Dynamics of Aerosol Particles in Stationary, Isotropic Turbulence
Grant Agreement: NAG3-2470

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1 Task Description

A detailed study of the dynamics of sub-Kolmogorov-size aerosol particles in stationary isotropic turbulence has been performed. The study combined direct numerical simulations (DNS; directed by Prof. Collins) and high-resolution experimental measurements (directed by Prof. Meng) under conditions of nearly perfect geometric and parametric overlap. The goal was to measure the accumulation of particles in low-vorticity regions of the flow that arises from the effect commonly referred to as preferential concentration. The grant technically was initiated on June 13, 2000; however, funding was not available until July 11, 2000. The grant was originally awarded to Penn State University (numerical simulations) and SUNY-Buffalo (experiments); however, Prof. Collins' effort was moved to Cornell University on January 2002 when he joined that university. He completed the study there. Below is a list of the specific tasks that were completed under this study

- **Experimental measurement of turbulent collision frequency (Hui Meng)**

  1. Developed an atmospheric turbulence chamber capable of producing stationary, isotropic turbulence and allowing the introduction of sub-Kolmogorov-size particles.

  2. Characterized the turbulence in the chamber over the range of operating parameters.

  3. Measured the particle radial distribution function and conditionally averaged relative velocity using a 3-dimensional technique: holographic particle image velocimetry (HPIV).

- **Direct numerical simulations (DNS) of particles in stationary, isotropic turbulence (Lance R. Collins)**

  1. Developed a parallel DNS code that is capable of achieving higher Reynolds numbers and that incorporates interparticle collisions.

  2. Calculated statistical properties of the particle, fluid and cross phases over a broad range of parameters. Emphasis was placed on matching conditions from the experiments.

Name	Role	Period of Time
Lance R. Collins	Principal Investigator	06/13/00 – 12/31/03
Arun Keswani[†]	Grad Student	06/13/00 – 12/31/00
Aruj Ahluwalia	Grad Student	09/01/00 – 08/31/02
Gretchen Holtzer[†]	Grad Student	09/01/00 – 12/31/01
Sarma L. Rani[†]	Postdoc	03/01/03 – 09/30/04
Hui Meng	Principal Investigator	06/13/00 – 12/31/03
Xiangqun Song	Postdoc	06/13/00 – 01/31/02
Ye Pu[‡]	Grad Student	06/13/00 – 12/31/02
Gang Pan[†]	Grad Student	09/01/01 – 08/31/03
Lujie Cao	Grad Student	09/01/01 – present
Senior Collaborators		
Prof. Donald Koch, Chem. & Biomolecular Engr., Cornell		
Prof. Raymond Shaw, Physics, Michigan Tech. U.		
Dr. Iskender Gökalp, CNRS, FRANCE		

Table 1: Research team, including graduate students and postdocs who made significant contributions to the research effort. Financial support for the graduate students and postdocs was supplied in full or in part by this grant (partially supported personnel indicated by †) or they were funded from other sources (externally supported personnel indicated by ‡). Collaborators provided in-kind support (with no financial remuneration from this grant).

3. Made quantitative comparisons of particle statistics with experimental measurements at precisely the same conditions. DNS also was used to help interpret experimental measurements where necessary.

2   Research Team

The research team we assembled was a highly-talented group of graduate students and postdoctoral research associates (see Table 1). Different students were involved in different elements of the work; however, the group listed under Prof. Collins was principally responsible for the direct numerical simulations and the group under Prof. Meng was principally responsible for the experiments. Note that Gretchen Holtzer left Prof. Collins' group in December 2001 when he joined Cornell University. She is currently pursuing a PhD with another faculty member at Penn State. In addition to the graduate students and postdocs, we note there were important contributions to the work from several key collaborators.

3   DNS Accomplishments

3.1   Code Development

The flow solver for the DNS has undergone several important revisions. Most recently, a parallel version of the pseudo-spectral code capable of simulating both isotropic and homogeneous shear flow has been developed. The code has important advantages over traditional pseudo-spectral codes (1). First, it takes full advantage of modern developments in Fast Fourier Transforms (FFT). Secondly, for homogeneous turbulent shear flow, the code has eliminated the troublesome remeshing
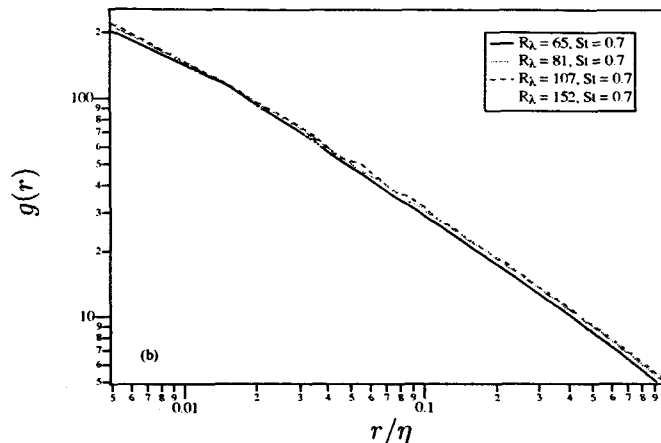
Figure 1: Radial distribution function $g(r)$ vs r/η for a Stokes number 0.7 and the indicated Reynolds numbers.

