

Ash & Pulverized Coal Deposition in Combustors & Gasifiers

Quarterly Report
October 1 - December 31, 1996

By
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Quarterly Technical Progress Report

(October 1, 1996 to December 31, 1996)

ASH & PULVERIZED COAL DEPOSITION

IN COMBUSTORS & GASIFIERS

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Submitted to

U.S. Department of Energy

Pittsburgh Energy Technology Center

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ASH & PULVERIZED COAL DEPOSITION IN COMBUSTORS & GASIFIERS

Grant Number: DE-FG22-94PC-94213

Project Period: September 1, 1994 to August 31, 1997

Contract Recipient: Clarkson University

Project Principal Investigator: Goodarz Ahmadi

DOE Project Officer: 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, 1996. In particular, 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.

The computational model for simulating particle transport in turbulent flows was used to analyze the dispersion and deposition of particles in a recirculating flow region.

The predictions of the particle resuspension 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. Considerable progress was also made in the direct numerical simulation of particle removal process in turbulent gas flows.

Experimental data for transport and deposition of glass fiber in the aerosol wind tunnel was also obtained.

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 gm 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 mitigation 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 July 1 to September 30, 1996 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 finds 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 discussed the simulation of the gas flow velocity field in complex passages with the use of the **STARPIG-RATE** computer code that makes use of an advanced anisotropic turbulence model. The particle equation of motion which includes all the forces relevant to the motion and deposition of particles in cold flows is also being used in the simulation studies. As noted before, the particle equation includes the Stokes drag, the turbulence dispersion effects, the lift force, as well as, the Brownian effects. 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 a recirculating flow are being studied. A summary of the progress made is presented in this section.

Particle Transport and Deposition In Recirculating Flows

The mean flow and turbulence intensity fields in a recirculating flow in a two-dimensional duct was described in earlier quarterly reports. Here, to provide an understanding of the deposition rate of particles which are shed uniformly from the back face of the block, a series of simulations are also performed. Two thousand particles are released with **Y** randomly distributed between 1.4 to 2 cm and **X** = 4.7cm (about 0.3mm away from the block). Thus,⁹ the initial concentration in this region is uniform. Simulations are performed for a duration of 9 seconds (9000 time steps). The distributions of the deposited 0.01 μ m, 1 μ m and 10 μ m particles on the upper wall are shown in Figure 1. The amplitudes shown in this figure correspond to the total number of deposited particles on the surface. It is observed that three hundred and ten 0.01 μ m and two hundred and forty five 1 μ m particles are deposited on the upper wall of the channel, while only one hundred seventeen 10 μ m particles are deposited on the same surface. Most of

0.01 μm and 1 μm particles are deposited in the distance range of $6 < X < 8\text{cm}$ near the reattachment point. As noted before, particles smaller than 1 μm generally follow the stream lines and are projected toward the wall. The 10 μm particles, however, follow their initial straight trajectories and deviate from the flow streamlines due to their relatively large inertia. Most 10 μm particles, therefore, follow their initial straight trajectories and leave the channel. It should also be pointed out that 80, 31 and 85 particles with diameters of 0.01 μm , 1 μm and 10 μm , respectively, deposit on the upper wall very near the block which are not shown in Figure 1. This high rate of deposition is due to the presence of the small clockwise vortex in the corner along side of the block which moves the particles toward the wall.

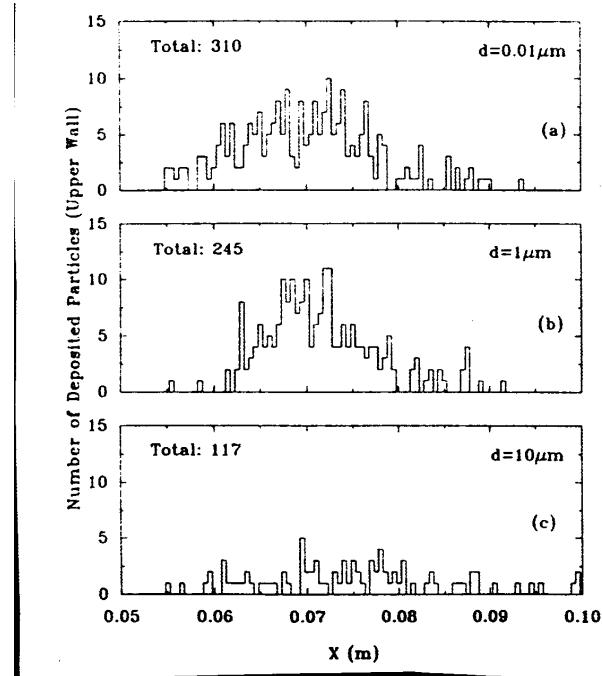


Figure 1. Distribution of deposited particles on the upper wall for particles which are shed uniformly from the block. (a) $d = 0.01\mu\text{m}$, (b) $d = 1\mu\text{m}$, (c) $d = 10\mu\text{m}$.

