PLATFORM FOR MODELLING AND DIRECT NUMERICAL SIMULATION OF MULTIPHASE FLOWS

The design of multiphase flow devices requires effective continuum models that describe the transport behavior. These models are needed to scale-up equipment in the same way that is done with traditional computational fluids approaches (i.e., Navier-Stokes equations).

The three common computational approaches for modeling of gas-solid flows are the continuum method, the discrete element method (DEM) and the direct numerical simulation method (DNS). The first approach is computationally the least demanding and therefore, at least partly for this reason, has been used extensively in the past. But, since it resolves flow at the coarsest scales (scales much larger than the size of particles) it cannot be easily used for understanding phenomena that are controlled by the particle-particle and gas-particle interactions. The last approach, which has become viable only in the past few years, is computationally most demanding, as it resolves flow at the finest scales. This powerful methodology simulates dynamics at scales much smaller than the size of particles, and thus could be used to understand previously unexplained phenomena such as the formation of plugs in gas-solid flows. The DEM approach resolves flows at intermediate scales requiring models for the gas-particle and particle-particle interactions. This technique also has been only partly successfully, as the models for interaction between the phases are approximate and thus may not correctly include all particle scale features.

The results of DNS simulations performed in small domains (~100 particle diameters) can be compared directly with those obtained by DEM simulations, thus providing direct comparisons of predicted structures at the smallest relevant length scale (i.e., the particle diameter). DEM simulations performed with much larger domains (~ 1000 particle diameters) and larger numbers of particles allow observation of structures at the next larger scale (namely, tens of particle diameters), as well as the determination of effective closure models for continuum approaches. Such hierarchical calculations represent a powerful and essential approach to modeling and simulation of industrial scale gas-solid flow problems.

The above hierarchical approach for studying momentum transfer in multiphase flows can be expanded to model heat and mass transfer as well in chemical reactors by including appropriate conservation equations.