HYDRODYNAMIC MODELS FOR SLURRY BUBBLE COLUMN REACTORS

Final Technical Report

This report also includes the Quarterly Technical Report for period: 01/01/97 - 03/31/97.

Reporting Period: 06/01/94 - 06/01/97

Principal Author: Dimitri Gidaspow

Report Issue Date: 08/15/97

DE-FG22-94PC94208--12

Illinois Institute of Technology
Dept. Of Chemical and Environmental Engineering
10 W. 33rd St.
Chicago, IL 60616

ABSTRACT

The objective of this study is to develop a predictive experimentally verified computational fluid dynamic (CFD) three phase model. It predicts the gas, liquid and solid hold-ups (volume fractions) and flow patterns in the industrially important bubble-coalesced (churn-turbulent) regime. The input into the model can be either particulate viscosities as measured with a Brookfield viscometer or effective restitution coefficient for particles.

A combination of x-ray and γ-ray densitometers was used to measure solid and liquid volume fractions. There is a fair agreement between the theory and the experiment. A CCD camera was used to measure instantaneous particle velocities. There is a good agreement between the computed time average velocities and the measurements. There is an excellent agreement between the viscosity of 800 μm glass beads obtained from measurement of granular temperature (random kinetic energy of particles) and the measurement using a Brookfield viscometer.

A relation between particle Reynolds stresses and granular temperature was found for developed flow. Such measurement and computations gave a restitution coefficient for a methanol catalyst to be about 0.9.

A transient, two-dimensional hydrodynamic model for production of methanol from syn-gas in an Air Products/DOE LaPorte slurry bubble column reactor was developed. The model predicts downflow of catalyst at the walls and oscillatory particle and gas flow at the center, with a frequency of about 0.7 Hertz. The computed temperature variation in the rector with heat exchangers was only about 5 ^{o}K, indicating good thermal management.

The computed slurry height, the gas holdup and the rate of methanol production agree with LaPorte’s reported data.

Unlike the previous models in the literature, this model computes the gas and the particle holdups and the particle rheology. The only adjustable parameter in the model is the effective particle restitution coefficient.

EXECUTIVE SUMMARY

The objective of this investigation is to convert our "learning gas-solid -liquid" fluidization model into a predictive design model . This model is capable of predicting local gas , liquid and solids hold-ups and the basic flow regimes: the uniform bubbling , the industrially practical churn-turbulent (bubble coalescence) and the slugging regimes . Current reactor models incorrectly assume that the gas and the particle hold-ups (volume fractions) are uniform in the reactor . They must be given in terms of empirical correlations determined under conditions that radically differ from the reactor operation . In the proposed hydrodynamic approach these hold-ups are computed from separate phase momentum balances . Furthermore , the kinetic theory approach computes the high slurry viscosities from collisions of the catalyst particles . Thus particle rheology is not an input into the model . See Gidaspow, "Multiphase Flow and Fluidization, Continuum and Kinetic Theory Description," Academic Press, 1994.

Our program was reviewed by DOE and Air products team who visited us January 31 , 1995 . DOE FETC is sponsoring a multi-year program at Air Products and Chemicals on development of alternative fuels from coal derived syngas using slurry bubble column reactors . Air Products use stirred tank reactor models for analyzing their data . Our model predicts the flow patterns .

The new model we developed should help the industry to optimize their reactors, since it predicts the hydrodynamics under operating conditions. Our newly developed CCD camera technique can measure the velocity and the turbulence in a cold model of the reactor. This new method can be used to further verify our hydrodynamic model.

A combination of x-ray and γ-ray densitometers was used to measure solid and liquid volume fractions. There is a fair agreement between the theory and the experiment. A CCD camera was used to measure instantaneous particle velocities. There is a good agreement between the computed time average velocities and the measurements. There is an excellent agreement between the viscosity of 800 μm glass beads obtained from measurement of granular temperature (random kinetic energy of particles) and the measurement using a Brookfield viscometer.

A relation between particle Reynolds stresses and granular temperature was found for developed flow. Such measurement and computations gave a restitution coefficient for a methanol catalyst to be about 0.9.

A transient, two-dimensional hydrodynamic model for production of methanol from syn-gas in an Air Products/DOE LaPorte slurry bubble column reactor was developed. The model predicts downflow of catalyst at the walls and oscillatory particle and gas flow at the center, with a frequency of about 0.7 Hertz. The computed temperature variation in the rector with heat exchangers was only about 5 ^{o}K, indicating good thermal management.

The computed slurry height, the gas holdup and the rate of methanol production agree with LaPorte's reported data.

TABLE OF CONTENT