The distributions of the deposited particles on the block are shown in Figure 2. It is observed that about fifteen hundred 0.01 μm and 1 μm particles are deposited on the back face of the block, while about twelve hundred 10 μm particles have reached the surface of the block. The deposited particle distributions on the block are roughly uniform.

Figure 3 shows the distribution of particles at the outlet of the channel. It is observed that two hundred and twenty nine 0.01 μm , two hundred and forty four 1 μm , and six hundred and thirty seven 10 μm particles leave the channel. As mentioned before, at first few time step, all particles roughly follow the local flow streamlines. However, as the streamlines bend due to the presence of the recirculation zone, very small particles, which follow the streamline, fall into the recirculation zone due to their Brownian motion and turbulence fluctuations. As a result more of the smaller particles are captured by the recirculating flow, and are deposited on the upper wall of the channel and/or on the back side of the block.

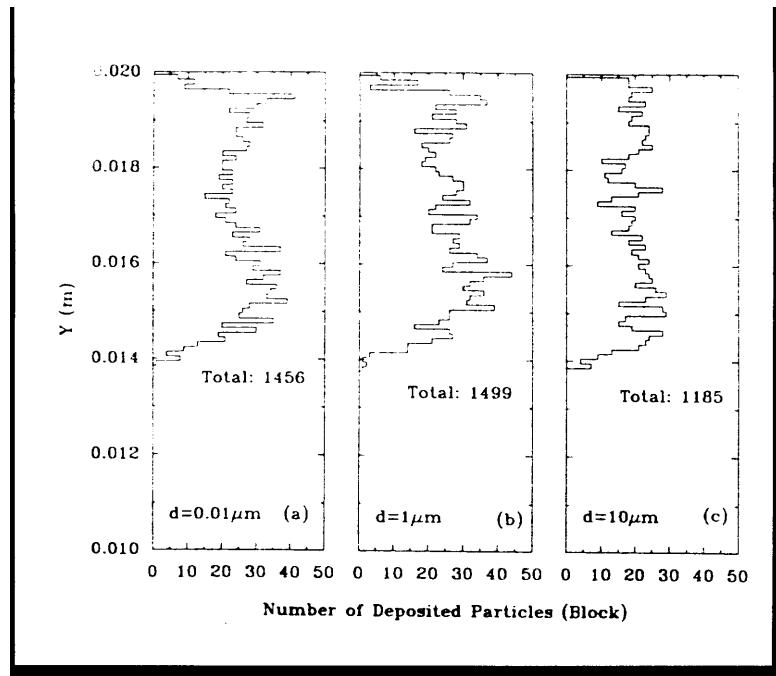


Figure 2. Distribution of deposited particles on the face of the block for particles which are shed uniformly from the block. (a) $d = 0.01 \mu\text{m}$, (b) $d = 1 \mu\text{m}$, (c) $d = 10 \mu\text{m}$.

