TITLE: COMPUTATIONAL AND EXPERIMENTAL MODELING OF SLURRY-BUBBLE-COLUMN REACTORS

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GRANT NO.: DE-FG-2698-FT40117

PERIOD OF PERFORMANCE: Sept 1, 1998 – July 30, 2001 DATE: April 20, 1999

ABSTRACT

OBJECTIVE

The overall objective of this research is to develop predictive hydrodynamic models for gas-liquid-solid catalyst reactors using momentum balances for each phase. The unique feature of our approach is the modeling of turbulence of the catalyst particles using kinetic theory.
This project is a collaborative effort between the University of Akron, Illinois Institute of Technology and two industries: UOP and Energy International.
The tasks involve the development of transient two and three dimensional computer codes for Fischer-Tropsch synthesis in slurry-bubble-column reactors, optimization,

comparison to data, and measurement of input parameters, such as the catalyst viscosity and effective restitution coefficients. Heat and mass transfer rates will be measured in the IIT two-story riser by injection of liquid nitrogen into an air-catalyst stream.

ACCOMPLISHMENTS TO DATE

A considerable progress has been achieved in understanding three-phase slurry-bubble-column reactors from the point of view of kinetic theory. Our paper describing the basic approach using kinetic theory to predict the turbulence of catalyst particles in a slurry-bubble-column reactor, based mainly on the work accomplished in a previous UCR grant, has been accepted for publication in a refereed journal. The simulation predicted the existence of multiple vortices in the LaPorte Air Products methanol reactor. We have searched and found analytical solutions for the existence of multiple circulation cells which support our numerical simulations. The essence of the solution is as follows. Suppose the frequency of the oscillation of the gravity wave in the slurry-bubble-column is one Hertz. (We computed 0.7 Hz). The pseudo-sonic velocity of the particles is about 1 m/sec. Then the wavelength is 1 m. Hence in a 5 m reactor there may be 5 circulation cells. However, if we neglect the particles the sonic velocity for the gas-liquid column is of the order of 10 m/sec. Then we obtain only one circulation cell as reported in the literature.

The thermal conductivity of FCC particles was calculated using the energy balance for the mixture. This procedure was very similar to the method of computation of FCC viscosity from measurement of radial velocity profiles. Similarly to the viscosity, the conductivity is a function of the volume fraction of FCC particles. At 5% particles, the kinematic viscosity is 0.15 cm^2/sec, while the thermal diffusivity is only 0.036 cm^2/sec. Hence the Prandtl number has a reasonable value of 4.2.

A simple collisional kinetic theory model for vaporization was developed and will be presented at the 1999 National Heat Transfer Conference. It gives large but reasonable vaporization rates.

SIGNIFICANCE TO FOSSIL ENERGY PROGRAMS

The world oil reserves are dwindling, while demand continues to increase. Hence, there is need to find domestic alternative sources for the fast depleting conventional petroleum and methanol gas for economic and security reasons. Coal liquefaction appears to be a good candidate. Slurry-bubble-column reactors are the preferred reactor type of synthesis gas conversion. Successful development of the hydrodynamic and Fischer-Tropsch kinetic models for slurry-bubble-column reactors will provide the needed base for design, scale-up and operation of less costly slurry-bubble-column reactors. As a consequence, the production of fuels from coal will proceed at a more efficient pace.

PLANS FOR THE COMING YEAR

The plan involves a combination of computational, experimental, and theoretical studies to gain an understanding of reacting fluid dynamics. The work will continue as described in the objective and work statement.

ARTICLES, PRESENTATIONS, AND STUDENT SUPPORT

Journal Articles (peer reviewed)

- Gamwo, I. K., Soong, Y., Lyczkowsky, R. W., "Numerical Simulation and Experimental Validation of Solid Flows in a Bubbling Fluidized bed", in press, *Powder Technology*, 1999

- Wu, Y. and D. Gidaspow, "Hydrodynamic Simulation of Methanol Synthesis in Gas-Liquid-Slurry Bubble Column Reactors", accepted, *Chemical Engineering Science*, 1999.

Conference Presentations

- Gamwo, I. K., "Modeling of Multiphase Reactors: Simulations and Experiments", Seminar, Dept. of Chemical Engineering, Ohio University, Athens, March 26, 1999

- Gidaspow, D., Mostofi, R., Neri A., and Wu, X., "Modeling Risers and Slurry-Bubble- Column Reactors using Kinetic Theory" to be presented at Fluid Particle Interactions V Engineering Foundations Conference, May 9-14, 1999, Santa Fe, New Mexico

- Gidaspow, D., " Fluidized Bed Hydrodynamics and Direct Contact Heat Transfer Using Kinetic Theory", to be presented at the 33rd National Heat Transfer Conference, August 15-17, 1999, Albaquerque, New Mexico

Students Supported under this Grant

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