DOE DE-FG26-99FT-40584

PROGRESS REPORT

November 2000

ADVANCED COMPUTATIONAL MODEL FOR THREE-PHASE SLURRY REACTORS

Grant Number: DE-FG26-99FT-40584

Goodarz Ahmadi

Department of Mechanical and Aeronautical Engineering
Clarkson University

Submitted to

U.S. Department of Energy

National Energy Technology Laboratory

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

PI: Goodarz Ahmadi

STUDENTS: A.R. Mazaheri, H. Zhang, C. He, J. Cao, W. Kvasnak

INSTITUTION: Clarkson University
Potsdam, NY 13699-5725
Tel: (315) 268-2322
Fax: (315) 268-6438
Email: ahmadi@clarkson.edu

GRANT NO.: DE-FG2699-FT40458

PERIOD OF PERFORMANCE: September 1, 1999 to August 31, 2002

DOE Project Officers: Dr. Donald Krastman

SUMMARY

In the first year of the project, solid-fluid mixture flows in ducts and passages at different angle of orientations were analyzed. The model predictions are compared with the experimental data and good agreement was found. Progress was also made in analyzing the gravity chute flows of solid-liquid mixtures.

An Eulerian-Largrangian formulation for analyzing three-phase slurry flows in a bubble column is being developed. The approach uses an Eulerian analysis of gas liquid flows in the bubble column, and makes use of the Lagrangian particle tracking procedure to analyze the particle motions.

Progress was also made in developing a rate dependent thermodynamically consistent model for multiphase slurry flows in a state of turbulent motion. The new model includes the effect of phasic interactions and leads to anisotropic effective phasic stress tensors. Progress was also made in measuring concentration and velocity of particles of different sizes near a wall in a duct flow. The formulation of a thermodynamically consistent model for chemically active multiphase solid-fluid flows in a turbulent state of motion was also initiated.

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.

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 and liquid fuel production equipment will be developed.

PROGRESS REPORT

GENERAL

Progress was made in various aspect of the research project. The highlight of the accomplishment is first summarized. This is followed by a description of the progress made.

HIGHLIGHT OF ACCOMPLISHMENTS

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

An Eulerian-Largrangian approach for analyzing three-phase slurry flows in a bubble column is being formulated. The plan is to use an Eulerian analysis of gas liquid flows in the bubble column, and make use the Lagrangian particle tracking procedure to study the particle flows.

Progress was made in developing 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 wall in a duct flow. Formulation of a thermodynamically consistent model for chemical active multiphase turbulent flows is also initiated.

TWO-PHASE FLOWS IN HORIZONTAL AND INCLINED DUCTS

Using the earlier developed thermodynamically consistent model, a computational procedure for solving dense and dilute two-phase flows in ducts at various angle was developed. Figure 1 shows the configuration of the flow domain. The computational model predictions for mean flow and particle velocities, and phasic turbulence intensities were compared with the experimental data of Tsuji et al. (1989) for a horizontal duct flow. In addition, the variations of phasic shear and normal stresses, as well as the phasic fluctuation energy production and dissipation were also evaluated.

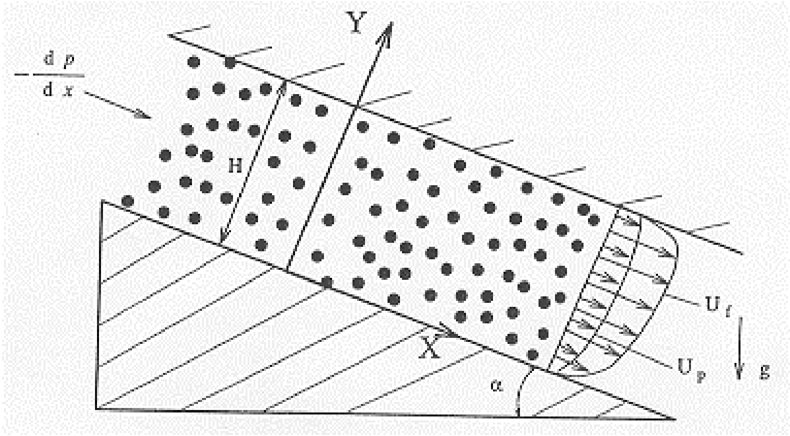

Figure 1. Configuration of the flow in duct an angle.