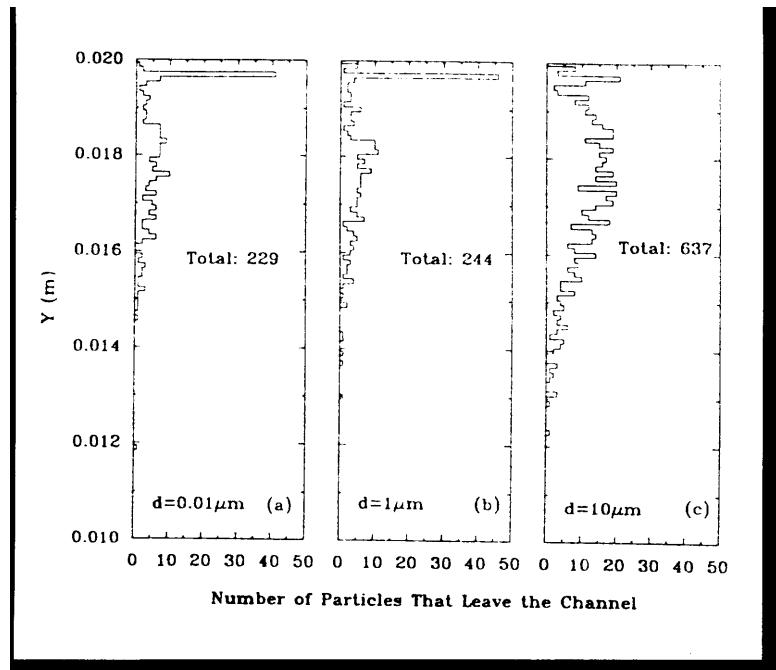


Figure 3. Particle concentration at the outlet of the duct for particles which are shed uniformly from the block. (a) $d = 0.01 \mu\text{m}$, (b) $d = 1\mu\text{m}$, (c) $d = 10\mu\text{m}$.

The particle concentration profiles at the channel exit shown in Figure 3 have large spreads roughly spanning the entire distance between the source location and the channel wall. There are also sharp peaks near the wall. These peaks appear to be due to turbophoresis phenomena as described by Reeks. Accordingly, particles with higher velocity fluctuations perpendicular to the wall are transported into the region with lower fluctuation velocities closer to the wall. At distances very close to the wall the turbulent fluctuation velocity becomes negligibly small and therefore, the particle dispersion mechanism becomes ineffective. That, in turns, leads to an increase in concentration of particles in neighborhood of the wall.

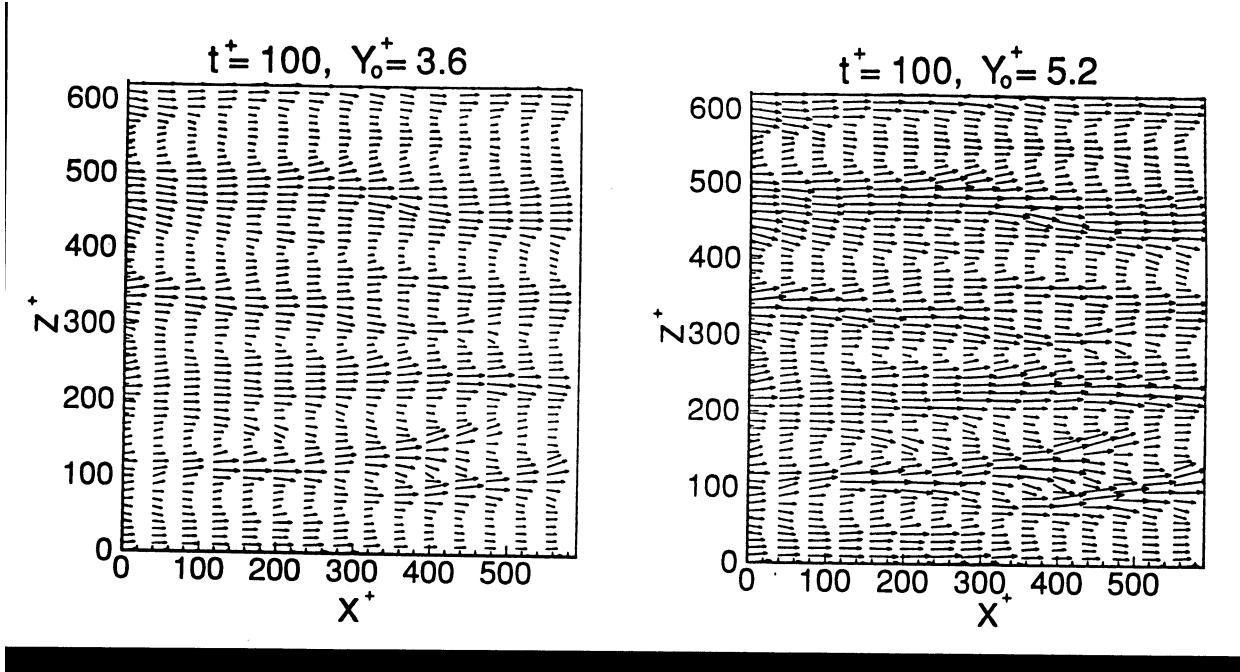


Figure 4. Sample velocity vector field in the xz-plane near the upper wall at $t^+ = 100$.

