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CFD CODE DEVELOPMENT FOR PERFORMANCE EVALUATION OF A PILOT-SCALE FCC RISER REACTOR*

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ABSTRACT

Fluid Catalytic Cracking (FCC) is an important conversion process for the refining industry. The improvement of FCC technology could have a great impact on the public in general by lowering the cost of transportation fuel. A recent review of the FCC technology development by Bienstock et al. of Exxon [1] indicated that the use of computational fluid dynamics (CFD) simulation can be very effective in the advancement of the technology. Theologos and Markatos [2] used a commercial CFD code to model an FCC riser reactor. National Laboratories of the U.S. Department of Energy (DOE) have accumulated immense CFD expertise over the years for various engineering applications. A recent DOE survey [3] showed that National Laboratories are using their CFD expertise to help the refinery industry improve the FCC technology under DOE's Cooperative Research and Development Agreement (CRADA). Among them are Los Alamos National Laboratory with Exxon and Amoco and Argonne National Laboratory (ANL) with Chevron and UOP. This abstract briefly describes the current status of ANL's work.

The objectives of the ANL CRADA work are (1) to use a CFD code to simulate FCC riser reactor flow and (2) to evaluate the impacts of operating conditions and design parameters on the product yields. The CFD code used in this work was originally developed for spray combustion simulation in early 1980 at Argonne. It has been successfully applied to diagnosing a number of multi-phase reacting flow problems in a magneto-hydrodynamic power train [4]. A new version of the CFD code developed for the simulation of the FCC riser flow is called Integral CRacKing FLOw (ICRKFLO). The CFD code solves conservation equations of general flow properties for three phases: gaseous species, liquid droplets, and solid particles. General conservation laws, expressed by elliptic-type partial differential equations, are used in conjunction with rate equations governing the mass, momentum, enthalpy, and species for a multi-phase flow with gas species, liquid droplets, and solid particles. Phenomenological models are used to characterize multi-phase interactions, including interfacial drag and heat transfer, droplet evaporation, and droplet and particle dispersion. The codes also include a two-parameter multi-phase turbulence model, and a hybrid chemical kinetic coupling technique that is numerically stable. The droplet dispersion and evaporation model divides the size distribution of liquid droplets into a number of size groups, calculates the evaporation rates of the droplets, and translates the evaporation rates into a droplet size distribution shift.

Unique features of the ICRKFLO code developed for the FCC riser flow simulation include: (1) a flow simulation of all gas, liquid and solid phases [5], (2) an integral approach for bridging the different time scales of flow and reaction [6], (3) a coke formation/transport model [7]; (4) a particle-solid model for the stratified particle flow in a riser, and (5) a hybrid approach to incorporate detailed petroleum cracking reactions into the hydrodynamic calculation. In parallel with the computer simulation work, experimental work on a pilot scale FCC riser unit was conducted. A test matrix that covers the main operating conditions was carefully selected. The operating parameters include reactor exit temperature, catalyst/oil ratio, catalyst activity, and

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pressure. Among these tests, some results were used to develop a kinetic model for the petroleum cracking processes and the others were used to validate the computer code. The kinetic model for the FCC riser flow simulation defines oil products with lumped subspecies and employs Ahrrenius type formulae to correlate the cracking reaction rates of a subspecies with local variables, i.e., temperature T, subspecies concentration f_i, catalyst volume fraction θ_p, and coke concentration f_k. A general formula is shown in the following,

$$\frac{df_i}{dt} = k_{o,i}\, e^{-(E_i/R)(1/T-1/T_r)}\, e^{-\alpha f_k}\, (\theta_p/\theta_{po})^{n_i} \times [f_i] \qquad (1)$$

Empirical constants in this formula include a pre-exponential constant $k_{o,i}$, an activation energy E_i, a catalyst reaction order n_i, and a deactivation constant α. All these constants need to be extracted from test data. Iteration routines were used to determine the kinetic constants for the many-species kinetic model. Due to the highly non-linear nature of the problem, not all iteration routines can generate a set of kinetic constants for predicting the test data. After many trials, a methodology was developed to generate a set of kinetic constants from selected test data [8]. At this point, the ICRKFLO code with a new petroleum kinetic model was completed. Next, ICRKFLO was validated by comparing calculated results against experimental data. Good agreements were found in the comparisons of various riser exit temperatures, catalyst/oil ratios, catalyst activities, and pressures. Finally, a CFD code ICRKFLO is ready to be used to evaluate the impact of operating conditions and design parameters on the product yields for the selected pilot-scale FCC unit. The work will be extended to include the simulation of commercial-scale FCC units.

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