Using a Laser-Doppler Velocimeter (LDV), Tsuji et al. (1989) reported measurements of the phasic flow properties in a fully developed, two-phase turbulent flow in a horizontal channel with a height of 25 mm. In their experiments, polystyrene spheres with density of 1038 kg/m^3 and an average diameter of 1.1 mm were used. A restitution coefficients of r = 0.93 for particle-particle collisions, and a coefficient of dynamic friction $\mu = 0.28$ between a particle and the wall were used in the present study. These values are identical to those reported by Tsuji et al. (1989).

The phasic mean velocities, turbulence intensities and solid volume fraction profiles for a mass loading of m = 1 of 1.1-mm polystyrene spheres are shown in Figure 2. In this case, the channel mean velocity was = 7 m/s. Figure 1a shows that the mean particulate velocity has a nearly uniform distribution and is generally smaller than the fluid mean velocity. The fluid velocity develops an asymmetric distribution with the peak velocity drifting to above the centerline. This is because the particle drag retardation of the fluid phase is larger near the lower wall due to higher concentration there. Figure 2a shows that the predicted fluid phase velocity is in good agreement with the experimental data while the particulate phase mean velocity is somewhat underestimated.

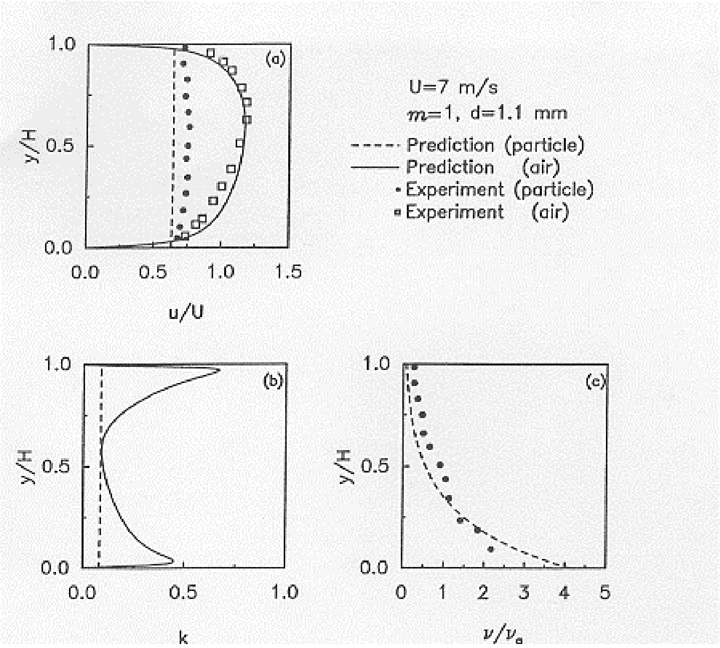

Figure 2. Variations of mean velocities, fluctuation kinetic energies and solid volume fraction profiles in a horizontal duct. Comparison with the data of Tsuji et al. (1989).

Figure 2b presents the predicted phasic fluctuation kinetic energy profiles. It is observed that the fluctuation kinetic energy for the fluid phase has peaks near both walls. The peak near the upper wall is larger than that near the lower wall. This implies that the presence of high concentration of particles reduces the fluid turbulence intensity. The particulate fluctuation kinetic energy profile is quite flat and smaller than that of the fluid phase, particularly near the walls. The solid volume fraction profile shown in Figure 2c clearly shows the strong segregation of particles toward the bottom wall. Clearly the gravity causes the heavier solid particles to migrate toward the lower wall of the horizontal channel. The experimental data for solid volume fraction, as reported by Tsuji et al. (1989), is reproduced in Figure 2c for comparison. It is observed that the agreement of the model predictions with the experimental data is quite good.

