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CORRELATING GAS–LIQUID MASS TRANSFER IN A STIRRED-TANK REACTOR

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A correlation is developed for the volumetric gas–liquid mass transfer coefficient (k_La) in stirred-tank reactors (STRs) using results from the literature. The volumetric mass transfer coefficient is correlated on the basis of the relative dispersion parameter (N/N_{CD}) for similar impeller hydrodynamics and operating regimes. Using a bench-top STR of diameter $T = 0.211$ m, gas–liquid mass transfer data are also obtained and found to follow the proposed correlation when the appropriate hydrodynamic conditions are satisfied. A STR scale-up technique from bench-scale ($T = 0.211$ m and $D/T = 0.35$) to industrial-scale (up to $T = 2.7$ m) is proposed using a normalized hydrodynamic flow regime map and shown to be useful in understanding the range of operational conditions for the successful scale-up of STRs.

Keywords: bioreactors; hydrodynamics; mass transfer; scale-up; stirred-tank reactor.

INTRODUCTION

The purpose of this paper is to use knowledge of stirred-tank reactor (STR) hydrodynamic regimes to correlate the volumetric mass transfer coefficient (k_La). STRs are used in a variety of process industries, but the prediction of k_La is extremely difficult because of the complexity of the gas–liquid hydrodynamics. Various investigators have correlated k_La values to power density (P_g/V) and superficial gas velocity (U_g) over one or two similar vessel sizes. Published results in air–water systems show a large scatter when plotted in the form

$$k_La = C_1\left(\frac{P_g}{V}\right)^{\alpha} U_g^{\beta} \tag{1}$$

where the exponents α and β range from 0.3 to 0.7 and 0 to 1.0, respectively, as summarized by Stenberg and Andersson (1988) and Rushton and Bimbinet (1968). They suggested that correlations based on equation (1) were scale dependent and should have additional terms for successful scale-up. This is supported by the fact that in many scale-up attempts, equation (1) was shown to be unsuccessful in predicting industrial-scale results from laboratory trials, but was very successful in correlating data from similarly sized vessels (Lines, 2000; Stenberg and Andersson, 1988; Figueiredo and Calderbank, 1979; Chandrasekharan and Calderbank, 1981; Nienow and Wisdom, 1978; Rushton and Bimbinet, 1968).

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Successful scale-up of STRs requires knowledge of the fluid behaviour in terms of gas–liquid operating regimes, so that mass transfer coefficients can be determined in bench-top equipment and projected to large industrial-scale systems. There are flooding limits, complete dispersion transitions, cavity formations, and critical impeller speeds below which the impeller will not effectively disperse the gas into the liquid.

The following STR bulk flow regime transitions at constant gas flow rate with increasing impeller speed have been correlated in the literature: (1) at too high gas flow, gas dominates the flow and the impeller becomes flooded at an impeller speed N_F defined by (Nienow *et al.*, 1985):

$$(Fl_g)_F = 30(Fr)_F\left(\frac{D}{T}\right)^{3.5} \tag{2}$$

(2) for $N_F < N < N_{CD}$, the impeller is loaded but the gas is not completely dispersed and correlated by (Nienow *et al.*, 1977):

$$(Fl_g)_{CD} = 0.2(Fr)_{CD}^{0.5}\left(\frac{D}{T}\right)^{0.5} \tag{3}$$

(3) for $N_{CD} < N < N_R$, the gas is completely dispersed; and (4) when $N > N_R$, large amounts of gas recirculate throughout the vessel and is described by (Nienow and Wisdom, 1976):

$$(Fl_g)_R = 13(Fr)_R^2\left(\frac{D}{T}\right)^{5} \tag{4}$$

where $(Fl_g)_i$ and $(Fr)_i$ represent the gas flow number and the corresponding Froude number at flooding, complete dispersion, and recirculation, respectively. For efficient operation, the impeller speed N should be greater than the impeller speed at which complete gas dispersion occurs ($N > N_{CD}$).

van't Riet (1975) studied the cavity formation on the impeller blades in detail and defined three cavity forms that depend on the stirrer speed and gas flow rate: (1) vortex cavities, (2) clinging cavities, and (3) large cavities. Warmoeskerken *et al*. (1984a, b) reported that 3-3 cavity structures directly affect the power demand of the impeller, which in turn will influence other process variables such as gas holdup and gas–liquid mass transfer. The transition from the vortex-clinging cavities to the first large cavity occurred at a gas flow number given by (Smith and Warmoeskerken, 1985):

$$Fl_g = 3.8 \times 10^{-3} \left(\frac{Re^2}{Fr}\right)^{0.067} \left(\frac{T}{D}\right)^{0.5} \quad (5)$$

where Re is the Reynolds number.

