TITLE: **ADVANCED COMPUTATIONAL MODEL FOR THREE-PHASE SLURRY REACTORS**

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ABSTRACT

OBJECTIVES

The general objective of this project is to provide the needed fundamental understanding of three-phase slurry reactors in Fischer-Tropsch (F-T) liquid fuel synthesis. The other main goal is to develop a computational capability for predicting the transport and processing of three-phase coal slurries. The specific objectives are:

- To develop a thermodynamically consistent rate-dependent anisotropic model for multiphase slurry flows with and without chemical reaction for application to coal liquefaction. Also to establish the material parameters of the model.

- To provide experimental data for phasic fluctuation and mean velocities, as well as the solid volume fraction in the shear flow devices.

- To develop an accurate computational capability incorporating the new rate-dependent and anisotropic model for analyzing reacting and nonreacting slurry flows, and to solve a number of technologically important problems related to Fischer-Tropsch (F-T) liquid fuel production processes.

- To verify the validity of the developed model by comparing the predicted results with the performed and the available experimental data under idealized conditions.

ACCOMPLISHMENTS TO DATE

A computational model for two-phase flow was developed and the flows in horizontal and inclined ducts were analyzed. The results were compared with the available experimental data and earlier model predictions and good agreements were observed. A computational model for analyzing two-phase solid liquid flows at various mass loading ratios was also developed and was successfully used to predict flow parameters down an inclined chute.

Progress was also made in studying two-phase bubbly flows with using the volume of fluid approach of FLUENT code. The Largragian trajectory of a dilute concentration of the solid phase is also studied. In a related modeling effort, progress was made in developing a rate dependent thermodynamically consistent model for slurry flows. The new model includes the effect of phasic interactions and appears to lead to anisotropic effective stress tensor. The formulation is being extended to cover three-phase liquid-gas-solid flows.

Progress was also made in analyzing turbulent heat transfer in turbulent two-phase. We are using an Eulerian/Lagrangian approach including the two-way interaction for two-phase flows. The model considers the thermal turbulent field characteristics and includes equations for temperature fluctuation in addition to the velocity turbulent kinetic energy and time scales of flow and thermal filed fluctuations.

Progress was also made in measuring concentration and velocity of particles of different sizes near a solid wall in a duct flow. The result shows that small particles have diffusion dominated concentration profiles near the wall, while the larger particles could acquire an inertial dominated counter gradient profile. We are also developing an experimental set-up for generating a plane bubble column for detail studies.

SIGNIFICANCE TO FOSSIL ENERGY PROGRAM

Converting coal to liquid hydrocarbon fuel by direct and indirect liquefaction processes has been of great concern to the development of coal-based energy systems. While the direct hydrogenation has been quite successful and was further developed in various forms, use of slurry phase Fischer-Tropsch (F-T) processing is considered a potentially more economical scheme to convert synthesis gas into liquid fuels. Slurry transport and processing and pneumatic transport of particles play a critical role in the operation, efficiency, safety and maintenance of these advanced coal liquefaction and coal-based liquid fuel production systems. Therefore, a fundamental understanding of reacting coal slurries will have a significant impact on the future of environmentally acceptable liquid fuel generation from coal.

Particle-particle and particle-gas/liquid interactions strongly affect the performance of three-phase slurry reactors used in coal conversion processes and are crucial to the further development of coal-based synthetic hydrocarbon fuel production systems. The scientific knowledge base for these processes, however, is in its infancy. Therefore, most current techniques were developed on an *ad hoc* and trial and error basis. This project is concerned with for providing the needed fundamental understanding of the dynamics of chemically active slurries and three-phase mixtures. In particular, a computational model for predicting the behavior of dense mixtures in coal liquefaction, gasification and liquid fuel production equipment will be developed.

PLANS FOR THE COMING YEAR

- To complete the thermodynamical consistent and anisotropic model and extend to multiphase slurry flows. To evaluate the model parameters for the cases of practical interest to liquid fuel production from coal.
- To further develop the volume of the fluid model for bubbly flows and to simulate technologically important problems related to Fischer-Tropsch (F-T) liquid fuel production processes.
- To complete the fabrication of the experimental setups for simple shear flow and bubble plane bubble column. To perform experimental measurements of the phasic properties in the simple shear flow device and in the plane bubble column.

ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Journals Articles (peer reviewed)

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G. Ahmadi, K. Elliott and W. Kvasnak, "An Experimental Study of Granular Flow in a Couette Flow Device," 1999 ASME Mechanics and Materials Conference, Blacksburg, VA, June 27-30, 1999.

C. He and G. Ahmadi, "Modeling of Particle Dispersion and Deposition with Thermophoresis in a Controlled Profile Combustor," 18th Annual Conference of the American Association for Aerosol Research, AAAR '99, Tacoma. WA, October 11-15, 1999.

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P.V. Skudarnov, L.L. Regel, W. R. Wilcox and G. Ahmadi, "Numerical Modeling and Flow Visualization in the Gradient Freeze Configuration During Centrifugation," Fourth International Workshop on Materials Processing at High Gravity, Clarkson University, Potsdam, NY, May 29-June 2, 2000.

A.R. Mazaheri, H. Zhang and G. Ahmadi, "A Centrifual Filtration Concept for Hot-Gas Cleaning," Fourth International Workshop on Materials Processing at High Gravity, Clarkson University, Potsdam, NY, May 29-June 2, 2000.

G. Ahmadi, "Advanced Computational Model for Three-Phase Slurry Reactors," Abstract and Research Accomplishments of University Coal Research Projects, pp. 91-91, University Coal Research Contractors Review Conference, NETL, Pittsburgh, PA, June 6-7, 2000.

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Students and Collaborators

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