Ash & Pulverized Coal Deposition in Combustors & Gasifiers

**Quarterly Report
October 1 - December 31, 1997**

**By
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Quarterly Technical Progress Report

(October 1, 1997 to December 31, 1997)

**ASH & PULVERIZED COAL DEPOSITION
IN COMBUSTORS & GASIFIERS**

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Submitted to:

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Project Period: September 1, 1994 to August 31, 1998

Contract Recipient: Clarkson University

Project Principal Investigator: Goodarz Ahmadi

DOE Project Officers: Dr. Norman Holcombe and Dr. Rodney A. Geisbrecht

DOE Program Administrator: Dr. Eric T. Bell

SUMMARY

Further progress in achieving the objectives of the project was made in the period of October 1 to December 31, 1997. The direct numerical simulation of particle removal process in turbulent gas flows was continued. Variations of vorticity contours which are averaged over a short time duration are studied. It is shown that the near wall vortices profoundly affect the particle removal process in turbulent boundary layer flows.

The sublayer model for evaluating the particle deposition in turbulent flows was extended to include the effect of particle rebound. A new more advance flow model for the near wall vortices is also used in these analysis. Sample particle trajectories are obtained and discussed.

Experimental data for transport and deposition of fibrous particles in the aerosol wind tunnel was obtained. The measured deposition velocity is compared with the empirical correlation and the available data and discussed.

Particle resuspension process in turbulent flows are studied. The model is compared with the experimental data. It is shown that when the effects of the near wall flow structure, as well as the surface roughness are included the model agrees with the available experimental data.

OBJECTIVE AND SIGNIFICANCE

In this section the objective of the project and its significance to the fossil energy program are outlined.

Objectives

The general goal of this project is to provide a fundamental understanding of deposition processes of flyash and pulverized coal particles in coal combustors and coal gasifiers. The specific objectives are:

- i) To provide a fundamental understanding of deposition mechanisms for coal and ash particles via digital simulations of turbulent flow conditions in a coal combustor and/or gasifier and the Lagrangian particle trajectory analysis.
- ii) To develop a semi-analytical model for wall deposition rate of coal and flyash particles in complex flow and thermal conditions of coal combustors and gasifiers.
- iii) To assess the relative significance of turbulent dispersion, Brownian diffusion, thermophoretic, electrostatic and surface forces, as well as particle collision and agglomeration under different conditions.
- iv) To assess the significant effects of nonsphericity of coal and ash particles on their transport and wall deposition processes.
- v) To provide a detail understanding of wall deposition mechanisms for relatively compact, as well as elongated flyash and pulverized coal particles via a direct numerical simulation of near-wall turbulent flows.
- vi) To experimentally verify the validity of the simulation and analytical results for deposition rates of flyash and pulverized coal particles in the size range of 2 to 100 μm in the upgraded MAE Aerosol Wind Tunnel.

Significance to Fossil Energy Program

Transport and deposition of particles play a critical role in operation, efficiency, safety and maintenance of coal combustors and gasifiers. Turbulent mixing of pulverized coal significantly affects the efficiency of combustion, pyrolysis and gasification processes. Deposition of flyash and other particles on the wall leads to the formation of coal slag. Corrosion by coal slag is a serious problem in coal-gasification and combustion systems. Presence of particulate contaminant in the combustion product is also a major source of air pollution in coal energy systems.

No completely satisfactory model describing the motion of a coal or ash particle in the highly transient turbulent flow and thermal conditions in coal combustors and gasifiers exists. More importantly, the controlling mechanisms for deposition of particles on surfaces in a turbulent stream with strong temperature gradients are not

fully understood. Without such an adequate understanding, providing n-litigation measures against slag formation and/or improving the efficiency of coal combustors are not possible.

The general goal of this research is to provide a fundamental understanding of transport and deposition mechanisms of ash and pulverized coal particles in complex turbulent flow conditions in a coal-fired combustor or in a coal gasifier. The other main objective is to develop an accurate computational model for simulating motions of ash, pulverized coal, and soot particles in complex geometries of coal (gas turbine) combustors and gasifiers. Availability of these tool and knowledge base will be indispensable for developing an environmentally acceptable coal energy system.