step. Standard codes solve the equations on a mesh that deforms with the mean velocity gradient. This allows a standard FFT to be used, since the fluctuations are strictly periodic in this reference frame. However, to reduce aliasing errors that arise when the mesh becomes highly skewed, the domain is periodically "remeshed" or mapped onto a coordinate skewed in the opposite direction. Each remeshing step introduces errors due to the remapping procedure. Our approach eliminates this step by remaining in the orthogonal reference frame throughout (2; 3). A highly-optimized, parallel version of this code is able to simulate up to 1024^3 grid points on a modest Beowulf cluster containing 64 Pentium IV processors.

We have implemented a parallel algorithm for describing the motion of up to several million particles. This work was initiated in the Masters theses of Arun Keswani and Aruj Ahluwalia and was recently made more efficient by Sarma L. Rani. The code can track several million particles and uses arbitrary-order interpolation schemes to determine the force on each particle. These algorithmic breakthroughs were essential for allowing us to test theories under development in the group, as they enabled us to achieve the necessary statistical convergence.

3.2 Reynolds Number Study

One of the main goals of the numerical work was to extend the range of Reynolds numbers to investigate the effect of this parameter on particle clustering. This is especially important for applications such as meteorology, where the Reynolds number (based on the Taylor microscale) can exceed 10^4. We were not able to reach values that large, but we could explore the trend over the range 50–160 and look for whether we see continued growth of the clustering with increasing Reynolds number or an approach to an asymptote. The most significant measure of particle clustering is the radial distribution function (RDF), $g(r)$, defined as the number of pairs at a given separation distance divided by the expected number of pairs. $g(r)$ is normalized to unity if the system is uniformly distributed. Figure 1 shows a result from our recent publication (4) for a Stokes number of 0.7 The curves appear to converge with increasing Reynolds number suggesting saturation is occuring. We plan to test this hypothesis using experimental data.
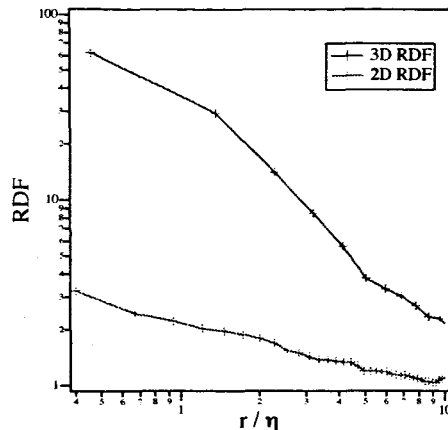
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Figure 2: Two-dimensional (red) and three-dimensional (blue) RDF from experimental measurements at $St = 0.88$ and $R_\lambda = 185$. Notice the large attenuation of the signal in the 2D measurement.

3.3 DNS to Support Experiments

The simulations, beyond providing data for comparison with experiments, were used to test different configurations of the experiment. Initial measurements of the RDF were performed by passing a laser sheet through the box and imaging the particles that lie within the sheet in *two* dimensions using a charged coupled device (CCD) camera oriented perpendicularly to the sheet. This 2D measurement of particle pairs also could be binned to produce a 2D RDF. This was considered a preliminary measurement on our way to 3D measurements using holography. Interestingly, the RDF signal was found to be much smaller than was expected (see Fig. 2). This provided motivation for a study to understand the origin of this discrepancy; that work culminated in an analysis showing lower-dimensional measurements are fundamentally incapable of determining the 3D RDF (5). The 2D signal (or 1D, sampling probe measurement used in clouds (6)) was shown to be equivalent to a weighted integral of the 3D RDF, making the inverse problem ill posed. We proposed a procedure for inverting 2D (or 1D) data, but there is inherent risk and increased errors in this procedure. This result underscores the need for 3D measurements of particle positions.

