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Title: Developing Drag Models for Non-Spherical Particles through Machine Learning

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Final Report

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Executive Summary

This project focused on advancing the understanding of aerodynamic drag on non-spherical particles in dense gas-solid flows through the development of experimental and numerical datasets. Direct numerical simulations (DNS) were conducted for a range of particle shapes, concentrations, and Reynolds numbers, generating large datasets. These simulations provided detailed insights into the behavior of particles and formed the basis for identifying critical parameters influencing drag forces.

To validate the numerical findings, high-resolution experiments were performed in a controlled drop tower environment, where Reynolds numbers and particle concentrations were carefully regulated. This setup allowed for the generation of experimental data that closely matched the conditions of the simulations, minimizing wall effects and other external influences. The resulting datasets from simulations and experiments were then used to train deep neural networks in TensorFlow, testing various architectures with at least three hidden layers to develop an accurate drag model.

The outcome of the project is a comprehensive and validated drag model for non-spherical particles in dense gas-solid flows, along with a robust dataset for future research. This work provides critical insights into two-phase flow behavior, enabling improved understanding and modeling of processes involving non-spherical particles.

Project Activities Summary

This project aimed to advance the understanding of aerodynamic drag on non-spherical particles in dense gas-solid flows through a combination of computational modeling, experimental validation, and machine learning. The overarching goal was to develop a general drag model to support the accurate prediction and optimization of fluidized beds and chemical looping reactors. The project comprised four main thrusts: Direct Numerical Simulations (DNS), parameter reduction, high-resolution experiments, and TensorFlow-based machine learning. These activities, carried out over several years, resulted in significant progress in both fundamental understanding and practical application of particle drag models.

Direct Numerical Simulations (DNS)

The project began with three initial DNS test runs to explore the effects of varying particle concentrations, aspect ratios, and Reynolds numbers. Each simulation generated over 100,000 samples, as every particle and time step provided a unique data point. These initial runs were completed ahead of schedule in January 2020 and offered critical insights into drag behavior under controlled conditions.

Building on these results, a detailed analysis was performed to identify computational parameters suitable for further simulations. This was achieved by comparing DNS outputs with preliminary experimental results, culminating in the finalization of a robust parameter set in July 2021. Once these parameters were established, a comprehensive campaign of DNS simulations was conducted, resulting in a complete dataset of aerodynamic drag data by mid-2022. This dataset formed the foundation for subsequent machine learning activities and was disseminated through publications to benefit the broader scientific community.

Parameter Reduction

To enhance the efficiency of data analysis and reduce computational complexity, parameter reduction techniques were employed. The inputs and outputs from the DNS simulations were systematically reorganized to facilitate dimensionality reduction using the Diffusion Maps (DMAPS) algorithm. This effort, completed in October 2021, resulted in the identification of functional forms for a lower-dimensional manifold. These simplified representations were used to guide both experimental designs and machine learning model development, ensuring that only the most relevant parameters were considered.

Experimental Activities

High-resolution experimental validation was a critical aspect of the project, providing real-world data to corroborate the findings from DNS. The construction of a drop tower system, designed to control parameters such as Reynolds number and particle concentration, was completed in mid-2021. This system offered a unique capability to observe particle behavior under free-fall conditions, avoiding wall effects and maintaining consistency with numerical simulations.

Characterization of particle size and aspect ratio distributions was initiated to ensure precise experimental inputs. Although the majority of this task was completed by early 2022, unexpected printing issues delayed its finalization. Similarly, systematic experiments to sweep Reynolds numbers and particle concentrations reached 98% completion but were delayed due to disruptions caused by the COVID-19 pandemic.

Machine Learning Integration

A critical goal of the project was to develop a robust workflow to integrate data analysis with machine learning. This workflow, completed in July 2021, enabled the seamless transfer of data from simulations and experiments into TensorFlow. Using the comprehensive datasets generated, deep neural networks with at least three hidden layers were trained and tested. The model development process involved feature selection methods, such as K-fold cross-validation, to identify the most impactful parameters for predicting aerodynamic drag.

By the end of the project, the machine learning framework successfully leveraged the DNS and experimental datasets to produce a generalizable drag model. This model provides a powerful tool for understanding and predicting two-phase flow behavior involving non-spherical particles.

Key Outcomes and Impact

The project delivered a robust drag model validated by high-resolution experimental data and trained on comprehensive simulation datasets. This model represents a significant advancement in the field of gas-solid flows, providing critical insights into the behavior of non-spherical particles in dense regimes. Additionally, the methodologies developed, including the use of dimensionality reduction and machine learning workflows, have broader applications in computational fluid dynamics and related disciplines.

Despite challenges such as printing delays and COVID-19-related disruptions, the project achieved its primary objectives, laying the groundwork for further innovations in particle drag modeling and multiphase flow research. The comprehensive datasets, validated models, and streamlined workflows developed during this effort will serve as valuable resources for future studies and practical applications.

Journal Published

Two peer-reviewed journal articles have been published.

Lu, J., Xu, X., Zhong, S., Ni, R., & Tryggvason, G. (2023). The dynamics of suspensions of prolate spheroidal particles—Effects of volume fraction. *International Journal of Multiphase Flow*, *165*, 104469.

Lu, J., Xu, X., Zhong, S., Ni, R., & Tryggvason, G. (2024). Shape effects on the local dynamics of suspensions of spheroidal particles. *Physics of Fluids*, *36*(9).