This paper will utilize various hydrodynamic flow regimes identified in a STR equipped with a Rushton impeller to develop a model for gas–liquid mass transfer scale-up. Initially, the STR scale-up correlation is developed from literature data for a range of STR sizes and geometric ratios. In addition, gas-liquid mass transfer data are collected and shown to fit the correlation when the required hydrodynamic flow conditions are satisfied.

METHODS AND MATERIALS

Experiments are carried out in a BioFlo 110 Fermentor (New Brunswick Scientific Co., Edison, NJ), which is a dished-bottom cylindrical vessel of diameter $T = 0.211$ m filled with water to a height (H) equal to the vessel diameter (T) (Figure 1). A six-bladed Rushton impeller of diameter $D = 0.0747$ m ($D/T = 0.35$) is used at a constant clearance ratio of $c = H/4$ above the tank base. The impeller blade dimensions and all other vessel geometric factors in the system correspond to the well known standard vessel configuration (Holland and Chapman, 1966). The STR is maintained at a constant temperature (25°C) using a heat blanket and recirculating water bath. The tank is also fitted with a dissolved oxygen probe (DO probe) and pH electrode. The impeller is driven by a variable-speed DC motor, which is connected to the primary control unit (PCU) of the BioFlo 110 Fermentor for dissolved oxygen measurements, or to an AC/DC converter for power measurements. Details of the power measurements are provided by Kapic (2005).

The volumetric gas–liquid mass transfer rate measurements are determined using a dynamic gassing-out method (Linek *et al.*, 1987; van't Riet, 1979; Zhu *et al.*, 2001). Dissolved oxygen concentrations are recorded using an InPro-6800 series polarographic type probe with a single layer silicon membrane cover for faster response (Mettler Toledo, Woburn, MA). Probe calibration is completed each time at the same operating conditions at which the measurements are obtained. The liquid is first deoxygenated by sparging nitrogen at the desired gas flow rate and impeller speed until a zero reading is reached on the DO probe. The nitrogen flow rate is then turned off and the impeller speed stopped to allow all the nitrogen bubbles to escape from the liquid. The impeller is then turned back on and a three-way valve is switched to the air supply. Dissolved oxygen concentrations are then determined as a function of time until saturated conditions are established.

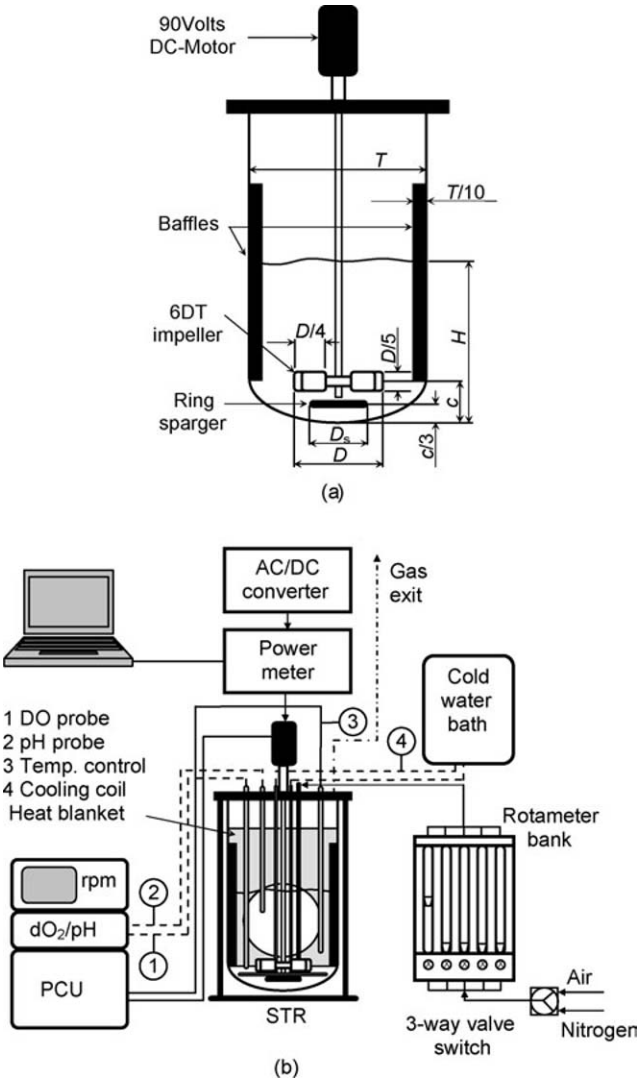

Figure 1. Experimental (a) stirred-tank reactor geometry and (b) facility setup.

Assuming the liquid phase is well mixed, gas absorption is liquid phase controlled, and oxygen concentration in the liquid at the gas–liquid interface is in equilibrium with the oxygen concentration in the gas, the volumetric mass transfer coefficient (k_La) can be determined from

$$\frac{dC}{dt} = k_La(C_i - C) \quad (6)$$

where C is the dissolved oxygen concentration in the liquid at time t, and C_i is the gas concentration at the gas liquid interface assumed to be in equilibrium with the bubble.