Direct Numerical Simulation of Particle Resuspension

As was noted in the last quarterly report, to provide a fundamental understanding of particle resuspension process in turbulent flows, a direct numerical simulation of Navier-Stokes equation is 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 report.

The velocity vector fields at $t^+ = 100$ in different planes at distances of $Y^+ = 3.6$ and $Y^+ = 5.2$ wall units away from the upper channel wall are shown in figure 4. Here, $Y^+ = 125 - y^+$ denotes the distance from the upper wall. While the flow is predominantly in the x -direction, the low and high

speed streaks are noticeable in this figure. This flow pattern is quite similar to those observed experimentally by Smith and Schwartz using a hydrogen bubble wire and a high speed video system. It is also observed that the locations of the high speed and low speed streaks remain almost unchanged at different planes near the wall. The magnitude of the velocity, however, increases linearly with distance from the wall, which is as expected. Figure 4 also shows that the roughly periodic distortion has a periodicity of about 100 wall units. Smith and Schwartz reported that the counter rotating vortices were observed to be always associated with a low speed streak, but not vice versa. The cause and effect relationship between the streamwise vortices and periodic flow structure can not be determined from the present simulation. That is, it is not quite obvious whether this periodic distortion is the consequence of the streamwise vortices, or the instability is the cause for generating the coherent vortices.

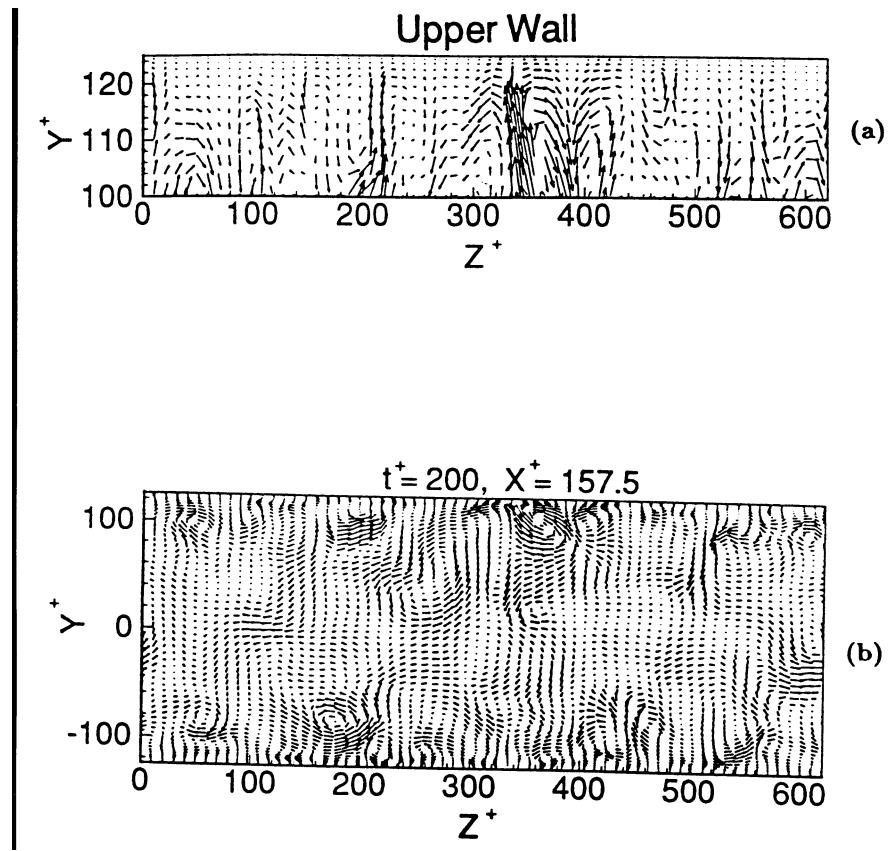


Figure 5. (a) The details of the velocity field within 25 wall units from the upper wall.
 (b) Instantaneous velocity vector field in the yz -plan.

Figures 5 and 6 show sample velocity fields in the channel in different planes at $t^+ = 200$. Compari-

son of figure 5(b) with the figure 3 of last quarterly report for $t^+ = 100$ shows that some of the streamwise vortices have decayed and some others have amplified or are newly born. Inspection of these figures indicates that most axial vortices appear as single vortices and very few pairs of vortices are discernible. This observation is consistent with the results of Moser and Moin, Robinson et al., Guezennec et al., and Brooke et al.

