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A Method for Deducing the Self-Diffusion Coefficient of a Single Analog Molecule within a Liquid-State Flow

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A Method for Deducing the Self-Diffusion Coefficient of a Single Analog Molecule within a Liquid-state Flow (Work in Progress)

Abstract

This work was conducted as part of the Shaping Experiential Research for Veteran Education (SERVE) program for undergraduate students. This program aims to engage veterans in engineering and STEM related topics that address US Navy research priorities by:

a) increasing the number of veterans obtaining graduate STEM degrees

b) providing these students with hands-on research experience, working alongside experienced faculty and graduate students.

Research conducted at UNC Charlotte, and funded by the Office of Naval Research, has demonstrated the viability of using vibrating grain beds as macroscopic analogs for studying dense, liquid-state molecular hydrodynamic flows.[1] Unlike other molecular hydrodynamic methods, vibrating grain beds allow direct observation of particle interactions in liquid flows. Previous experiments using this method have concentrated on observing the molecular interactions of particles in an entire flow-field.[2] However, the present inquiry concentrates on tracking the random displacements of a single grain, i.e., an analog atom or molecule, as it undergoes simultaneous transport by deterministic bulk fluid motion and random, thermally driven self-diffusive hops. The study objective centers on using these measurements to estimate the effective self-diffusion coefficient of a single, molecule-like grain within a vibrated granular fluid. Experimentally, this single grain is first heated in a convection oven and then introduced into a granular flow field having a lower, spatially uniform ambient temperature. The grain is then tracked with a thermal imaging camera, allowing direct observation of the grain's random path within the flow. The experiment is performed multiple times, with each realization processed into individual, digitized paths using PIV (Particle Image Velocimetry) software. The set of experimentally observed paths is then averaged, creating a mean particle path. To extract the self-diffusion coefficient, individual grain paths will be modeled as single realizations of a stochastic Weiner process. Finally, using the estimated self-diffusion coefficient, the effective grain fluid viscosity will be determined using the Stokes-Einstein relation.

Education Program Introduction

The SERVE (Shaping Experiential Research for Veteran Education) program aims to engage veterans in research experiences that address US Navy research priorities and increase the number of veterans with graduate level STEM degrees. This program is funded by the ONR (Office of Naval Research) through a grant to provide research mentorship and guidance as students gain experience exploring topics that are of interest to national security. This program also operates as a research exchange program for veterans interested in STEM careers between

The University of Tennessee and The University of North Carolina at Charlotte, allowing student veterans to gain research experience at both institutions. This program proved the funding and mentorship necessary to bring this project to its current status and continues to provide financial and technical support.

Research Background and Objectives

The dynamics of dense fluids, when considered on length-scales exceeding several molecular diameters, can be treated as a continuum; if length-scales do not exceed several molecular diameters, the interactions between molecules must be considered.[1] Present methods of studying molecular hydrodynamics include light scattering, molecular dynamic simulations, and neutron scattering; however, these methods do not allow for direct observation of molecular interactions.[2]

This research continues the development of an analog technique in which vibrated grain beds serve as an analog for studying dense molecular flows. The technique, an alternative for studying molecular hydrodynamic systems, allows direct analog observation of molecular flow and particle interactions.[2] Unlike previous studies, this research focuses on the movement of a single grain acting as an analogue for a molecule.

The present study focuses on obtaining the self-diffusion coefficient for a grain liquid comprised of 2 mm spheres. Given the self-diffusion coefficient, the grain liquid viscosity can then be determined. This viscosity will then be compared to the viscosity measured earlier via fluid drag force measurements studies in the same vibrating grain bed. This poster details the first step in this determination: measurement of a discretized mean path taken by 100 single heated spheres with our vibrated grain bed.

Research Description

The experimental setup in Figure 1 shows a Fluke TiX580 thermal imaging video camera suspended over the annular polyurethane bowl of a vibratory polishing system. Figure 2 shows the perspective of the camera when set to view visible light; this same perspective was used when switched to thermal imaging mode, as seen in Figure 3. Figure 3 has been altered to provide a visual of how the grain flows across the vibrating bed over time; multiple dots and arrows were added to the figure for visualization purposes only.

