FLUIDIZED BEDS

I-10. Investigation of Catalytic Gas-Phase Olefin Polymerization Reactors - Radioactive Particle Tracking and CFD Studies RPT-CFD

A. Problem Definition

Bubbling gas-solid fluidized beds have found widespread application in the chemical process industries. An important process based on gas-solid fluidization is the UNIPOL process for the production of polyolefin's. Polymerization is extremely exothermic and the rate at which the heat generated can be removed determines the production capacity, even in a fluidized bed with its excellent heat transfer characteristics. The rate of heat removal is to a large extent determined by the macroscopic circulation patterns of the emulsion phase in a fluidized bed. Unfortunately, a profound understanding of the prevailing mechanisms is still lacking and quantitative information on the macro-scale circulation patterns in fluidized bed reactors is still quite scarce[1]. In this project the mechanisms causing the macro-scale circulation patterns are being studied using advanced experimental techniques and detailed modeling. To describe the hydrodynamic behavior of industrial scale bubbling fluidized reactors, a 3D Discrete Bubble Model (DBM) has been developed. In the DBM, an Euler-Lagrangian model, the larger bubbles are regarded as discrete elements and the bubble trajectories are tracked individually by integrating the equations of motion, accounting for possible bubble-bubble interactions. The emulsion phase is considered as a continuum and is described with the continuity and Navier-Stokes equations. The computation time to simulate large scale columns with Euler-Euler models, that completely resolve the bubbles (e.g. using the Kinetic Theory of Granular Flow), is prohibitively large. The main advantage of the DBM is that it fully accounts for the two-way coupling, i.e. the bubbles rising through the emulsion phase will affect the dynamics of the emulsion phase and, visa versa, the emulsion phase velocity patterns will be influenced by the drag exerted by the bubbles on the emulsion phase. Thus, the DBM can be used to investigate the macroscopic circulation patterns in fluidized beds, provided that good closures for the bubble behavior and bubble-bubble interactions are available (to be obtained from CARPT experiments). Another strong advantage of DBM is that in the DBM no *a priori* assumptions are required on the bubble encounter frequency, an important factor determining the bubble coalescence rate.

B. Objectives

The main objective of this project is to develop a profound and fundamental understanding of particle mixing and circulation patterns in mono- and poly-dispersed gas-solid fluidized beds resulting in a predictive model for up-scaling of fluidized beds. These phenomena will be studied using Computational Fluid Dynamics (CFD) using the Discrete Bubble Model (DBM) validated with Computer Aided Radioactive Particle Tracking (CARPT) experiments in cold flow set-ups.

C. Accomplishments and Current Work

To investigate the macroscopic circulation patterns in fluidized beds, a Discrete Bubble Model has been developed[2], which is able to simulate bubbles that can grow to a size larger than an Eulerian grid cell so that very wide bubble size distributions and high gas velocities can be simulated. The coalescence model in the Discrete Bubble Model has been improved in such a way that it is able to handle multiple coalescence events in a single time step. In addition, the interaction that a leading bubble has on a tailing bubble (bubble-bubble interaction) has been incorporated. Figure 1 shows a typical result from a simulation. In this figure a snapshot of the bubble phase and the corresponding time-averaged emulsion phase velocity plot after 110 seconds is presented.

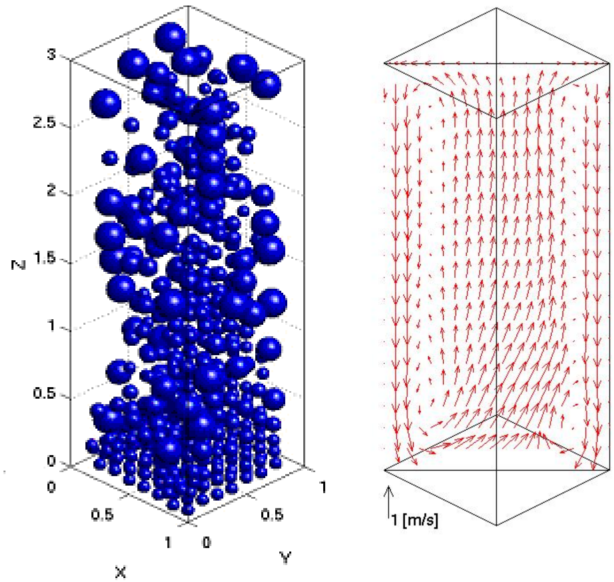

Figure 1: Snapshots of the bubble phase, at superficial gas velocities of respectively 0.25 and corresponding time-averaged emulsion phase velocity profile.

To validate the Discrete Bubble Model, several CARPT experiments have been carried out on an 18-inch diameter reactor in the CREL. The second part of the experimental program is currently being performed.

D. Future Work and Milestones

On the basis of the CARPT experiments data, the closure of the DBM will be evaluated and improved if necessary.

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E. Acknowledgements

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F. References

1. Bokkers, G.A., *Multi-Level Modelling of Hydrodynamics in Gas Phase Polymerisation Reactors*, PhD thesis, University of Twente, Enschede, The Netherlands, 2005.
2. Bokkers, G.A., Laverman, J.A., van Sint Annaland, M., and Kuipers, J.A.M., *Modelling of large-scale dense gas-solid bubbling fluidized beds using a novel Discrete Bubble Model*, Chemical Engineering Science, In press.

I-11. Experimental Investigation of the Hydrodynamics of Fluidized-Bed Reactors.

A. Problem Definition

Fluidized bed reactors are used in chemical, petroleum and petrochemical industries for various applications such as ammoxidation of propylene. Its main advantages are the ability to process large volumes of fluid and to provide low temperature gradients due to well mixed particles. The lack of understanding of the fundamentals of gas-particle flow and, in particular, the effects of gas-particle, particle-wall and particle-particle interactions on the flow dynamics, has led to the challenges in the scale-up and design of industrial gas-solid fluidized bed reactors. Therefore, improved understanding of the flow field and hydrodynamics of these reactors is essential to achieve better performance, control and operation of the currently used industrial reactors and for proper design (Mabrouk et al., 2005; Matsen, 1996).

B. Research Objectives

The overall objective of this work is to advance the understanding of the fluidized bed reactors at conditions pertinent to acrylonitrile synthesis by experimentally investigating the flow field, solids mixing and detailed fluid dynamic parameters using the advanced measurement techniques such as: computer automated radioactive particle tracking (CARPT), gamma ray computed tomography (CT), gamma ray densitometry, fiber optical probe, gas phase tracer, and pressure transducers.

C. Research Accomplishments

A literature review has been initiated and it is currently in progress. The goal of this review is to present the state-of-art regarding the recent advances made on gas-solid fluidized catalytic reactors.

D. Future Work

This project is supported by Innovene and hence, the future work will be finalized with them. However, preliminary work will be conducted by implementing CARPT on the current 18 inch column fluidized bed with 7 ft height using air and glass beads to provide beach-mark data for CFD evaluation and validation.

E. Acknowledgements

The financial support provided by Innovene is acknowledged.

F. References

Mabrouk, R., Radmanesh, R., Chaouki, J., and Guy, Ch., "Scale effects on fluidized bed hydrodynamics", International Journal of Chemical Reactor Engineering, Vol. 3, 1-11 (2005).

Matsen, J.M., "Scale up of fluidized bed processes: principle and practice", Powder Technology, Vol. 88, No. 3, 237-244 (1996).

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