the ENERGY lab

PROJECT FACTS

Crosscutting Research

Development, Verification, and Validation of Multiphase Models for Polydisperse Flows

Background

A fundamental understanding and numerical representation of multiphase flow (e.g., dense solid/gas flow) is important for the development of clean energy coal-based power systems, by allowing models and simulations to describe the complex interactions of reacting solid and gas media, including flow patterns, species, and temperature distributions. Reactors used in the conversion of coal to energy have traditionally been designed using a build-and-test method, resulting in suboptimal performance in terms of both efficiency and carbon emissions. First-principles models can help to overcome such obstacles, yet their application to practical systems has remained limited due to simplifying assumptions. For example, coal feedstock is characterized by a distribution of particle sizes (polydisperse); such a distribution is known to significantly impact reactor performance, yet most existing models assume identical particles (monodisperse). It is anticipated that accurate, verified, and validated models have been successfully applied to the design, scale up, and evaluation of clean energy systems (e.g., transport gasification, chemical looping). The application of these models will lead to a reduction in cost associated with the development and commercialization efforts.

In alignment with the Coal Utilization Sciences Program's mission, the National Energy Technology Laboratory (NETL) selected the University of Colorado to develop, verify, and validate simulation codes for polydisperse flows.

Project Description

The University of Colorado partnered with Iowa State University, Princeton University, and Particulate Solid Research Inc. to develop fundamental descriptions of poly-disperse multiphase flows, including gas-solid interactions, solid-solid interactions, and turbulence. The project aimed to bridge micro-scale effects to macro-scale behavior via simulations ranging from direct numerical simulations (DNS) to continuum models. This multi-scale approach was designed to ensure that important physics are retained upon scale-up.

This project developed a fully-specified continuum gas-solid model targeted specifically at materials with differences in size and/or density. A combination of theory, simulations, and experiments was utilized to develop simulation code for polydisperse flows. Specifically, in early efforts of the project, both Kinetic Theory

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PARTNERS

Particulate Solid Research Incorporated
Princeton University
Iowa State University

PROJECT DURATION

Start Date
05/16/2007

End Date
12/31/2011

COST

Total Project Value
$ 2,534,699

of Granular Flows (KTGF) and Direct Quadrature Method of Moments (DQMOM) techniques were systematically derived for solid-solid polydisperse systems. Two variations of these theories were implemented into the Multiphase Flow with Interphase eXchanges (MFIX) software suite, developed by NETL, to assess the relative merits. The Lattice Boltzmann Method (LBM) and the Discrete Time Immersed Boundary Method (DTIBM) were used to derive the gas-solid drag force for a polydisperse system over a wide range of conditions. The effect of polydispersity on instabilities in the gas-phase and solid-phase were also be explored using direct numerical simulation and coarse-graining techniques. Finally, a variety of test cases were used to validate model predictions for arange of vessel sizes and operating conditions. Discrete-element simulations were also be used to generate validation data for both granular and gas-solid systems using both NETL codes and MFIX. Experimental data was obtained from existing low-velocity and high-velocity systems.

Goal and Objectives

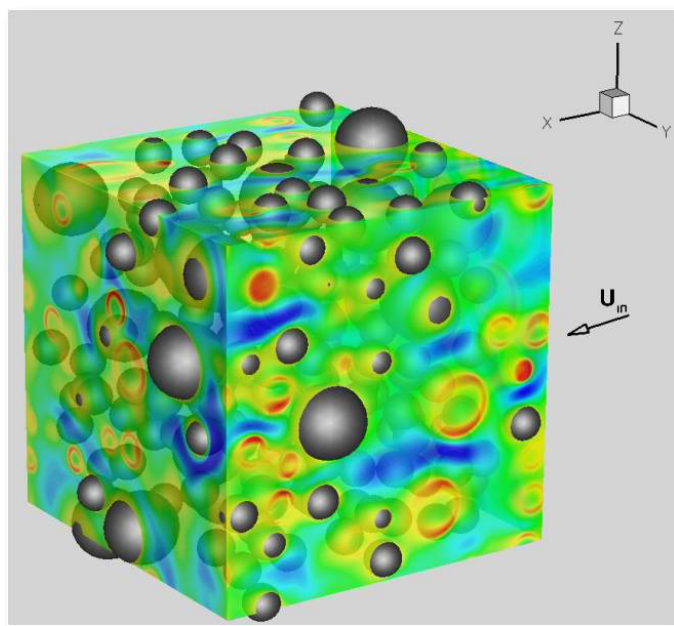
The goal of this project was to develop first-principles into MFIX. The goal was achieved using state-of-the-art methodologies tailored to polydisperse systems. The objectives of this effort were (1) to derive constitutive relations for a polydisperse solid phase that are not restricted by typical assumptions and which do account for the evolution of particle properties, (2) to develop a drag law for polydisperse flows that accounts for random particle motion and a mean relative motion between unlike particles, (3) to extend gas-phase turbulence models to account for polydisperse particles, and (4) to incorporate the resulting Computational Fluid Dynamic (CFD) model into MFIX and validate it via several industrially motivated test cases. Successful completion of the project will resulted in a fully specified model in which all of the necessary closures were developed specifically for polydisperse systems and the demonstration of the predictive ability of the model.

Accomplishments

This project has been completed. Two new polydisperse models KTGF and Discrete DQMOM have been developed and both have been fully incorporated and tested in the DOE NETL code MFIX. Experimental validation studies have also been completed, making up a suite of data from low-velocity (bubbling) and high-velocity (circulating) fluidized beds, as well as small- and large-scale units. The experiments, which were performed using both binary mixtures and continuous size distributions, revealed new and qualitatively different behaviors between the two distribution types. The impact of polydispersity on clustering has also been investigated both experimentally and theoretically. Ongoing work will include further comparison between the CFD models in MFIX and the experimental data.

Benefits

The development of improved CFD models and simulations to describe the complex interactions of reacting solid and gas media provides a better understanding of multiphase flow. This capability to more accurately model the flow of polydisperse systems, such as those found in coal combustion or gasification, will lead to a reduction in costs associated with the development and commercialization efforts of clean energy coal-based power systems. Additionally, by enhancing the MFIX code to handle a distribution of particle sizes rather than a single particle size, researchers have improved the accuracy of model predictions.



Direct numerical simulation of flow past a bi-disperse suspension of spheres as used to develop polydisperse drag laws.