PROGRESS REPORT

This section outlines the progress made in the period of October 1 to December 31, 1997 in accomplishing the tasks of the project. We have made considerable progress in modeling the particle transport, deposition and resuspension processes in turbulent gas flows, and the experimental study of deposition of nonspherical particles. This quarterly report describes our new findings for particle removal and particle transport and deposition in turbulent recirculating flow fields. In addition, the progress made in direct digital simulation of particle removal in duct flows is described.

COMPUTATIONAL MODELING

In the earlier reports, we have described the simulation of the gas flow velocity field in complex passages with the use of the STARPIC-RATE computer code that makes use of an advanced anisotropic turbulence model. The particle equation of motion which includes the Stokes drag, the turbulence dispersion effects, the lift force, as well as, the Brownian effects was also used in the simulation. The instantaneous turbulence fluctuations are simulated as an anisotropic continuous Gaussian random vector process. The computational model have been tested earlier for several cases and its accuracy was verified. Studies concerning dispersion and deposition from a point source of particles in a turbulent air flow and deposition from uniform concentration in a circular cylindrical duct and in recirculating flow region were studied before. The details of flow in a duct using a direct numerical simulation procedure and the corresponding particle resuspension are being studied. A summary of the progress made is presented in this section.

Direct Numerical Simulation of Particle Resuspension

To provide a fundamental understanding of particle resuspension process in turbulent flows, a direct numerical simulation of Navier-Stokes equation was performed. The Navier-Stokes equation is solved directly using a pseudo-spectral computational scheme. The computational grid and the numerical procedure used was outlined in the earlier reports. The velocity vector fields at different times and different planes and the equation governing the motion of particles were presented in the earlier reports. The iso-vorticity contours and the structure of near wall flow were discussed in the last

quarterly report. A series of computer simulations for particles that were initially distributed (with a statistically uniform distribution) on the xy-plane at a distance of $Y_0 = 1$ wall unit from the upper wall were performed. It was shown that the locations of ejected particles (that reach different levels) form lines with spacings of about 100 to 150 wall units. These variations appeared to be consistent with the available flow visualization results for the streaky structures in the viscous sublayer. It was also observed that these lines shifted to new locations for time duration of 200 to 400 wall units. It was conjectured that the shifting of lines is due to the break-up (or lifting) of vortices and formation of new ones at other locations as time progresses. Those results suggested that the near wall streamwise structure (coherent vortices) plays a dominant role in the particle entrainment process.

Figures 1-3 show sample trajectories corresponding to the particle line-up near $z^+ 530$ in the figures of earlier reports. These particles reach to a distance of 4 wall units away from the upper channel wall in a time duration of 200 wall units. Figure 1 shows that the ejected particles originate from a region in the xz-plane which has an area of about 10×20 in wall units. The particles also drift to the left during their transport along the channel. Figure 2 shows the yz-projection of particles trajectories. A side way motion is observed from this figure. Figure 3 shows the particle trajectories in the xy-plane. It is observed that the particles lift-off initially, with a slope of approximately $1/100$ for a distance of about 1 wall unit (in the Y_0 -direction), and then their trajectory slope becomes sharper and reaches to about $1/50$.

Figure 1. Particle trajectories in the xz-plane corresponding to the particle lineup near $z^+ = 530$.

Figure 2. Particle trajectories in the yz-plane corresponding to the particle lineup near $z^+ = 530$.

Figure 3. Particle trajectories in the xy-plane corresponding to the particle lineup near $z^+ = 530$.

The particle statistics in the yz-plane are shown in figure 4. To perform the analysis for different groups of particles, their trajectories are translated (in the z-direction) so that the particles have a common location at the last time step. The mean,

the standard deviation and the absolute maximum and minimum trajectories are then evaluated. It is observed that the statistical trajectories of particles are inclined to one side. The results presented in Figs. 1-4 show that a single streamwise vortical structure, with its accompanying upflow, is responsible for the entrainment of this group of particles. This vortex is also observed in the averaged vorticity plot of the last report.