Figure 5(a) shows the near wall velocity vector plot in the yz -plane within 25 wall units from the wall. The sequence of inward/outward flow patterns is clearly observed from this figure. Interestingly, these instantaneous flow patterns are only occasionally associated with specific counter rotating vortices. The flow variation shown in figure 5(a) is strikingly similar to the near wall flow patterns obtained by Aubry et al. using the proper orthogonal decomposition and dynamical system theory. The velocity vector field in the $Y^+ = 3.6$ ($y^+ = 121.4$) plane is shown in figure 6. Similar to figure 4, the high and low speed streaks are clearly observed from this figure. In particular, certain regions (parts of the streak) have very high or very low velocities, which are conjectured to be due to the burst/inrush events. The peak instantaneous streamwise velocities in figure 6 are statistically analyzed. The sample mean, maximum and minimum are evaluated. Accordingly, in wall units, the sample mean is given by

$$u^+ = 1.84y^+ \quad (1)$$

and the sample maximum and minimum are

$$u_{\max}^+ = 2.14y^+, \quad u_{\min}^+ = 1.6y^+. \quad (2)$$

Equation (1) is in reasonable agreement with the peak velocity estimates during burst/inrush events, reported by Johnson and Alfredsson.

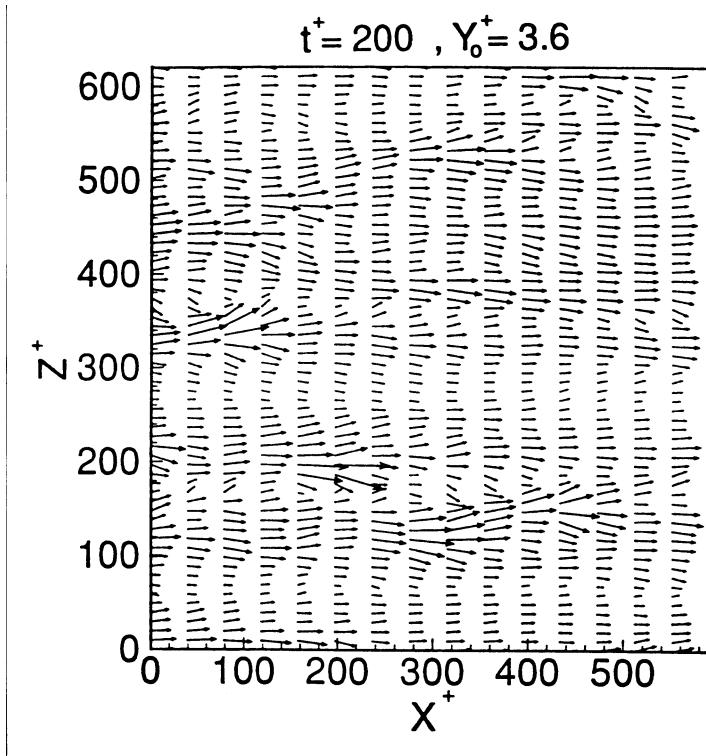


Figure 6. Velocity vector field in the xz-plan near the upper wall at $t^+ = 200$.

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 was described in the earlier reports.

The aerosol used in the experiment was generated by dispersing approximately 1 gram of particles over a duration of 10 seconds. This corresponds to a loading of about 0.2% which is far less than the one percent limit for the assumption of dilute flow. The test section concentration was sampled over a 1 minute time span, and the particles deposited on the filter in the isokinetic probe were analyzed by the image processing procedure described in detail by Kvasnak et al. (1993). Thirty digital images having an area of 480 μm by 512 μm were averaged for each particle size.

The average deposition velocity of particles on the collection plate over a period of 1 minute was evaluated in these experiments. The deposition velocity is defined as the flux of particles to the wall over the concentration of the free stream. That is

$$u_d = J/C_o, \quad (3)$$

where u_d is the deposition velocity, J is the flux of particles to the wall, and C is the free stream concentration. It is assumed that the two dimensionality of the flow allows the particles to deposit uniformly on the channel wall so that any area provides a representative statistical sample. The particle flux J (number deposited per unit area per unit time) to the wall may be evaluated from the number of deposited particles on an image, and the area under the microscope. Thus, the deposition velocity may be evaluated directly by counting the number of particles that are deposited on the filter of the isokinetic probe and on the test specimen.

