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

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GRANT NO.: DE-FG2699-FT40458

PERIOD OF PERFORMANCE: September 1, 1999 to August 31, 2002 **DATE:** April 2000

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 also 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 loadings was also developed and was successfully used to predict flow parameters down an inclined chute.

Progress was made in developing a rate dependent thermodynamically consistent models for slurry flows. The new model includes the effect of phasic interactions and appears to lead to anisotropic effective stress tensor.Progress was also made in measuring concentration and velocity of particles of different sizes near a solid wall in a duct flow.

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 is 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 initiate simulating technologically important problems related to Fischer-Tropsch (F-T) liquid fuel production processes.
- To initiate the experimental measurements of the phasic properties in the simple shear flow device.

ARTICLES, PRESENTATIONS AND STUDENT SUPPORT

Journal Articles (peer reviewed)

He, C. and Ahmadi, G., "*Particle Deposition in a Nearly Developed Turbulent Duct Flow with Electrophoresis*," J. Aerosol Science, Vol. 30, pp. 739-758 (1999).

Cao, J. and Ahmadi, G., "*Gas-Particle Two-Phase Flow in Horizontal and Inclined Ducts*," Int. J. Engng. Sci, (In press).

Conference Presentations

G. Ahmadi and J. Cao, "*Anisotropic Model for Granular and Dense Two-Phase Flows*," 1999 ASME Mechanics and Materials Conference, Blacksburg, VA, June 27-30, 1999.

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.

H. Zhang and G. Ahmadi, "*Aerosol Particle Removal and Re-entrainment in Turbulent Channel Flows*," 18th Annual Conference of the American Association for Aerosol Research, AAAR '99, Tacoma. WA, October 11-15, 1999.

H. Zhang and G. Ahmadi, F. Fan and J.B. McLaughlin, "*Analysis of the Motion of Ellipsoidal Particle in Turbulent Channel Flows*," 52st Annual Meeting of American Physical Society, Division of Fluid Dynamics, New Orleans, LA, November 21-23, 1999.

Students and Collaborators

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