Figure 3 presents the model predictions for a gas-particle two-phase flow in a horizontal channel with a loading of m=3, an average solid fraction $\nu_a = 0.0062$ and a comparison with the corresponding experimental data of Tsuji et al. (1989). The rest of the parameters used in this simulation are kept the same as those used in Figure 2. Figure 3a shows the variation of phasic mean velocity profiles. It is observed that the particulate phasic mean velocity is almost constant across the channel and is about one half of the fluid mean velocity. Fluid mean velocity has an asymmetric profile with a peak in the upper part of the duct. Comparing Figures 3 and 2, it is observed that as loading, m, increases from 1 to 3, the particulate mean velocity remains nearly unchanged. The mean fluid velocity profile also has the same trend of variation, while the location of the peak mean velocity is drifted closer to the upper wall. As expected, the retardation effect of particle drag on the fluid phase increases with the increase of mass loading. Figure 3a also shows that the model predictions for the particulate mean velocity are in close agreement with the experimental data of Tsuji et al. (1989). Unfortunately, the experimental data for the fluid velocity was not reported for additional comparison.

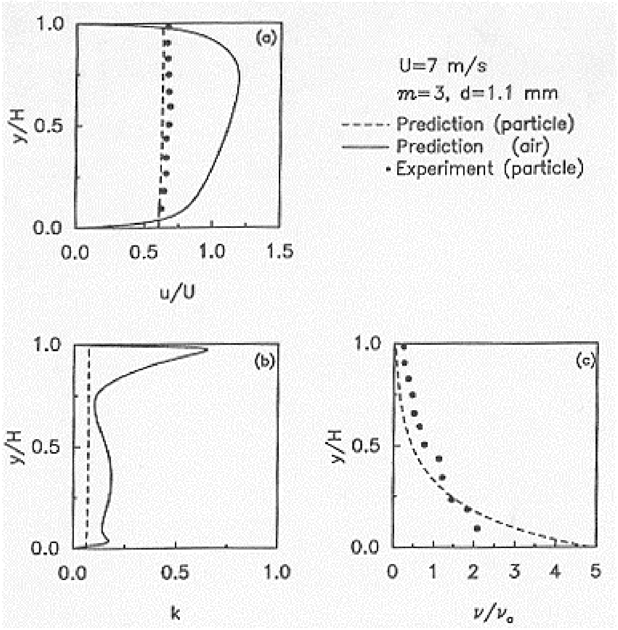

Figure 3. Variations of mean velocities, fluctuation kinetic energies and solid volume fraction profiles in a horizontal duct. Comparison with the data of Tsuji et al. (1989).

The corresponding phasic fluctuation kinetic energy profile for m=3 ($\nu_a = 0.08$) is shown in Figure 3b. It is observed that, while the particulate fluctuation kinetic energy is uniform and remained nearly unchanged, the fluid fluctuation kinetic energy has now a highly asymmetric distribution. Comparing Figure 3b to 2b, it is found that as the mass loading ratio increases, the fluid fluctuation kinetic energy near the bottom wall decreases, while that near the upper wall of the channel is not affected significantly. This is because the local concentration of the particles is quite low near the upper wall even at the higher loading of m=3. The solid volume fraction profile plotted in Figure 3c shows that the particle concentration is extremely high near the bottom wall. Figure 3c also shows that there is a reasonable agreement between the model prediction for the particle concentration and the experimental data of Tsuji et al (1989).

For a gas-particle mixture conveyed in a horizontal channel with a mass loading ratio of m=1 ($\nu_a = 0.0028$), and the mean average air velocity of U=15 /s, the model predictions for solid volume fraction are shown in Figure 4. There is a large particle concentration near the lower wall and the solid volume fraction decreases rapidly with increasing y/H (H being the height of the channel). The experimental data and the numerical simulation results of Tsuji et al. (1989) are also reproduced in this figure for comparison. Tsuji et al. (1989) used a Lagrangian trajectory analysis procedure for their particulate phase, which also allowed for collisional interactions. The present model prediction appears to be in good agreement with the simulation result of Tsuji et al. (1989). But both model predictions deviate somewhat from the experimental data. As pointed by Tsuji et al. (1989), this is mainly because the particles used in their experiment were not perfectly spherical. In fact, their experimental data showed that a small deviation of particle shapes from perfect spheres has a significant effect on the concentration profile.