The non-dimensional deposition velocity u_d^+ is defined as

$$u_d^+ = u_d / u^* \quad (4)$$

where u^* is the friction velocity defined as

$$u^* = (\tau_w / \rho)^{1/2}. \quad (5)$$

Here, τ_w is the wall shear stress and ρ is the density of air. The wall shear stress in the smooth channel is determined by measuring the pressure drop ΔP for a segment of the tunnel.

It is customary to present the deposition velocity data in terms of the non-dimensional relaxation time defined for spherical particles as

$$\tau_d^+ = S d^{+2} / 18 \quad (6)$$

where the non-dimensional particle diameter is given by

$$d^+ = d u^* / \nu. \quad (7)$$

Here, S is the particle to gas density ratio, d is the particle diameter, and ν is the kinematic viscosity of air.

For fibers the definition of the relaxation time becomes more complicated. The relaxation time based on the minimum diameter, τ_d^+ may be defined by equations (6) and (7) with $d = 2a$, where a is the minimum radius of the fiber. The fiber is then characterized by τ_d^+ and the aspect ratio $\beta = L/d$, where L is the fiber length. Shapiro and Goldenberg (1993) used an equivalent relaxation time based on the orientation averaged resistance, τ_{eq}^+ . Accordingly, the equivalent relaxation time is defined as

$$\tau_{eq}^+ = m_p u_p^{*2} / \mu \nu K_{eq}^p \quad (8)$$

where m_p is the mass of the particle, μ is the coefficient of viscosity of air, and K_{eq}^p

$$K = 3(K_{xx}^{-1} + K_{yy}^{-1} + K_{zz}^{-1})^{-1}. \quad (9)$$

Here K_{xx} , K_{yy} , and K_{zz} are the components of the resistance tensor.

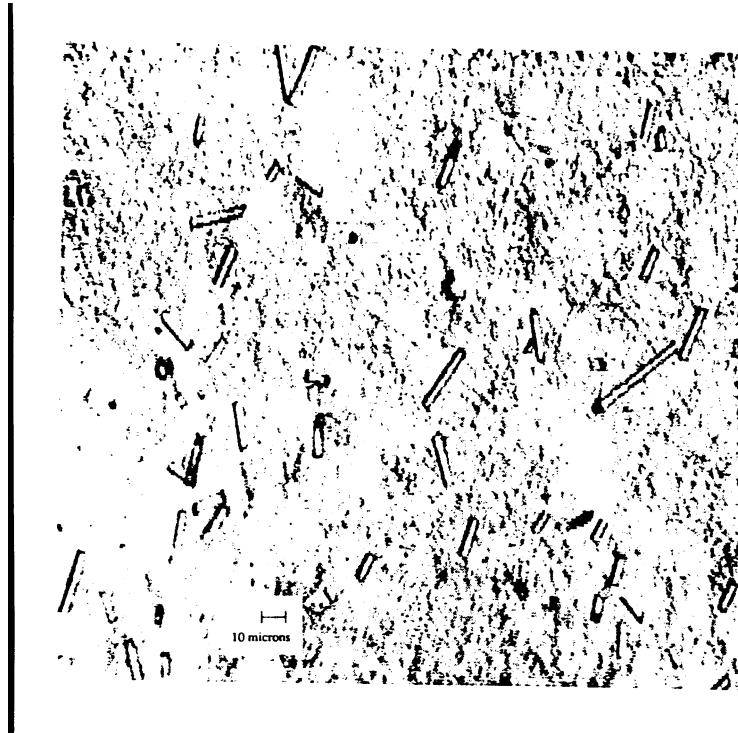


Figure 7. Micrograph of glass fibers

To measure the flux of aerosol particles to the wall, a clean plate was mounted to the lower wall of the test section in the wind tunnel. The plate was grounded to reduce electrostatic effects. The isokinetic probe with a membrane filter was also used. A specific amount of particles (roughly 0.02 grams) was prepared for the aerosol generation. Under a steady state air flow condition, the sample particles were dispersed into the wind tunnel with the aid of an aspirator over a duration of about 1 minute. Immediately after the run, the millipore filter and the test plate are removed from the probe and the tunnel test section and processed. The deposited particles were statistically analyzed using the image processing procedure described by Kvasnak et al. (1993). Each image is treated as an independent sample, and thirty images are used for obtaining the average deposition rate of fibers of different sizes and aspect ratios. As noted before the maximum and minimum dimensions of a particle on the image are used as estimates for the fiber length and diameter.

