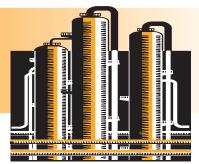
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Project Fact Sheet



DEVELOPMENT OF A COMPUTATIONAL FLUID DYNAMIC (CFD) MODEL OF FLUID CATALYTIC CRACKING (FCC)

BENEFITS

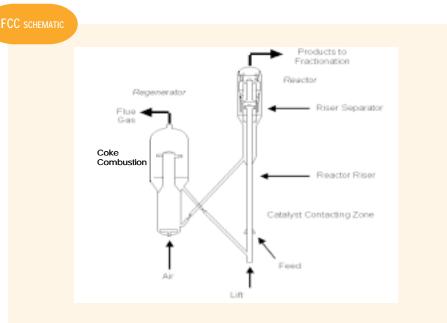
- Increase the yields of fluid catalytic cracker gasoline and alkylate by three to seven percent
- Achieve higher yields of transportation fuels per barrel processed
- Increase energy efficiency
- Reduce carbon dioxide (CO₂), sulfur oxides (SO_x), and nitrogen oxides (NO_x) emissions
- Reduce usage of crude oil

APPLICATIONS

Technology developed via this project will be available immediately to Chevron, the largest refiner in the United States. It will also be available to the remainder of the refinery industry from UOP, the world's leading supplier of fluid catalytic cracker technology. Existing fluid catalytic cracker units will be improved via revamps. Full penetration of the marketplace is targeted for 2010.

FCC MODEL CAN BE USED AS A TOOL TO GENERATE IMPROVEMENTS IN DESIGN AND OPERATING PARAMETERS, TO INCREASE PRODUCT YIELDS AND ENERGY EFFICIENCY, AND TO REDUCE EMISSIONS

Refiners are under pressure to adjust their product slate and/or specifications in response to market forces, changing crude supplies and environmental regulations, e.g., the 1990 Clean Air Act Amendment. The latter eventually required the refiners to reformulate their gasoline, and currently pressures are mounting to reformulate diesel fuels as well. The Fluid Catalytic Cracker is a key process in a refinery that can be used to alter product slates and/or increase yields. The key to achieving such changes is to develop a better understanding of the interaction of FCC riser hydrodynamics and cracking kinetics. OIT has supported the development of advanced FCC CFD models (analytical design tools) that can be used to define and evaluate optimized FCC operating conditions and potential hardware improvements to alter the FCC product mix. Recent advances at Argonne National Laboratory (ANL) in the development of two and three-dimensional reacting flow models (simulations) that integrate kinetics with hydrodynamics places ANL in an ideal position to further the development of the FCC design tool. ANL's research contribution and DOE's funding leverage the industry's investments; and they support the development of an advanced technology that meets DOE's mission for improved energy efficiency and reduced environmental impacts.





Fluid Catalytic Cracker schematic.

Project Description

Goal: Develop and validate a three-dimensional (3-D) integrated hydrodynamic-kinetic model that can be used as a design tool for modifying FCC hardware and processes to optimize operating conditions for specific feedstocks in order to obtain desired products, yields, and slates.

Current objectives are to:

- 1. Develop a cracking reaction kinetics model that will extend the operating range to short riser contact times (millisecond range).
- 2. Develop a 3-D, coupled hydrodynamic-cracking kinetics model that can be used in the design of advanced FCC units.
- 3. Validate the 3-D model with data derived from pilot plants, large-scale cold flow FCC mock-ups, and operating commercial FCC units.

Future objectives are to:

- 1. Develop a 3-D model of the regenerator that can be used to predict pollutant (NO,, SO) formation, coke combustion, etc.
- 2. Develop an overall FCC computer simulation, combining the validated riser and regenerator models.

Progress and Milestones

- ANL developed a 3-D, CFD code for the simulation of the FCC riser flow that encompasses three-phase flow and includes key submodels, such as:
 - a particle-solid interactions model
 - a hybrid flow-kinetics calculation routine
 - enhancements to intraphase mass, momentum, and heat transfer modelscoke formation and transport model
- Advanced numerical techniques have been developed and implemented to assure the integrity of the computational results which include:
 - an integral approach for handling multiple time scales
 - techniques for handling flow singularities and boundary conditions
 - sectional and blocked cell approach for handling long irregular riser geometries
- An experimental test program was conducted on Chevron's pilot scale FCC unit to provide data for developing kinetic cracking models and code validation.
- A new numerical iteration routine using the CFD calculations has been developed to extract kinetic constants from the test results. The numerical routine is able to extract a set of kinetic constants from a very limited set of runs -- approximately seven.
- The CFD code has been validated with pilot-scale test data. Currently the CFD simulation is being validated with data from a UOP commercial-scale FCC riser.
- A release version of the code is being prepared that uses advanced features of FORTRAN to provide for arbitrary grid sizes while using the minimum amount of memory necessary for a user-specified grid.



PROJECT PARTNERS

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