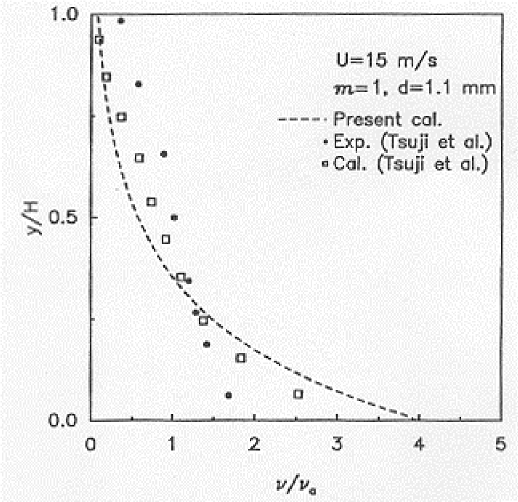

Figure 4. Variations of solid volume fraction profile in a horizontal duct. Comparison with the data and model of Tsuji et al. (1989).

EULERIAN-LAGRANGIAN ANALYSIS OF BUBBLE COLUMN

A combined Eulerian-Lagrangian model for analyzing the flow condition in the bubble column is being developed. The FLUENT code is being used to evaluate the unsteady liquid-gas flows in the bubble column. Lagrangian particle tracking approach is then used to analyze the motion of particles. The preliminary results of this approach are described in this section. The height of the column is 1 m with a width of 20 cm. Air enters from 1-mm holes at the bottom of the column. Figure 5 shows the concentration contours in the column at 1.16 second after the startup. (The gravity points from right to left in this figure.) The initial stages of air bubble formation are observed from this figure.

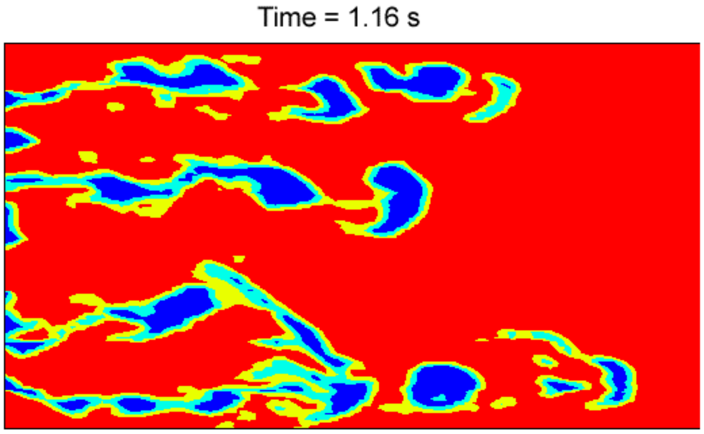

Figure 5. Concentration contours in the bubble column at t = 1.16 s.

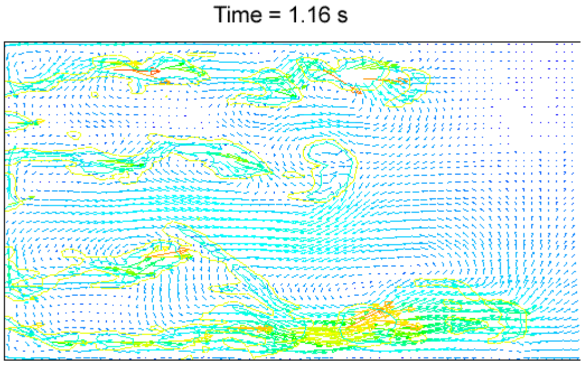

Figure 6. The velocity vector plot and concentration contours in the bubble column at t = 1.16 s.