3.4 Theory[1]

A collaborative effort involving Prof. Koch, Jaehun Chun (former graduate student of Prof. Koch), Aruj Ahluwalia and Sarma Rani yielded a new theory of particle clustering (7). The theory considered the dynamics controlling a pair of particles with small (but finite) Stokes numbers in a turbulent flow field. Particles drift together due to the biased sampling of strain over rotation experienced by particle pairs with finite inertia. The drift is eventually balanced by (non-local) diffusion, which acts in the opposite direction once a gradient is established. The statistical theory predicts the RDF to be a power-law function of the particle separation, in agreement with DNS (8). Moreover, it is able to predict the exponent in quantitative agreement with DNS. The theory explains (and predicts) why bidisperse particles (i.e., particles with different response times) have a strongly attenuated RDF. Differences in particle inertia give rise to a second diffusion process due to the difference in response of the two particles to local fluid accelerations. This second diffusivity causes the RDF to deviate from the power law at separations below a critical separation, r_c. The

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[1]This activity was not part of the original proposal work statement.

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theory predicts r_c in quantitative agreement with DNS.

3.5 Summary of DNS Effort

In summary, the project has achieved all of the goals laid out in the original proposal. A summary of the comparisons between DNS and experiments is given in §4.3. The funds supported, in part, two Masters degrees (9; 10), one PhD candidate for one year and a postdoc for one year. This work has lead to five journal publications (8; 11; 5; 7; 4), eleven invited lectures and six contributed talks.

4 Major Experimental Accomplishments

4.1 Isotropic Turbulence Chamber

An atmospheric air turbulence chamber with a $40 \times 40 \times 40$ cm^3 cavity has been built. Fans were attached to the eight corners of the box and they were adjusted to provide nearly isotropic turbulence in the center of the chamber. The design is similar to the one used by Birouk et al. (12) to study droplet vaporization.

The flow in the chamber was extensively analyzed using two-component laser doppler anemometry (LDA) and particle image velocimetry (PIV). The turbulent kinetic energy was found to be nearly isotropic and easily correlated with the fan speed. The integral length scale of the turbulence was roughly independent of fan speed. A critical measurement for this study was the energy dissipation rate, ϵ, used to set parameters such as the particle Stokes number. According to the Kolmogorov theory, the second-order structure function, defined as $\left\langle [u_i(\mathbf{x}) - u_j(\mathbf{x} + \mathbf{r})]^2 \right\rangle$, is proportional to $\epsilon^{2/3}$ within the inertial range. We fitted this function and back-calculated ϵ following the procedure in Voth et al. (13). Additionally, higher-order statistics of the velocity fluctuations (e.g., skewness and flatness) were analyzed and found to be in reasonable agreement with wind tunnel data at similar Reynolds numbers.

4.2 3D Particle Imaging and Identification

3D HPIV, with the goal of describing the instantaneous motion of *individual* particles, must contend with aberations that result from the reconstruction process. Figure 3 shows two holographically reconstructed images; the one on the left was obtained by optical reconstruction of an actual hologram (i.e., inverting the reference laser beam) while the one on the right was obtained from a Mie scattering calculation of an "idealized" hologram. What is readily apparent is that the spherical shape is lost in the reconstruction process, even for an ideal hologram (right image).

To assist in locating the centroids of the particle images, our group has developed two pieces of sofware: Concise Cross Correlation (CCC) and Particle Reconstruction by Edge Detection (PRED) (14; 15; 16). These packages use edge detection to help identify the boundaries of the particle and then perform a weighted average to obtain an estimate of the location of the particle centroid. The computational expense associated with this step of the process is significant; we estimate 40 hours on a single 600 MHz Pentium-grade computer. We therefore ported CCC and PRED to a computer cluster with 4 nodes (8 Pentium processors) using MPI and we see a nearly linear speed up (processing times of approximately 5 hours).
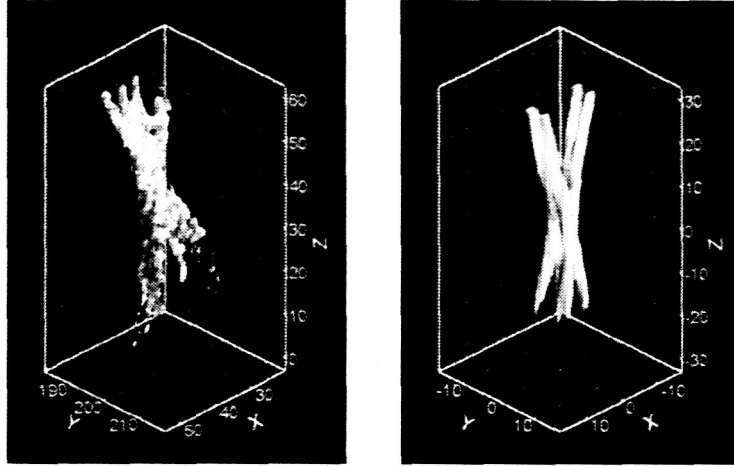
Figure 3: Particle image from an optical reconstruction of a hologram (left) and from a mathematical reconstruction of an ideal holographic image (right).