Figure 4. Particle trajectories statistics in the yz-plane corresponding to the particle lineup near $z^+ = 530$.

EXPERIMENTAL STUDY

The goal of the experimental study is to provide the much needed data base on deposition rates of (generally nonspherical) coal and flyash particles. The experimentation is being performed in the horizontal aerosol wind tunnel and for glass fiber transport and deposition. The geometry of the wind tunnel and the experimental procedure were described in the earlier reports. In the earlier report, the experimental data for the non-dimensional deposition velocity versus the non-dimensional equivalent particle relaxation time, τ_{eq}^+ (based on the orientation averaged resistance) were presented. Use of the τ_{eq}^+ -scaling clearly shows the significant increase of the deposition velocity with aspect ratio of the fiber. This observation is as expected because the increase in aspect ratio increases the wall capture efficiency by the interception mechanism. The flyash particles are nonspherical and, generally, irregular in shape. To provide an understanding of the transport of this kind of particles, the experimental results for the deposition rates of irregular shaped paper fibers using τ_{eq}^+ -scaling are described in this section.

Figure 5 shows a micrograph picture of deposited paper fibers on the gold plate. It is observed that the particles are irregular shape and vary in size from 1 to 20 μm with

aspect ratios of 3 to 10. In processing of images, the limit on resolution was determined to be about $1.0\text{ }\mu\text{m}$. Therefore no particles smaller than $1\text{ }\mu\text{m}$ were considered in either the concentration or the deposition measurements. Furthermore, due to the lack of sufficient statistical samples, particles with aspect ratios larger than 10 were also discarded.

Figure 5. Micrograph of irregular shaped paper fibers.

Figure 6 shows the non-dimensional deposition velocity versus the non-dimensional equivalent particle relaxation time (based on the orientation averaged resistance) for the paper fibers. The experimental data of Shapiro and Goldenberg (1993), along with the prediction of the empirical relation given by equation (26) for fixed minimum diameter of 1, 2, and $5\text{ }\mu\text{m}$ are presented in this figure for comparison. It is observed that the experimental data for the paper fibers are clustered around those for the $5\text{ }\mu\text{m}$ minimum diameter glass fibers with a few being near the data for the $2\text{ }\mu\text{m}$ glass fibers. Figure 6 also shows good agreement between the experimental data and the model predictions. This figure also indicates the increase of the deposition velocity with particle aspect ratio.

SUBLAYER MODEL FOR PARTICLE DEPOSITION

The significance of streamwise coherent vortices in the turbulent shear flows on particle deposition and removal processes was emphasized in the earlier reports. A simplified sublayer flow model for analyzing particle deposition including the effects of rebound from surfaces was described in the earlier reports. The present study is concerned with evaluating the particle deposition rate based on their motions in the near wall vortices. The equations for particle motion in the turbulence near-wall vortices were described in our earlier works. The details of the interactions of particles

with the near wall eddies were described in the last quarterly report, where a number of sample trajectories were also presented.

Figure 6. Measured deposition velocity of paper fibers versus equivalent relaxation time for different effective minimum diameters.

Particle motion and rebound analyses in shear layer vortices described earlier is applied to the turbulent deposition processes. In particular, the particle deposition velocity, which is defined as the particle flux to the wall divided by the particle concentration far away, is evaluated.

The particle deposition due to inertia-interception process may be evaluated based on the limiting trajectory and the rebound pattern. Here, it is assumed there are several regions of escape within the distance of limiting trajectory z_{L12}^+ along the line $y^+ = 12$. The particle concentration is assumed to remain uniform for $Y^+ > 12$ and is given by C_0 . The limiting trajectories for particles of different sizes are evaluated and the results are used for estimating the inertial deposition rates.