The velocity vector field in the bubble column and the concentration contours at t = 1.16s are shown in Figure 6. It is noticed that the formation of gas bubble leads to rather complex flow pattern in the column. Figure 7 shows the corresponding concentration contours and sample trajectories for 100 μm particles. It is observed that some particles paths ends up in the bubble, while some others pass through the gas bubbles. This depends on the relative velocity between the bubble and the particle. (Here the mean particle trajectories were analyzed using the frozen field approach.)

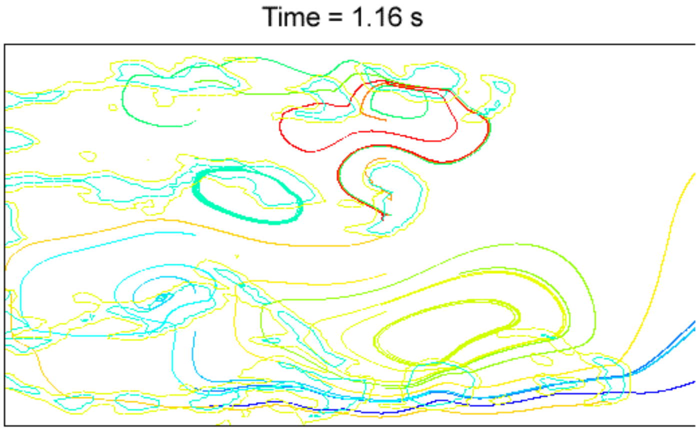

Figure 7. Concentration contours and sample particle trajectories in the bubble column at t = 1.16 s.

Figure 8 shows the variation of the velocity vector field and the concentration contours at t = 9.3 s. The bubble column is nearly fully developed at this time and contains many large and small gas bubbles. Formation of several recirculating flow regions in the bottom of the vessel can be clearly seen from this figure. Sample mean trajectories for 100 μm particle are also shown in this figure for comparison. The mean particle trajectories form loops in the recirculating flow regions. Figure 9 shows the corresponding particle trajectories when the effect of turbulence dispersion is included in the analysis. It is observed that the turbulence fluctuation field causes the particle to significantly disperse.

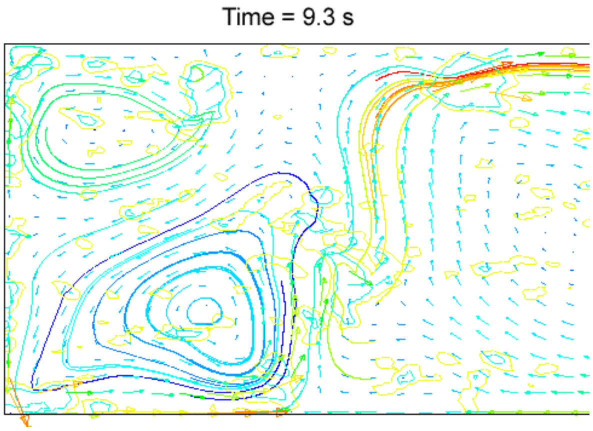

Figure 8. Concentration contours, velocity vector plot and sample mean particle trajectories in the bubble column at t = 9.3 s.

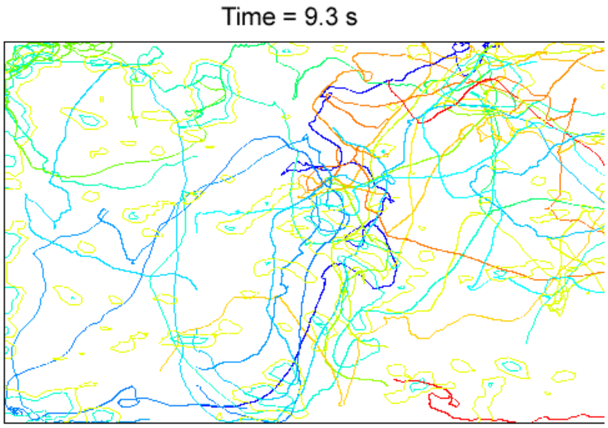

Figure 9. Concentration contours and sample random particle trajectories in the bubble column at t = 9.3 s.