4.3 RDF Comparisons

A comparison between the DNS and measured RDF is shown in Fig. 4. The symbols are two sets of measurements (obtained using different filters) and the solid lines are three DNS runs: monodisperse particles with diameters equal to the number-weighted mean diameter (black line); monodisperse particles with a diameter equal to the volume-weighted mean diameter (green line); and polydisperse particles with a size distribution chosen to match the experiment (magenta). The RDF for both the experiments and DNS reflect the local accumulation effect—the RDF increases with decreasing r at small separations. Indeed, this is the first experimental confirmation of the DNS to date. However in general, the DNS seems to under-estimate the RDF at all separations. The best agreement is obtained using the volume-weighted diameter, although this may be fortuitous.

There are several possible explanations for the disagreement. First, there may be a significant error in the estimate for ϵ in the turbulence box. The RDF is very sensitive to the Stokes number, which in turn is proportional to $\epsilon^{1/2}$. We followed Voth et al. (13) and fitted the measured second-order structure function and backed out the value of ϵ from the fit. The values are lower than scaling would suggest (i.e., u'^3/L). A second possibility is there are other forces acting on particles in close proximity to each other that are not accounted for by the simulations. For example, electrostatic charging may create additional interparticle forces. We are still working to refine this comparison.

4.4 Progress Towards digital HPIV[2]

While HPIV provides an instantaneous 3D volumetric measurement, its widespread use has been limited by the laborious process required to chemically develop the film, optically reconstruct the hologram and mechanically scan the image to determine the particle positions. Furthermore, we recognized that a process this cumbersome could not be considered for a flight experiment. This motivated us to initiate development of a digital version of HPIV, in which the hologram is recorded directly on a CCD camera and the reconstruction process is accomplished mathematically.

Our current setup uses an in-line configuration. The image is recorded on a 12-bit CCD camera (PCO SensiCam) with 1280×1024 pixels of size 6.7 μm, and a total area of 8.6 mm $\times$ 6.9 mm.

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[2]This activity was not part of the original proposal work statement.
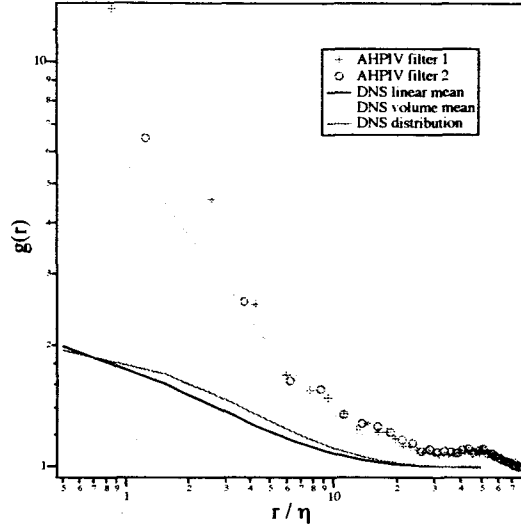
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Figure 4: Comparison of RDF obtained from Gemini HPIV system (symbols) and DNS (solid lines). There are two filters used in the experiments. The simulations are for monodisperse particles with the number-mean diameter (black), monodisperse particles with the volume-weighted mean diameter (green) and polydisperse particles (magenta).

The digital hologram is numerically reconstructed to obtain the reconstruction wave in the image volume. Particle position and size are extracted from the reconstruction wave using a complex amplitude-based method we developed known as PECA (17). By taking advantage of the complex amplitude uniquely available in mathematical reconstruction, PECA greatly reduces the error resulting from the lower resolution of the CCD camera to values comparable to the particle diameter in all three directions. At this stage, PECA is viewed as competitive in terms of accuracy with optical in-line holography, and will continue to improve as the pixel density of CCD cameras increases. Finally, using two briefly-spaced exposures, the particle velocity is obtained. The particle matching algorithm we use was originally developed by Stellmacher & Obermayer (18).

4.5 Summary of Experimental Effort

In summary, the project has achieved the goals laid out in the original proposal. This work has lead to four peer-reviewed publications (17; 19; 20; 21), five refereed conference proceedings (22; 23; 24; 25; 26) and two contributed talks. Additionally, two doctoral students have been supported by the grant, including one completed degree (27).

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