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The following report (which will be submitted as a topical report) from Washington University for the period July-September 1996 contains the following chapters:

1. Introduction
2. Objectives
3. Gas Holdup Measurement
4. Tracer Experiments
5. Modeling
6. Parameter Estimation
7. Comparison with the Results from Tracer Studies in the Methanol Synthesis Slurry Bubble Column
8. Conclusions
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Slurry Bubble Column Hydrodynamics

Tracer Studies of the La Porte AFDU Reactor:

Dehydration of Isobutanol to Isobutylene

Topical Report

(6th quarterly report)

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Abstract

Radioactive tracer data, acquired in the slurry bubble column reactor during dehydration of isobutanol to isobutylene at the Alternative Fuels Development Unit (AFDU) of La Porte, Texas, was interpreted based on the axial dispersion model (ADM). The tracer experiments were conducted using Manganese⁵⁶ oxide particles (slurry, 50 μm) as liquid phase tracer and Ar⁴¹ as gas phase tracer. The liquid and gas phase axial dispersion coefficients and the liquid volumetric mass transfer coefficient were estimated by fitting the experimental responses with the model predictions. Both the liquid phase and gas phase axial dispersion coefficients showed an increase with gas superficial velocities. It was also found that the model is not sensitive to the volumetric mass transfer coefficient, leading to a wide spread in the range of this estimated parameter. The results obtained are consistent with the findings obtained in interpreting tracer data during methanol synthesis. Alternative models were proposed.

Executive Summary

Radioactive tracer experiments were conducted at the AFDU slurry bubble column reactor during the dehydration of isobutanol to isobutylene at La Porte, Texas, to investigate the flow pattern and back mixing of the liquid and gas phase. Impulse injections of radioactive Mn^{56} particles of 50 μm mean diameter (in a slurry) were made at two different axial positions along the column to monitor the mixing of the slurry phase (batch). Impulse injections of radioactive Ar^{41} were made at the inlet of the bubble column reactor to monitor the gas phase flow. Four sets of scintillation detectors, each of which consists of four detectors placed at 90° to each other at the same plane, were arranged along the column to measure the responses. The axial dispersion model was used to interpret the tracer data of both liquid and gas phases.

The objectives of the present study were: (a) to investigate the flow pattern and backmixing information from the actual pilot plant slurry bubble column reactor operating at high temperature (300° C) and elevated pressure (25 psig) under reaction conditions; (b) to examine the dependence of the axial dispersion coefficients, D_g and D_l , on the superficial gas velocity; (c) to assess the suitability of the axial dispersion model for describing the backmixing in slurry bubble column reactors. Further, the goal was to compare the findings of this study to those obtained during methanol synthesis.

The obtained results can be summarized as follows:

- 1) The axial dispersion model cannot describe with a consistent axial dispersion coefficient the flow pattern and back mixing of the liquid phase in the bubble column. The model predictions were only fitted to data that show no overshoots. An alternative phenomenological model is suggested.
- 2) The estimated average axial dispersion coefficients for liquid, D_l , are 3258 and 3612 cm^2/s at inlet superficial gas velocities of 7.0 cm/s and 12.2 cm/s , respectively,

indicating a reasonable extent of backmixing of the liquid (slurry) phase. The liquid axial dispersion coefficient shows an increase with superficial gas velocity.

- 3) For the gas tracer experiments, the axial dispersion model can yield reasonably good fits of the experimental responses. However, the estimated parameters, such as the gas phase dispersion coefficient, D_g and the volumetric mass transfer coefficient, k_1a , have a very wide range. This is especially true for k_1a . The values of k_1a vary from 0.002 to 18.0 (1/s), meaning that the model is not sensitive to the mass transfer parameters. A new model developed at CREL is recommended to describe the flow pattern and back mixing for the present system.
- 4) The available correlations for predicting the axial dispersion coefficients were tested to get an approximate estimate of the parameters. For the liquid phase, the predicted D_l is about 50% lower than the values obtained in this study. For the gas phase, the predicted D_g is much higher than the values obtained in this study, about 4 ~ 9 times larger. The correlations clearly would be not applicable under the conditions investigated..
- 5) The average values of the estimated parameters are shown in the table below:

Run No.	P, psig	T, °C	$\bar{\epsilon}_g$	\bar{U}_g , cm/s	D_l , cm ² /s	D_g , cm ² /s	k_1a , s ⁻¹
R82-1	25.0	300	0.19	10.4	3260±2020	6750 ±1580	1.87 ±1.77
R82-2	25.0	300	0.19	10.4	3260±2020	7140 ±1770	1.38 ±1.54
R86-1	25.0	300	0.25	18.1	3610±2070	8350 ±2010	2.04 ±2.86
R86-2	25.0	300	0.25	18.1	3610±2070	8180 ±1590	2.11 ±2.74

- 6) Comparison of the results between the methanol synthesis runs and the present dehydration of isobutylene studies suggests that the expansion of gas in the column, in the present case, results in larger values for both the liquid and gas phase dispersion coefficients.

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