EXPERIMENTAL STUDY

The earlier research provided a significant level of understanding of the process of particulate transport and deposition processes in turbulent flows. Accordingly, particles are transported by the mean flow field and are dispersed by turbulent diffusion. Near the wall, particles are entrained in the coherent wall vortices, which are the dominant flow structure in the sublayer. The downflow region of the vortices transport the particles to the wall. We plan to provide experimental data for particle concentration profile and velocity characteristics in the near wall region of a turbulent channel flow. Measurements are to be made up to very short distances from the channel wall. The nonintrusive, technique of Phase-Doppler Anemometry will be used in the experimentation. The technique allows for the simultaneous measurement of particle size and velocity.

CHEMICALLY ACTIVE TWO-PHASE FLOWS

Progress is made in the formulation of a thermodynamically consistent model for chemically active multiphase flows. The equations governing the phasic conservation of mass and energy, as well as the balance of momentum and fluctuation energy are being derived. The appropriate form of the mean entropy inequality is being derived. The entropy equation will be used for formulating thermodynamically consistent constitutive equations for chemically active multi-phase mixtures in a turbulent state of motion in the bubble column.

PLANS FOR THE COMING YEAR

- To complete the thermodynamical consistent and anisotropic model and extend the model to multiphase slurry flows in a bubble column.
- 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

Journals 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, Vol. 38, pp. 1961-1981 (2000).

Zhang, H. and Ahmadi, G., Aerosol Particle Transport and Deposition in Vertical and Horizontal Turbulent Channel Duct Flows, J. Fluid Mechanics, Vol. 406, pp. 55-88 (2000).

Fan, F-G. and Ahmadi, G., Wall Deposition of Small Ellipsoids from Turbulent Air Flows-A Brownian Dynamics Simulation, J. Aerosol Sci., Vol. 31, pp. 1205-1229 (2000).

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.

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.

G. Ahmadi and H. Zhang, "Resuspension of Particles in Turbulent Flows," Seventh International Symposium on Particles on Surfaces: Detection, Adhesion and Removal, Newark, NJ, June 19-21, 2000.

G. Ahmadi and H. Zhang, "Hot-Gas Flow and Particle Transport and Deposition in the Filter Vessel at Wilsonville," Seventeenth Annual International Pittsburgh Coal Conference, Pittsburgh, PA, September 11-14, 2000.

A.R. Mazaheri and G. Ahmadi, "Computational Modeling of a Centrifual Filtration System," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

D.J. Schmidt, G. Ahmadi, and G. Schmidt, "Dispersion of Droplets in a Turbulent Spray," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

M. Shams, G. Ahmadi and H. Rahimzadeh, "Transport and Deposition of Flexible Fibers in Turbulent Flows," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

H. Zhang, G. Ahmadi, R. Han and B.J. Greenspan, "Impact Breakup of Particle Pairs," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

H. Zhang, G. Ahmadi, R. Han and B.J. Greenspan, "Breakup of Pairs of Attached Particles in Simple Shear Flows," 19th Annual Conference of the American Association for Aerosol Research, AAAR 2000, St. Louis, MO, November 6-10, 2000.

Students and Collaborators

- A.R. Mazaheri, graduate (Ph.D) student, Mech. & Aero. Engineering, Clarkson University
- J. Cao, graduate (Ph.D) student, Mech. & Aero. Engineering, Clarkson University
- X. Zhang, visiting scholar, Mech. & Aero. Engineering, Clarkson University
- H. Zhang, graduate (Ph.D) student, Mech. & Aero. Engineering, Clarkson University
- C. He, graduate (Ph.D) student, Mech. & Aero. Engineering, Clarkson University (Curently with Corning)
- W. Kvasnak, graduate (Ph.D) student, Mech. & Aero. Engineering, Clarkson University (Currently with Pratt & Whitney)