

TITLE PAGE

**ENGINEERING DEVELOPMENT OF SLURRY BUBBLE COLUMN
REACTOR (SBCR) TECHNOLOGY**

**Quarterly Technical Progress Report No. 24
For the Period 1 January – 31 March 2001**

FINAL

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ENGINEERING DEVELOPMENT OF SLURRY BUBBLE COLUMN REACTOR (SBCR) TECHNOLOGY

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Project Objectives

The major technical objectives of this program are threefold: 1) to develop the design tools and a fundamental understanding of the fluid dynamics of a slurry bubble column reactor to maximize reactor productivity, 2) to develop the mathematical reactor design models and gain an understanding of the hydrodynamic fundamentals under industrially relevant process conditions, and 3) to develop an understanding of the hydrodynamics and their interaction with the chemistries occurring in the bubble column reactor. Successful completion of these objectives will permit more efficient usage of the reactor column and tighter design criteria, increase overall reactor efficiency, and ensure a design that leads to stable reactor behavior when scaling up to large diameter reactors.

Abstract

Washington University's work for the quarter involved the study of the dynamic simulations of bubble columns in three dimensions. Work was also done in dynamic simulations of two-phase transient flow using CFDLIB. Ohio State measured the axial dispersion coefficients of the liquid phase. The steady-state thermal dispersion method was used to obtain the measurements. Iowa State followed the last quarter's work by using CFDLIB to simulate conditions described in the literature, with the objective of validating the simulation result. The group's work also led to a determination of the adequacy of periodic boundary conditions in representing small columns.

Executive Summary

In the twenty-fourth quarter's work, Washington University's team studied three-dimensional dynamic simulations of bubble columns. Numerical simulation was utilized to capture the significant features of column flows. Washington University also reported completion of 3D dynamic simulations for three sizes of bubble columns operating at different superficial gas velocities. The simulations were performed in CFDLIB, which was developed by the Los Alamos labs. The predicted overall gas holdup in each case was in good agreement with the experimentally measured value. Numerical liquid-phase particle tracking simulations covering columns of two different sizes were performed using CFDLIB. Numerically predicted axial diffusivities agreed well with the measured values calculated from CARPT data.

Ohio State measured the axial dispersion coefficients of the liquid phase in high-pressure columns by the steady-state thermal dispersion method. It was found that the axial temperature distribution in terms of $\ln[(T-T_0)/(T_m-T_0)]$ is almost linear at various gas velocities. The axial dispersion coefficient increases significantly with increasing gas velocity. The effect of liquid velocity on the axial liquid mixing is small compared to the effect of gas velocity. Ohio State also initiated the study of flow fields and Reynolds stresses at high pressures using a two-dimensional laser Doppler velocimetry (LDV) system calibrated under ambient conditions. In addition, Ohio State measured the axial liquid velocity profiles at different gas velocities under ambient conditions for the air-water system using the LDV technique. The regime transition was identified based on the liquid velocity measurement, and the transition superficial gas velocity obtained was about 4 - 6 cm/s in the air-water system.

Iowa State used 3D CFDLIB in simulating conditions described in the literature. In order to improve the resolution obtained through the first set of simulations, a second set was performed under the same conditions as the first, but with a smaller grid. This produced a high-resolution set of 3D simulations that the Iowa State group expects to be of great value in the work ahead.