The experimental results for the deposition rates of cylindrical glass fibers are described in this section. The minimum diameters of the glass fibers was $5 \mu\text{m}$. Each set of data displayed is the average of

6 separate experiments with 30 samples per experiment.

Figure 7 shows a micrograph picture of glass fibers on a gold surface. It is observed that the glass fibers have a constant minimum diameter of 5 μm and a wide range of aspect ratios from 1 to over 100. Due to the rather low concentration used, practically no clustering of the deposited fibers on the gold tile or the isokinetic probe filter was observed. In this study the deposition rates for glass fibers with an aspect ratio in the range of 3 and 20 are presented. While their number were few, most fibers longer than 100 μm were found to cross the edge of the images. This could cause considerable inaccuracy and, therefore, such large size fibers were excluded from the present study. Similarly, particles with aspect ratio's smaller than 3 were not included due to the insufficient number of samples.

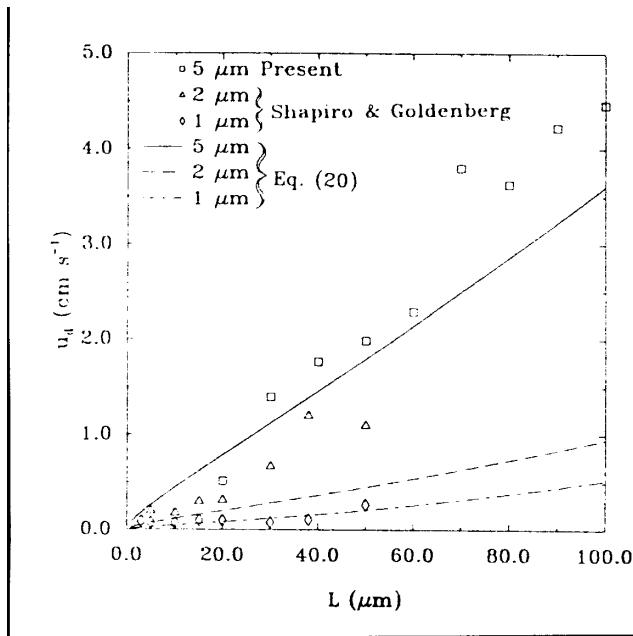


Figure 8. Measured deposition velocity of glass fibers

Figure 8 shows the measured deposition velocities for 5 μm glass fibers deposited on the lower wall of the channel versus the fiber length. The data of Shapiro and Goldenberg (1993) for 1 and 2 μm glass fiber deposition are reproduced in this figure for comparison. The predictions of our empirical equation for different values of diameter are also shown in figure 8. A value of $u^* = 0.3$ for the flow conditions in the aerosol wind tunnel is used to express the model predictions in dimensional form. It is observed that the deposition rate increases as the fiber length increases. Good agreement is also seen between the empirical relation and the experimental data. Shapiro and Goldenberg also suggested a limit $\tau_{\text{relax}} < 6$ for using their empirical equation. However, figure 8 shows that our empirical equation holds for much larger relaxation times.

PARTICLE RESUSPENSION IN TURBULENT FLOWS

In the previous reports, a model for particle resuspension was described. In this section the model predictions are compared with the experimental data of Zimon for resuspension of glass particles. The experimental data of Zimon was for entrainment of glass particles which were lying on a steel wall and the particles were removed by blowing air.

Figure 9 shows the variation of the critical shear velocity as a function of particle diameter for detaching glass particles from a steel substrate in according to the rolling detachment mechanism as predicted by the sublayer and burst models. Experimental data of Zimon for removal of glass particles from steel surface are also reproduced in this figure for comparison. Since Zimon only reported the critical free stream detaching velocities, the corresponding shear velocities were estimated using, $u^* = 0.04U$. The critical detaching velocity was obtained by Zimon using the assumption of a log-normal distribution of the adhesion force. Figure 12 shows that the experimental data are in good agreement with the model prediction for $\Delta = 0.9$. This value of Δ corresponds to roughnesses of $\sigma = 2 \text{ } \mu\text{m}$ and $8 \text{ } \mu\text{m}$ for particle diameters of $d = 10 \text{ and } 100 \mu\text{m}$, respectively. For seemingly smooth surfaces, such small values of roughness may be expected to be present.

