## 3.4 Coarse-Grid Simulation of Reacting and Non-Reacting Gas-Particle Flows

Peter N. Loezos (pnloezos@princeton.edu, 609-258-0543)
Anuj Srivastava (anujs@princeton.edu, 609-258-0543)
Sankaran Sundaresan (sundar@princeton.edu, 609-258-4583)
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544

**Abstract**

The principal goal of our project, funded under the *DOE Vision 21 Virtual Demonstration Initiative* is virtual demonstration of circulating fluidized bed (CFB) performance. Virtual demonstration of CFB performance requires modeling and simulation of the entire spectrum of gas-particle flow conditions ranging from dense phase flows in standpipes to dilute phase flow conditions of risers.

We had proposed a *virtual demonstration tool*, which is based on the open-domain Computational Fluid Dynamics (CFD) code MFIX (Multiphase Flow with Interphase eXchange), originally developed at NETL (National Energy Technology Laboratory). MFIX is based on a model framework in which the gas and particle phases are treated as interpenetrating continua. The general structure of Eulerian equations of motion for each of the phases is well understood, although specific constitutive equations describing the rheological behavior of gas-particle suspensions are still being developed. MFIX includes the capability to carry out reactive flow simulations, so the tool that we have set out to develop will permit both cold flow and reactive flow simulations. The principal challenge funded through this grant is to devise and implement in MFIX sound physical models for the rheological characteristics of the gas-particle mixtures.

The volume fraction of particles in dense fluidized beds, standpipes and valves is usually sufficiently large that the particles make enduring contact with multiple neighbors. In such instances, stress transmission between particles, and between particles and bounding solid surfaces occurs predominantly through frictional interactions. In this regime of flow, when the strength of frictional interaction between particles becomes sufficiently weak, flow of gas-solid suspension becomes unstable and a bubbly suspension results. Once formed, these bubbles dictate the macroscale flow characteristics, and therefore detailed CFD simulation of suspensions in this regime should account for the dynamics associated with the gas bubbles. This is possible only if frictional stresses are modeled properly. One of the objectives of our research is to develop a robust scheme for capturing the frictional stresses and a methodology to determine experimentally the parameters in such a model. We have now developed and implemented in MFIX a constitutive model for the rheology of granular materials in the dense, friction-dominated regime, and have shown that the key parameters in the frictional model can be estimated from fluidization-defluidization experiments. Such experiments have been performed with many different particle systems to demonstrate the viability of the procedure and the model itself.

The second objective of our research is to develop methodologies for practical simulation of gas-particle flows in fast-fluidized beds and risers, where the particle concentration is typically in the range of 1-30 vol %. In our past research, we have shown that meso-scale structures that take the form of clusters and streamers, which have been observed in risers, can be captured qualitatively through transient integration of continuum equations for the gas and particle phases. These structures arise as a result of two instability mechanisms, both of which are accounted for in a rheological model deduced in the literature by adapting the kinetic theory of gases to gas-particle mixtures. These meso-scale structures are too small in size to be resolved in simulations of flow in large process vessels, and are invariably invisible in the coarse-grid simulations. Yet, they affect

the flow characteristics profoundly; in particular, they alter the effective interaction force that couples the gas and particle phases, and dramatically increase the effective viscosities of the two phases. We had proposed to develop a more practical approach, where we simulate the dynamics of only the large clusters using coarse grids and account for the effects of smaller, unresolved clusters through suitable sub-grid approximations. Specifically, we had proposed to develop such sub-grid models and implement them into our *virtual demonstration too*l. To this end, we have carried out computational experiments which involve highly resolved simulations of meso-scale structures arising in dilute gas-solid flows, from which we have developed a sub-grid model to capture the effects of these structures in coarse-grid simulations of riser flows.

We have also examined the role of meso-scale structures on gas dispersion in gas-particle flows, so that one can begin to interpret tracer gas dispersion data. We found that macro-scale dispersion characteristics are governed by the macro-scale velocity and concentration fluctuations which are resolved in coarse-grid simulations. Consequently, a coarse-grid simulation of flow and dispersion only requires hydrodynamic sub-grid models and the sub-grid correction for the dispersion process only has a small influence on the overall behavior.