The effect of diffusion deposition may be obtained by analyzing the convection-diffusion equation for particle concentration in the shear layer vortices. According to Cleaver and Yates (1975), the resulting diffusion deposition velocity is given as

$$(ud^+)d = 0.084 Sc^{-2/3}, \quad Sc = \nu/D,$$

where Sc is the Schmidt number and D is the Brownian diffusivity. Although the vortical flow model used by Cleaver and Yates (1975) is not identical to that used in this study, the above expression is expected to provide a reasonable approximation for the diffusion-controlled deposition. The total deposition velocity is then given by the

summation of the contributions due to the inertia-interception and the diffusion processes.

Figure 7 shows the predicted deposition velocities with particle relaxation time. A particle-to-air density ratio of 857 (corresponds to that of polystyrene beads) and a friction velocity of 0.3 m/sec are used. The experimental data of Friedlander and Johnstone (1957), Schwendiman and Postma (1961), Sehmel (1968), Wells and Chamberlain (1967), Ilori (1971), Liu and Agarwal (1974), and Forney and Spielman (1974) for particles depositing in vertical channels as collected by Papavergos and Hedley (1984) are displayed in this figure by various symbols for comparison. The flow conditions and procedures used in these experiments were summarized by Cleaver and Yates (1975) and McCoy and Hanratty (1977), and hence, need not be repeated here. The solid line shown in Figure 7 displays the variation in deposition velocity with particle relaxation time for a vertical channel in the absence of gravity. It is observed that, for $0.1 < \tau^+ < 10$, the deposition velocity increases very rapidly with particle size. For $\tau^+ > 10$, the deposition velocities remain almost constant with a value of about 0.17.

Figure 7. Particle deposition velocity versus relaxation time for a vertical channel in the absence of rebound for $S = 857$.

There are two dot-dashed lines accompanying the solid line. The one above the solid line corresponds to the system in which the gravity is in the direction of flow (a down-flowing wind tunnel), while the one below the solid line is for the system in which the gravity direction is opposing the flow (an up-flowing wind tunnel). Figure 7 shows that the deposition rate strongly depends on the flow direction for $0.05 < \tau^+ < 5$ with the deposition velocity for a down-flowing duct being much higher than that for an up-flowing condition. For the up-flowing tunnel, the dot-dashed lines in Figure 7 do not cover

the entire range of τ^+ considered. As noted in previous studies (Fan and Ahmadi, 1993 and 1994), this implies that the shear induced lift prevent the particle deposition.

The model prediction of Fan and Ahmadi (1994) for vertical channel under $\mathbf{g} = 0$ condition is reproduced in Figure 7 by the dashed line for comparison. It is observed that both deposition models predict the trend shown by the experimental results. However, the present model provides a somewhat better agreement with the available data. The differences in model prediction arise from the variation in the flow fields and the lift forces used in the two models. In the earlier work of Fan and Ahmadi (1994), a sequence of plane stagnation point flow and the Saffman lift force were used.

Figure 8. Particle deposition velocity versus relaxation time for different coefficients of restitution and density ratios.

Figure 8 shows the deposition velocities for various particle sizes, density ratios and coefficients of restitution. The deposition velocities denoted by $r = 0$ in this figure are for the case of no rebound. The small dots in this figure correspond to the experimental data shown in Figure 7. It is observed that the model predictions are in reasonable agreement with the experimental data. For the coefficients of restitution considered, small particles within their limiting trajectory eventually deposit on the wall (either with or without rebounds). As a consequence, deposition velocities for various coefficients of restitution coincide. For larger relaxation times ($\tau^+ > 5$), some particles within the limiting trajectory may bounce off from the wall and escape from the flow region. It is noticed that, generally, the deposition rate reduces as the particles become more elastic. It is also observed that, due to the complex rebound patterns (described in the last quarterly report), variations of deposition rates for $\tau^+ > 5$ are quite complex and are no longer monotonically increasing functions of τ^+ . The rather wide spread of the predicted deposition velocities for $5 < \tau^+ < 100$ may explain the scatter of the experimental data in this region. It should be noted that a stationary flow picture is

used in the present model. The intensity of turbulence and the size of the near-wall coherent vortices, however, vary randomly. This stochastic variation, which was not included in the present model, may smooth out the complex variations of the deposition rates with particle relaxation time as shown in Figure 8.

