OBTAINING INTRINSIC KINETICS FOR GAS-LIQUID REACTIONS IN LABORATORY- AND PILOT-SCALE STUDIES: GAS-INDUCING IMPELLERS

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Abstract

The kinetics of gas-liquid reactions are often measured in small-scale stirred vessels, regardless of the commercial reactor configuration. Overcoming transport limitations such as gas-liquid mass transfer is critical in order to obtain intrinsic reaction kinetics useful for reaction scale-up. Gas-inducing impellers are commonly used in such laboratory studies to both agitate the mixture and entrain gas in the liquid phase, but are potentially more sensitive to transport limitations than other reactor configurations. This paper evaluates the performance of gas-inducing impellers through a combination of hydrodynamic experiments, kinetic measurements on surrogate reaction chemistry, and reactor modeling. The combined analysis provides a generalized framework for measuring intrinsic reaction kinetics in gas-liquid systems.

Keywords

Gas-inducing impellers, Gas-liquid reactions, Stirred vessels

Introduction

Stirred vessels are widely used in laboratories and pilot plants to investigate novel condensed phase reactions and their kinetics. It is preferred to operate these reactors in a kinetically-limited regime with minimal transport effects. For gas-liquid reactions, mass transfer limitations will obscure the intrinsic kinetics and confound attempts to translate kinetic observations to different process scales. Uniform dispersion of the gas and liquid phases are also important in ensuring that the reactor may be modeled as a well-mixed reactor. Thus, an accurate characterization of the hydrodynamics and mass transport at the laboratory and pilot reactor scales is critical to effective reaction scale-up.

For small-scale vessels, vendors often provide hollow shaft gas-inducing impellers (see Figure 1) to entrain gas from the reactor headspace and disperse it in the liquid phase. The spinning impeller reduces the dynamic head at the impeller tip; this enables gas suction from the headspace through hollow shaft and into the impeller discharge. Quality gas dispersion and mixing requires understanding the minimum required impeller speed for gas induction. Since gas-inducing impellers are often provided as standard options for purchased autoclaves, they are widely used without a proper understanding the appropriate operating conditions. The limited literature available on the subject (Joshi and Sharma, 1977, Patwardhan and Joshi, 1999, Poncin et al., 2002, Zieverink et al., 2006) provides general guidance; developed correlations are not universally predictive but rather application-specific. Impeller effects for small-scale stirred vessels are not often scalable because of the relative influence of the walls on the hydrodynamics.

This paper presents studies of the hydrodynamics of stirred vessels with gas-inducing impellers to enable decoupling of the transport effects. The performance of proprietary ParrTM and Autoclave Engineers™ impellers are evaluated in 1L, 2L, and 4L stirred vessels. The paper
shows impact of impeller choice and vessel size on gas induction, gas holdup and gas-liquid mass transfer. These effects are compared to traditional impellers to demonstrate the scenarios in which gas-inducing impellers are preferred and also indicate when they should be avoided.

Using this data, a multiphase stirred tank reactor model is developed to show the relative impact of the measured transport effects on the apparent reaction kinetics, which can be used to identify the vessel configurations and operating conditions necessary to obtain intrinsic kinetics. The model is then applied to a surrogate gas-liquid reaction chemistry to identify those appropriate operating conditions. The model results are compared to experimental measurements of the apparent reaction kinetics to show its applicability. The combined framework of hydrodynamic experiments, kinetic experiments and modeling are then summarized to show the requirements for obtaining reliable measurements of gas-liquid reaction kinetics.

Figure 1. Gas-inducing impeller

References


