Recent Advances in CFD Modeling Of Multiphase Reactors

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The accurate numerical simulation of multiphase chemical processes represents a challenge due to the complexity of the flows under consideration. Different flow behavior is observed depending on the inertia of the “particles” forming the dispersed phase(s), the mass loading, and whether the flow is laminar or turbulent. The disperse phase(s) can also undergo aggregation, breakage, nucleation and chemical reactions. While the carrier phase can be described using conventional computational fluid dynamics (CFD), the behavior of the disperse phase(s) is more difficult to capture. In general, a disperse phase can be described by means of a statistical approach, where a number density function (NDF) is introduced to describe the evolution of the phase properties in space and time. The evolution of the NDF is described by a generalised population balance equation (GPBE). The solution of the GPBE can be approximated using quadrature-based moment method (QBMM). This approximation allows complex phenomena such as aggregation, breakage, nucleation and chemical reactions to be accurately represented, without incurring unreasonably high computational costs. We have developed a suite of CFD tools, based on QBMM and OpenFOAM, to perform flow simulations of multiphase reactors, such as stirred tanks, bubble columns and fluidised beds. During this presentation, I will give an overview of these tools and the activities of the Center for Multiphase Flow Research and Education (CoMFRE) at Iowa State University.