PARTICLE RESUSPENSION IN TURBULENT FLOWS

In the previous reports, a flow structure-based model for particle resuspension from rough surfaces in turbulent streams were developed. The effect of surface roughness was included in the analysis. It was assumed that the real area of contact is determined by elastic deformation of asperities and the effect of topographic properties of surfaces were included. The JKR adhesion model was used to analyze the behavior of individual asperities. The theories of rolling and sliding detachment were used and the flow induced resuspension was studied. The effects of the near wall coherent eddies, and turbulence burst/inrush motion were included in the model development. The critical shear velocities needed to detach different size particles from rough surfaces under various conditions were evaluated and discussed. The model predictions were compared with the available experimental data and good agreement was obtained. The results indicated that particle removal from rough surfaces could be achieved by both rolling and sliding mechanism. Spherical particles, however, are more easily dislodged by the rolling motion in comparison with the sliding mechanism.

PARTICLE TRANSPORT AND DEPOSITION IN RECIRCULATING FLOWS

The mean flow and turbulence intensity fields in a recirculating flow in a two-dimensional duct in addition to particle dispersion and deposition patterns were described in earlier quarterly reports. The effect of gravity and its direction was also studied. For small particles, it was shown that the recirculating flow pattern and turbulence dominates the particle deposition rate and the effect of gravity is not as significant.

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F.G. Fan and G. Ahmadi, "Brownian Dynamics of Ellipsoidal Particles in Turbulent Flows," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

G. Ahmadi, T. Chen, C. He, H. Ban and J. Stencel, "Particle Transport in a Triboelectric Coal/Ash Separator," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

W. Kvasnak and G. Ahmadi, "Dispersion of Deforming Fuel Droplets in a Spray - A Computational Modeling Approach," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

D.H. Smith, V. Powell and G. Ahmadi, "Behavior of the Filtration System in an Integrated Gasification and Cleanup Facility - II: Incomplete Filter Cleaning," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

G. Ahmadi and D.H. Smith, "Particle Transport and Deposition in Hot-Gas Cleanup Filter Vessels: A Computational Modeling Approach," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

G. Ahmadi, M. Soltani, F.G. Fan, and S.C. Hart, "Detachment of Fibers From Flat Surfaces," Sixteenth Annual Conference of the American Association for Aerosol Research, AAAR '97, Denver, CO, October 13-17, 1997.

Seminar and Lecture Presentations

"Particle - Turbulence Interactions - Part I, Dilute Flows," Morgantown Energy Technology Center, U.S. Department of Energy, Morgantown, WV (September 13, 1995).

"Particle - Turbulence Interactions - Part II, Dense Flows," Morgantown Energy Technology Center, U.S. Department of Energy, Morgantown, WV (September 20, 1995).

"Modeling of Granular and Dense Two-Phase Flows," Department of Mechanical Engineering, University of Pittsburgh, Pittsburgh, PA (October 26, 1995).

"Particles Transport and Deposition in Turbulent Flows," Department of Mechanical Engineering, West Virginia University, Morgantown, WV (November 29, 1995).

"Recent Advances in Computational Modeling of Particle Transport, Deposition and Resuspension," Center for Applied Energy Research, University of Kentucky, Lexington, KY (December 18, 1995).

"Computational Modeling of Particles Transport, Deposition and Resuspension in Industrial Systems," MEMC, St Louis, MO, (June 27, 1997).

"Some Ideas for Computational Modeling of Dilute and Dense Turbulent Two-Phase Flows," FLUENT, Lebanon, NH, (July 17, 1997).

"On Computational Modeling of Particles Transport and Deposition in Hot-Gas Filter Vessels," Federal Energy Technology Center, Morgantown, WV (August 6, 1997).

"Recent Advances in Particle Transport, Deposition and Removal," ASYST Technologies Inc., Fremont, CA (October 13, 1997).