OPTICAL MEASUREMENTS IN GAS-LIQUID STIRRED TANKS

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Summary

The thrust of this research is to provide innovative, in-situ, optical techniques that can accurately obtain bubble dynamics in a G-L ST, readily track liquid level height to determine the volumetric expansion of CXLs, and determine the phase transition of fluids from the subcritical to the supercritical state – all across a wide range of operating pressures, temperatures, and fluids. The knowledge and understanding of optical probes and G-L STs as well as supercritical and dense phase reactors will be advanced, valuable knowledge for CFD modeling will be provided, and new engineering science will be generated in systems at elevated conditions never before reported in the literature.

Keywords

Multiphase and particulate reactors, Multiscale analysis, Environmental reaction engineering, Green CRE

Introduction

Multiphase reactors are used throughout the petroleum, chemical, mining, biochemical and pharmaceutical industries to contact reactants that are in different. Stirred tanks are used widely in chemical production (polymerization, alkylation, oxidation, chlorination, fermentation etc.) because they reliably allow for high levels of backmixing, for efficient contacting between liquid and gas to ensure good mass transfer, for the suspension of solids, and for ease of heat transfer leading to isothermal operation. However, in systems that are highly reactive or contain very active catalysts, it is often difficult to remove mass transfer limitations, which can adversely affect the rate of reaction. Poor yields and reduced selectivities due to inefficient mixing can cause excessive production of byproducts requiring disposal or unproductive downstream processing, excessive separation costs, greater use of harsh solvents – all of which reduce profitability of the process and create a large environmental footprint.

The ability to understand, properly model and design fluid flow within a multiphase stirred tank (ST) would allow for better reactor scale-up and therefore maximize reactor performance and decrease waste due to inadequate reactor design. More than 15 years ago, Tatterson et al.[1] estimated that nearly half of the $750 billion annual output from the chemical industry alone passed through a ST at one point and that losses incurred by inadequate reactor design were on the order of tens of billions of dollars. Unfortunately, things have not improved much in the past couple of decades.

Reactor scale-up – from the laboratory scale reactor, to the pilot plant reactor, and all the way up to the industrial scale reactor – is the single biggest challenge with multiphase reactors. As reactors are scaled up to larger sizes geometric, bubble, mixing and kinetic lengths and characteristic times do not scale in proportion.

Rather than beginning with the mass, energy, and momentum transport equations within a multiphase stirred tank, flow models with empirical correlations are generally used to describe the multiphase flow in the reactor. This approach has provided a foundation for reactor design and scale-up; however, care must be taken that the correlations are appropriately used. The empirical information available for modeling usually describes global properties in the system of interest (overall gas holdup, etc.) but often does not provide the detailed information regarding local properties that are important for the design and scale-up of process equipment.

In the age of ever increasing computing power, computational fluid dynamic (CFD) models have been developed to provide quantitative descriptions of flows in multiphase STs. Yet, even the most powerful CFD models require experimental validation. Guha et al.[2] have shown that current CFD attempts fail to properly capture flows in liquid-solid systems and Rammohan et al.[3-4] have documented the same for gas-liquid STs. Clearly, more experimental evidence is essential for guiding the improvement in the CFD codes. It is on this experimental front that data for G-L STs is lacking – especially concerning bubble dynamics. CFD models are inadequate, and there simply is not enough data to empower the predictive capabilities of CFD for multiphase stirred tank reactors.

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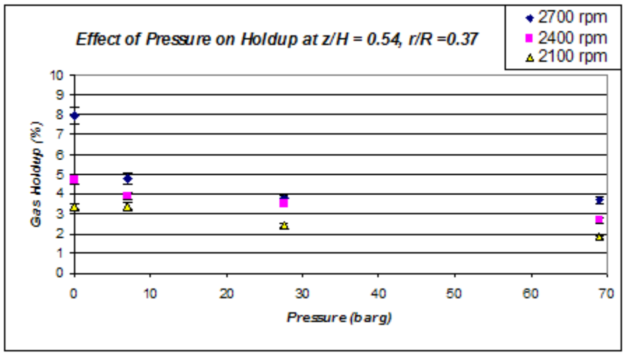
With the rising government regulation and global awareness of the type and scale of industrial impact on the environment, green engineering has rightly moved to the forefront in the design of chemical processes. To transform the manufacture and use of chemicals into inherently safe, ecologically responsible, and economically viable processes, one of the visions of the green engineering is to either eliminate or significantly replace the harsh, conventional mineral acids as well as organic and chlorinated solvents used in catalytic processes with benign solvents such as carbon dioxide. Dense phase carbon dioxide (CO_2), including liquid and supercritical CO_2, has been gaining acceptance for potential use in industrial applications due to benefits of pressure-tunable density and transport properties, ease of separation, solvent replacement, enhanced miscibility of reactants, optimized catalyst activity, and increased product selectivities, all of which decrease waste and pollution[5-6]. Carbon dioxide expanded liquids (CXL's) also provide the benefit up of to 80% solvent replacement with dense phase carbon dioxide. However, the basic information – such as how much organic solvent can be replaced with CO_2 at a given condition or when the supercritical phase change occurs in the mixture – is scant in the literature.

To add to the complexity of investigating G-L STs, most of the experimental thrusts in the literature use techniques that either require transparent vessels operating at low gas holdups, or are often expensive, or can be used only under limited conditions. Industrial STs are often opaque (stainless steel construction and high holdups) and operate at temperatures and pressures well outside the range of atmospheric conditions – rendering many of the experimental techniques outlined in the literature useless for industrial investigations. Therefore, relatively inexpensive tools are needed that can be used to capture local, quantitative information at industrially relevant conditions.

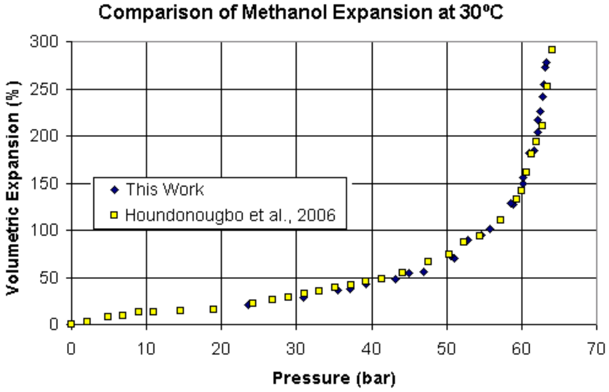
Results

Optical probes have been developed which can capture gas holdup, bubble velocity, chord-length and specific interfacial area of bubbles as small as 1 mm in diameter. Local gas holdup profile as a function of pressure is shown below for an air/water system in a 1-L autoclave equipped with a hollow shaft stirrer.



The optical probe results have also been confirmed visually with the use of in-situ borescopy coupled with high-speed photography.

Volumetric expansion and phase transition in CXL systems have also been quantified using optical probes. The volumetric expansion of methanol with CO2 is compared to work done by Houndonougbo et al.[7] below.



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