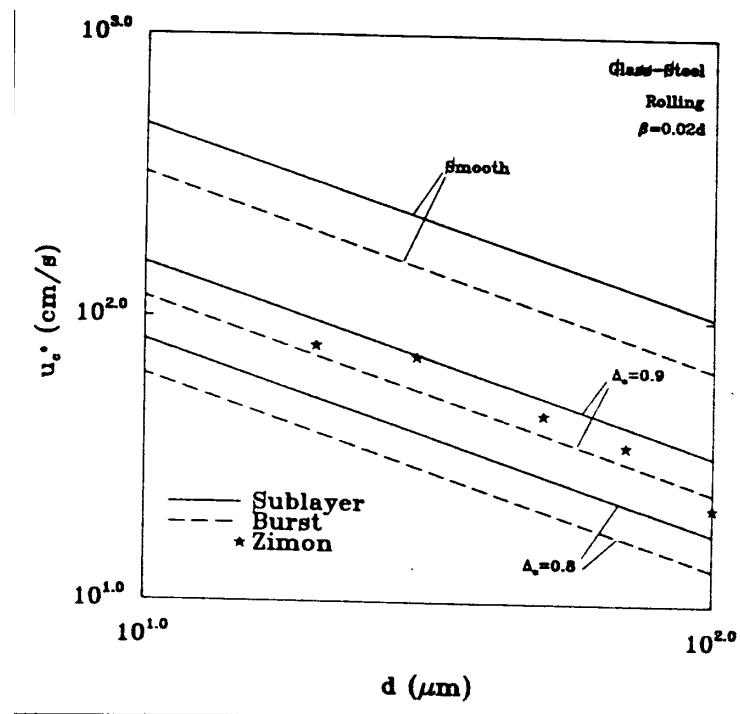


Figure 9. Comparison of the critical shear velocities as predicted by the rolling model with the experimental data of Zimon for glass particles on a steel substrate

SUBLAYER MODEL FOR PARTICLE DEPOSITION

The presence of streamwise coherent vortices in the turbulent shear flows is well documented. Numerous flow visualizations (e.g., Kline et al., 1967; Bakewell and Lumley, 1967; Blackwelder and Eckelmann, 1979) and numerical simulations (e.g., Kim, 1983 and Kim et al., 1987) showed that turbulent near-wall flow is a region of strong dynamic interaction dominated by streamwise vortices and roughly cyclic bursting phenomena. The mean lateral spacing of these vortices is about a hundred wall units. Using Proper Orthogonal Decomposition (POD) modes and dynamic systems theory, Aubry et al. (1988) reconstructed the near-wall turbulence structures and reported observations of dominating counter-rotating vortices and some isolated ones. The direct numerical simulations of Ounis et al. (1991 and 1993) confirmed the suggestion of Owen (1969) that these vortical motions are the main mechanism that carry the particles to the wall. A simplified sublayer flow model is being developed to analyze particle rebound from surfaces.

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G. Ahmadi and P. Nicoletti, "Computational Modeling of Hot-Gas Flows in Filtration System at Tidd," 27th Annual Meeting of the Fine Particle Society, and the 1996 Pharmaceutical Sciences and Technology Conference, Chicago, Illinois, August 6-8, 1996.

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G. Ahmadi and D. H. Smith, "Computational Modeling of Particle Transport and Deposition in Hot-Gas Cleanup Filter Vessels," Fifteenth Annual Meeting of the American Association for Aerosol Research, AAAR '96, Orlando, FL, October 14-18, 1996.

G. Ahmadi and Q. Chen, "Dispersion and Deposition of Particles in a Turbulent Pipe Flow with Sudden Expansion," Fifteenth Annual Meeting of the American Association for Aerosol Research, AAAR '96, Orlando, FL, October 14-18, 1996.

M. Soltani and G. Ahmadi, "Trajectory Statistics of Charged Particle Deposition in a Directly Simulated Turbulent Channel Flow," Fifteenth Annual Meeting of the American Association for Aerosol Research, AAAR '96, Orlando, FL, October 14-18, 1996.

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Seminar and Lecture Presentations

“Particle - Turbulence Interactions - Part 1, 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).