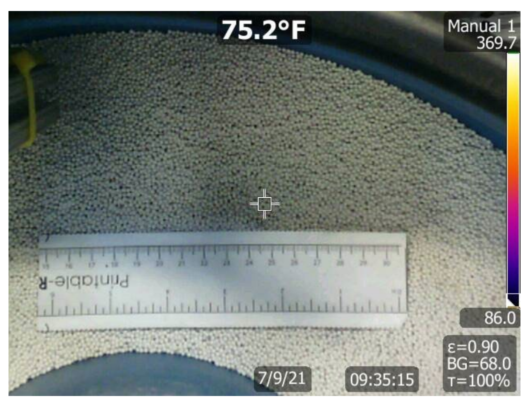

Figure 1: Visible Light Camera Perspective Calibration Image

The polisher vibrates using an unbalanced, single-speed motor that rotates at a constant 1740 RPM; a few moments after startup, the bowl's contents achieve a steady-flow, non-equilibrium flow condition.[1] These vibrations cause the media (2 mm ceramic spheres) to flow from the point of particle injection towards the center of the annulus, in an arc like motion (as observed from the camera perspective). Based on present and previous observations, grains appear to flow in a helical pattern around the annulus.

Due to our camera's 2-dimensional limitations, this experiment was conducted based on the visible surface of the grain bed. To differentiate a single, injected, self-diffusing grain from the other identical grains, the injected grain was heated in a standard convection oven to 350 °F for 2 minutes. The heated grain was then introduced ('injected') using a funnel and down tube to assure a consistent introduction location; this also ensured that the entire flow path was in the thermal camera's field of view. Using the Fluke TiX580 thermal imaging camera, we were able to track the heated grain (Figure 3,4); this experiment was then repeated 100 times and recorded in a .AVI video format.

The video files were then separated by frame into individual, time-stamped image files where each individual image was similar to that shown in Figure 3. For data analysis, the images needed to be converted to greyscale; Figure 4 shows the same image data presented in Figure 3, converted to grey-scale and ready to be experimentally processed. Figure 4 has also been altered to provide a visual of how the grain flows

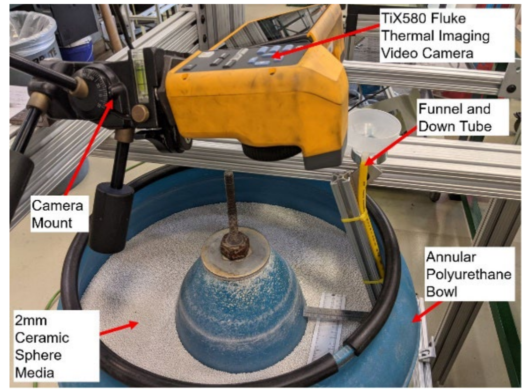

Figure 3: Experimental Setup

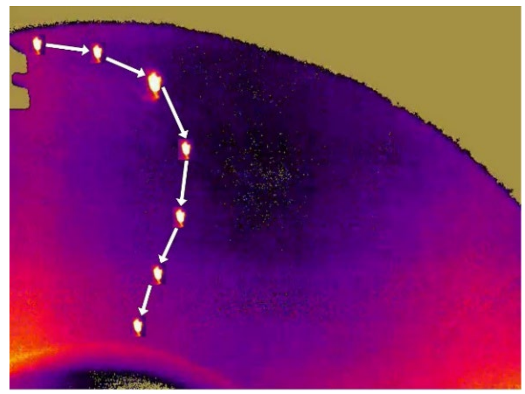
Figure 2: Thermal Camera Perspective with added Flow Path based of Visual Observation

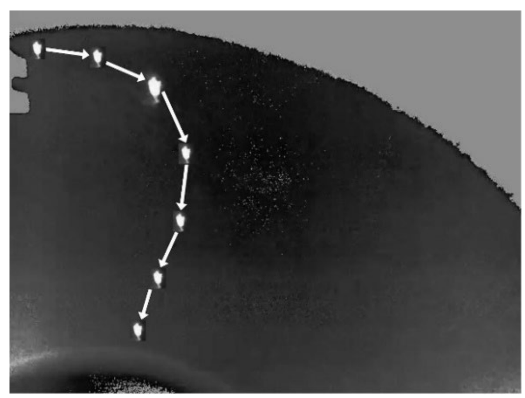
Figure 4: Thermal Camera Perspective with added Flow Path based of Visual Observation converted to Greyscale

across the vibrating bed over time. The greyscale images were then imported into a PIV (Particle Imaging Velocimetry) software package. This software uses two images from sequential timesteps to create an image pair, then detects the movement of objects, e.g., light spots of the individual grains, within the image pair. By providing the PIV software with a scale in the form of the ruler seen in Figure 2 and using the known time differential of the image pair based on the recording's frame rate, the velocity, position in the field of view, and direction of the moving object can be determined and expressed in vector form. Once all 100 runs of the experiment were processed, a MATLAB Program was created to sum all the velocity vectors across the length of the run to create a vector path; all 100 of these paths were then averaged, as shown in Figure 5.

