“Closures for Coarse-Grid Simulation of Fluidized Gas-Particle Flows”

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Grant No: DE-FG26-06NT42737
January 1, 2006 – May 31, 2007

OBJECTIVE(s)

Gas-particle flows in fluidized beds and riser reactors are inherently unstable, and they manifest fluctuations over a wide range of length and time scales. Two-fluid models for such flows reveal unstable modes whose length scale is as small as ten particle diameters. Yet, because of limited computational resources, gas-particle flows in large fluidized beds are invariably simulated by solving discretized versions of the two-fluid model equations over a coarse spatial grid. Such coarse-grid simulations do not resolve the small-scale spatial structures which are known to affect the macroscale flow structures both qualitatively and quantitatively. Thus, there is a need to develop filtered two-fluid models which are suitable for coarse-grid simulations and capturing the effect of the small-scale structures through closures in terms of the filtered variables.

The overall objective of the current study is to develop validated closures for filtered two-fluid models for gas-particle flows, with the transport gasifier as a primary, motivating example. In this study, highly resolved three-dimensional simulations of a kinetic theory based two-fluid model for gas-particle flows are performed and the statistical information on structures in the 100-1000 particle diameters length scale are extracted. Based on these results, closures for filtered two-fluid models will be constructed. The filtered model equations and closures will be validated against experimental data and the results obtained in highly resolved simulations of gas-particle flows.

ACCOMPLISHMENTS TO DATE

We have shown that filtering of the statistical data obtained from highly resolved 2-D and 3-D simulations – employing a kinetic theory based two-fluid model implemented into the MFIX platform – in a periodic domain is a fruitful way to develop closures for coarse-grid simulation of fluidized gas-particle flows. We completed several highly resolved 2-D and 3-D simulations in various domain sizes with different spatial resolutions to extract filtered quantities for various filter sizes (for the case of uniformly sized particles.) These simulations were carried out for 75 μm Fluid Catalytic Catalyst particles suspended in ambient air. Using the computational “data” generated through such simulations, we have extracted filtered drag coefficient and particle-phase stresses as functions of the local particle volume fraction and the size of the spatial averaging window (i.e. filter size).We found that both the filtered drag coefficient and the particle-phase stresses varied systematically with increasing filter width both in 2-D and 3-D simulations. We also demonstrated that the filtered statistics become less dependent on spatial resolution and essentially independent of the domain size for both 2-D and 3-D simulations provided that the filter size is appreciably smaller than the domain size and is much larger than the grid size.

We have also studied the effects of various model parameters on these filtered quantities and found that the dimensionless filtered drag coefficient should be modeled as a function of the dimensionless filter size and particle volume fraction.

FUTURE WORK

The results we have obtained thus far indicate that filtering of the statistical data obtained from highly resolved 3-D simulation in a periodic domain is a fruitful way to develop closures for coarse-grid simulation of fluidized gas-particle flows. However, we need to establish a rational basis for the choice of filter size.

In the coming year, we intend to “validate” that the coarse-grid simulations with the filtered equations yield the same macroscopic results as the highly-resolved simulations with the kinetic theory based two-fluid model. Then, we will study the effect of particle size distribution.

Published Articles and US Patents: We have not yet published any papers summarizing these results. We have not filed any patent applications.

Articles under Preparation: Y. Igci, A. T. Andrews IV, S. Pannala, T. O’Brien & S. Sundaresan, Filtered two-fluid models for fluidized gas-particle suspensions.

Completed/Future Presentations:

a) S. Sundaresan, A. T. Andrews IV & Y. Igci, Coarse-graining two-fluid models for fluidized gas particle suspensions, The 231st ACS National Meeting, Atlanta, GA, March 28, 2006.
b) S. Sundaresan, A. T. Andrews IV, Y. Igci, S. Pannala & T. O’Brien, Coarse-graining two-fluid models for fluidized gas particle suspensions, Fifth World Congress on Particle Technology, Orlando, FL, April 24, 2006.
c) S. Sundaresan, , Y. Igci, A. T. Andrews IV, T. O’Brien & S. Pannala, Filtered Two-Fluid Models for Gas-Particles Flows, The AIChE Annual Meeting, San Francisco, CA November 11-13, 2006.
d) Y. Igci, S. Sundaresan, S. Pannala, T. O’Brien & R. Breault, “Coarse-graining two-fluid models for fluidized gas particle suspensions,” Fifth International Conference on CFD in the Process Industry, CSIRO, Melbourne, Australia, Dec 13-15, 2006. (Includes a Proceedings manuscript.)
e) Two more presentations are anticipated for the 2007 AICHE Annual Meeting, Salt Lake City, November.

Ph.D. Student supported under this grant: Ms. Yesim Igci