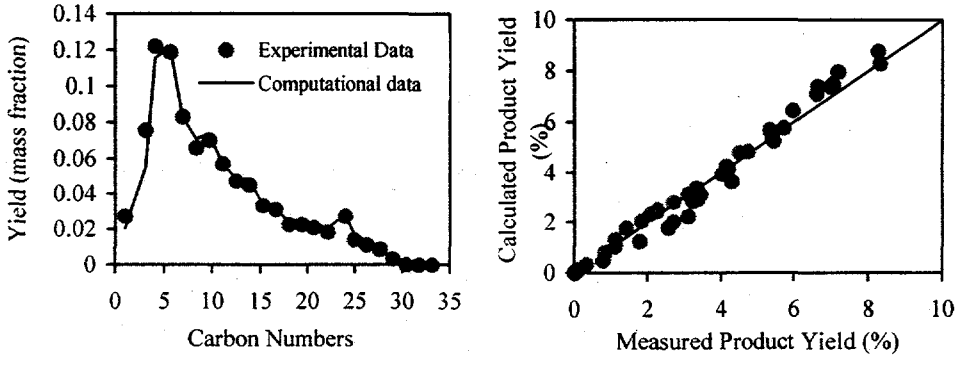
Cracking reactions in an FCC riser reactor produce thousands of oil species. Some of the reactions are well known but many are still under investigation. Lumped species consisting of a group of oil species and reduced kinetics of the lumped species are generally used in a CFD simulation. For example, a simple 4-lump cracking kinetics model [4] divides oil species into four lumps: heavy feed oil, light oil, dry gas, and coke. The model considers only two reduced reactions: (a) feed oil is converted to light oil, dry gas, and coke; and (b) light oil is further converted to dry gas and coke. In the above-mentioned pilot-scale tests, concentrations of the four lumps were measured in addition to the other flow properties. ICRKFLO used the 4-lump kinetics model to calculate species concentrations in these pilot-scale risers for various operating conditions. The computed results were in good agreement with the measured data.

The four oil lumps are not sufficient for the refining industry to determine the desired product yield distribution. Very few reaction models with more detailed lumping and cracking kinetic reactions are available in the literature. ANL has developed a methodology to extract kinetic constants for a general lumped cracking kinetics model from a few selected test data [5]. Based on the test data collected from a pilot-scale FCC riser unit, a general cracking kinetics model for many oil lumps was developed. The model assumed an oil species Y_i can be cracked into lighter species Y_j, j=1,i-1 and coke C_k is the by-product of the cracking.

$$Y_i \xrightarrow{k_i} \sum_{j=2}^{i-1} a_{ij} Y_j + a_{ik} C_k \tag{4}$$

$$k_i = k_{oi} \theta_p^{n_i} \exp(-E_i / RT) \tag{5}$$

in which a_{ij} are stoichiometric coefficients, k_{oi} is the pre-exponential constant, θ_p is the volume fraction of the catalyst particles, n_i and E_i are empirical kinetic constants derived from the test data, R is universal gas constant, and T is local gas temperature.



(a) (b)

Figure 3 Comparison of Calculated and Measured FCC Riser Product Yields

With the new lumped cracking kinetics model, ICRKFLO is used to calculate species concentrations along with other flow properties in an FCC riser reactor. The new kinetics model was validated with test data from pilot and commercial-scale FCC units. Figure 3a shows a case of comparison of the computed and measured species concentrations in an FCC riser. The agreement is excellent. Figure 3b shows a collection of computed and measured species for different risers and various operating conditions.

Applications

A validated CFD code can be an effective tool for the research and development of flow systems. The validated ICRKFLO code has been used to analyze the performance of FCC units in the following capacities: 1) trouble shooting, 2) parametric analysis, 3) performance optimization, and 4) evaluation of conceptual designs. The details of these applications are to be presented elsewhere.

SUMMARIES

Validation is a key to ensure accurate CFD analysis of multiphase flow systems. A CFD code and a validation process were developed for the simulation of multiphase reacting flow in an FCC riser reactor. New models including the interfacial interaction and cracking kinetics models were developed specifically for this application. The new models and the CFD code were validated with experimental and test data. Good agreements were obtained for several cases. The validated CFD code is now used to evaluate and improve existing as well as new FCC units.

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REFERENCES

[1] Chang, S.L., S.A. Lottes, C.Q. Zhou, B. Golchert, and M. Petrick, "Interactions of Multi-Phase Hydrodynamics, Droplet Evaporation, and Chemical Kinetics in FCC Riser Reactors," HTD-Vol. 357, Proceedings of the ASME Heat Transfer Division 1:261-269, the 7th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, Albuquerque, NM (June 15-17, 1998).

[2] 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, Proc. of the ASME Heat Transfer Division 4:17-27, International Mechanical Engineering Congress and Exposition, Atlanta, GA (1996).

[3] Chang, S.L., S.A. Lottes, and M. Petrick, *Development of a Three-Phase Reacting Flow Computer Model for Analysis of Petroleum Cracking,* Proceedings of 1995 Mid-America Chinese Professional Annual Convention, Itasca, IL, pp. 281-288 (June 23-25, 1995).

[4] 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).

[5] Chang, S.L., S.A. Lottes, and C.Q. Zhou, "Methodology for Extracting Local Constants from Petroleum Cracking Flows," U.S. Patent No. 6,013,172 (January 11, 2000).