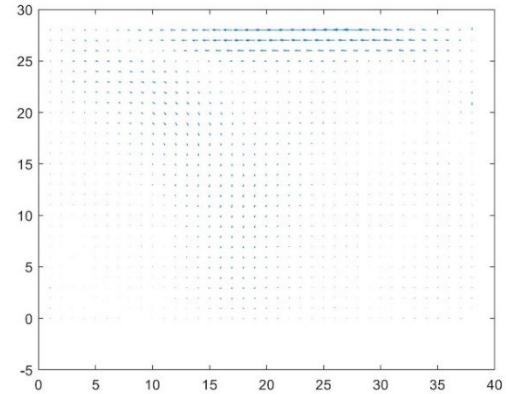

Figure 5: Average Vector Field of All PIV processed experimental data

Figure 5 shows the ensemble average of the flow paths in a vector field format. The x and y axis of the vector field is defined by the number of discretized interrogation areas created by the PIV software. By using this vector field, we can simulate a grain being introduced into that flow at a predefined location; this method, shown in Figure 6, is accomplished using the MATLAB streamlining function.

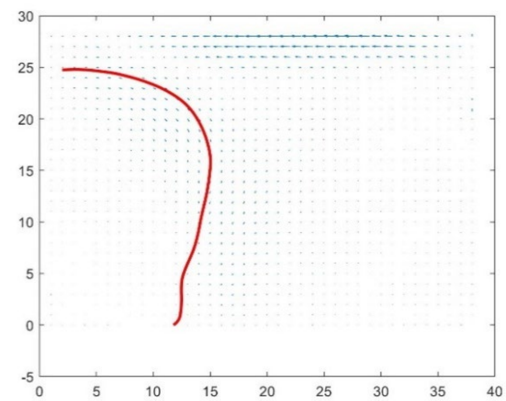

Figure 6: Streamline overlay of Average Vector Field of all PIV processed experimental data

Current Results

By overlaying Figure 6 on the original calibration image (Figure 2), Figure 7 was created.

This figure shows that the experimentally derived vector field and streamline closely resemble the expected flow path based upon visual observation (Ref. Figure 3,4). This similarity shows the accuracy of the PIV modeling process and proves that the discretized path data, along with the statistical spread and magnitude of the vector field will provide usable data for the next steps in the process.

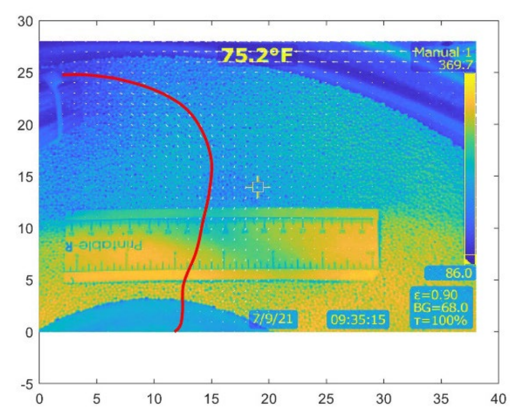

Figure 7: Streamline overlay of Average Vector Field of all PIV processed experimental data overlayed on Calibration Image

Future Plans

Moving forward, the discretized data from the streamlines path (Ref. Figure 6,7) will be used to derive the self-diffusion coefficient by modeling the collection of 100 random, heated grain paths as a stochastic Weiner process. Once the self-diffusion coefficient is solved for, it can be used to solve for the effective grain fluid viscosity using the Stokes-Einstein relation.

As research continues to show positive results for the use of vibrating grain beds as fluid analogs, eventually, the intent is to use the calculated grain-liquid properties in establishing a dimensional analysis correlation with the desired test fluid. This should allow vibrating grain beds testing to provide direct observation of the molecular interactions in fluid flow for a multitude of fluid types over a scaled version of the desired test geometry.

Acknowledgments

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