Looking Inside Multiphase Reactors: Some Recent Work on RPT, Euler-Euler-PBM and DEM Modeling

Shantanu Roy
Department of Chemical Engineering
Indian Institute of Technology - Delhi
Hauz, Khas, New Delhi 110019
(e) roys@chemical.iitd.ac.in
(t) 91 11 2659 6021
(f) 91 11 2658 1120

Dispersed gas-solid, gas-liquid and gas-liquid-solid systems, are of general interest in the multiphase reactor engineering community, owing to their wide applicability as reactors and separators in the petroleum refining, bulk and fine chemicals, and the downstream process industry in general. The flow pattern in these "real-world" systems is considerably more complex than what may be achieved in sanitized laboratory environments; consequently rigorous theoretical treatment of the flow in such systems is as yet elusive. This limitation poses a cap on predictive scale-up of such industrial vessels, whose design is primarily based on average flow rates, or more recently, on profiles of velocity and volume fraction of the phases. The fluctuations in the flow, generally multi-scale is nature, are not characterized well and thus that information is not incorporated into design and scale-up protocols today.

Radioactive Particle Tracking (RPT) has become popular in recent decades as a method for probing the velocity fields in opaque, multiphase systems non-invasively. Owing to the versatility of this technique, it has been variously used for probing multiphase reactors of interest. The basic idea in this method is to track the motion of a single tracer particle (made radioactive by incorporation of a suitable isotope) over many realizations of the flow, and then deriving ergodic means of the velocity profiles, RMS velocities, etc. In the past, much of the data treatment of RPT was done by projecting the data onto an Eulerian grid, since that was thought to be most useful from a reactor engineering perspective and also as validation data for CFD and other models. In principle, this experimental method is also "scaleable" (i.e., can be used in real industrial units), though there is almost no reported work thus far for use of this method in larger scale "real" multiphase reactors. Consequently, using RPT or otherwise, both experimentation and modeling of real industrial multiphase flows continues to be a challenge.

This presentation will focus of three different applications of RPT, and our attempts to develop appropriate computational fluid dynamics (CFD) models in each situation with RPT being the essential validation tool. The first two applications (laboratory scale) will be discussed with greater focus on the modeling aspects, while the third application will discuss more our experience and findings from "scaling-up" the RPT technique to industrial levels.

The first application that will be discussed will be a two-dimensional (rectangular) air-water bubble column operating at very low gas velocities. The gas in this column is introduced with a centrally placed distributor. First, we will discuss the key findings from the RPT experimentation and the different kinds of flow patterns observed by mapping the liquid velocity field. Next, conventional Euler-Euler simulation results will be presented with an assumed single bubble size and different combination of drag and lift forces. Finally, different population balance approaches coupled with CFD (Euler-Euler-PBM), namely Method of Classes (MOC), QMOM (Quadrature Method of Moments), MUSIG (MUltiple SIze Group) and DQMOM (Direct Quadrature Method of Moments) are implemented and validated against the RPT experimental observations. The results will be summarized and equivalence of the various population balance-CFD coupling methods will be shown.

The second application of RPT will focus on unary and binary batch fluidized beds, using glass and sago particles of different sizes. Classical observations of segregation and mixing in binary systems are cross-validated with the RPT observations, which actually present the velocity profiles in binary fluidized beds. A discrete element (DEM) model is implemented for this two-solids and gas system, and reasonably accurate predictions of the velocity profiles of either of the solids phases is reported. Importantly, we could show that the same closures used for predicting accurately the unary fluidized beds (of gas and either of the solids) could be employed for predicting the velocity profiles of both the solids phases (accounting only for the overall composition of the binary bed).

Finally, as a third application, the use of RPT for probing the flow pattern in an pilot plant scale bioreactor (for wastewater treatment) will be presented. Indeed, such an exercise threw up some unique challenges vis-a-vis implementation of RPT beyond laboratory scales, and these will be discussed. The experimental findings will be presented in brief, and future directions in experimentation for velocity measurement in industrial systems will be discussed. This would also be in keeping with the overarching theme of the workshop, *viz*. trends towards understanding "industrial multiphase" flows.