Mass transfer and shear rate in baffled surface aerator

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Abstract-The scale up or scale down of the process variables in a surface aerator requires information about the shear rate prevailing in the system. In fact, the performance of surface aerator depends upon the shear rate. Shear rate affects the mass transfer operation needed by the surface aerator. Theoretical analysis of shear rate suggests a nonlinear behavior with rotational speed of the impeller, which has been shown in the present work. Present work also shows that in a geometrically similar system of baffled surface aerator, shear rate can be used as a governing parameter for scaling up or down the mass transfer phenomena.

Key words: Mass Transfer Rate, Mixing, Power Number, Shear Rate, Surface Aeration

INTRODUCTION

Entrainment of gas from a gas-liquid surface is known as surface aeration. Stirred reactors designed for this type of gas-liquid contact, called surface aerators, are widely used in chemical, pharmaceutical, biochemical and wastewater industries. Their main purposes are to provide mixing for homogeneity with respect to biomass, nutrients and effective gas dispersion and aeration in order to meet the demands of respiring biomass. They are favorable mass transfer devices, since they provide a large gas-liquid interfacial area and high shear stress to enhance the mass transfer. In the case of surface aeration, the gas above the liquid surface can be entrained directly into the liquid by the surface aerating impeller, which eliminates the need for a recycle gas compressor [1]. The problem of shear in stirred tanks arises from the need to enhance the oxygen transfer rates. Stirred tanks have been the most versatile bioreactor system for large-scale cultivation of plant cells. These are highly effective for proper mixing of cell suspensions, the break-up of air bubbles for enhanced oxygenation and the prevention of large cell aggregates formation. The other advantages include adaptability of the existing industrial technology and ease of scale up. However, the high shear generated in these tanks due to rotation of impeller has been the major limitation for cultivation of plant cells [2]. For the cultivation of mammalian cells in stirred vessels, oxygen is often transferred by surface aeration [3]. Direct sparging with air sometimes causes foaming and other undesirable effects [4]. This is especially true for microcarrier culture and for relatively small scale suspension culture. To facilitate oxygen transfer through the liquid surface, a surface aerator can be used [5,6]. However, the processes involving shear-sensitive cells (mammalian, insect, and plant cell cultures) have created the need for considering shear stress as one of the parameters relevant in the design of such reactors [7,9].

For optimal design and operation of a surface aerator in terms of minimizing shear-related cell death, one would like to be able to predict cell damage directly from design parameters using a mechanistic model. This concerns knowledge about (i) the hydrodynamics in the reactor, (ii) the response of the individual cells in a cell population to hydrodynamic forces, and (iii) the mechanism by which the hydrodynamic forces interact with the cells. Because information on all three aspects mentioned above is not available, empirical models have been constructed just relating design parameters to cell death. The parameters of these models are determined from experiments. The main disadvantage of this approach is that scale up or scale down of the results to, for instance, different cell lines, medium formulations, and reactor scales is not allowed.

The determination of shear rate in a surface aerator is an important step in deciding their suitability to handle shear sensitive biosystems. At the same time, the objective of doing studies on a surface aerator is to interpret the laboratory result into the field installation. This requires a scaling up or down of geometric and dynamic properties of laboratory demonstration into a field installation. The issue of determining or quantifying the shear rate has been tried in the present work. The present work also aims to develop general scale up or scale down criteria for mass transfer rate based on the shear rate in the surface aerator.

SHEAR RATE

Shear rate is an important parameter in a surface aerator, but it is not easy to characterize. Knowledge of the shear rate is essential for the design and operation of surface aerators. The specific energy dissipation rate in a stirred tank is well known to depend on the shear rate γ and the shear stress τ [10,11], as follows [12]:

$$\frac{P}{V} = \tau \gamma \tag{1}$$

where P is the power input and V is the volume of the fluid in the tank. Furthermore, for Newtonian fluids, the viscosity μ is the ratio of shear stress and shear rate, i.e.,

$$\mu = \frac{\tau}{\gamma} \tag{2}$$

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Therefore, Eq. (1) can be written as follows:

$$\frac{P}{V} = \mu \gamma^2 \tag{3}$$

$$\gamma = \sqrt{\frac{1}{\mu V}}$$
(4)

Eq. (4) applies to laminar, turbulent and transitional flows. For agitation under laminar flow, the power number (N_p) and the agitator Reynolds number (R_p) are related [13,14] as follows:

$$N_p = \frac{C}{R_e}$$
(5)

where the constant C depends on the geometry of the tank and the impeller [13,14]. Power number and Reynolds number are defined as:

$$N_p = \frac{P}{\rho N^3 d^5}$$
(6)

$$R_e = \frac{\rho N d^2}{\mu}$$
(7)

where N is the rotational speed, ρ is density of the fluid and d is the impeller diameter. Substituting the definitions of the power number and Reynolds number in Eq. (5), the following equation can be obtained:

$$\frac{P}{\rho N^3 d^5} = C\left(\frac{\mu}{\rho N d^2}\right) \tag{8}$$

Volume of the fluid (V) can be assumed as proportional of d^3 . Thus Eq. (8) can be further written as:

$$\frac{P}{\mu V} = CN^2$$
(9)

Substituting Eq. (9) into Eq. (4), we get:

$$\gamma = \alpha N$$
 (10)

where α is a constant that depends only on the impeller geometry. Metzner and Otto [15] also defined the average shear rate (γ) in a stirred tank as a function solely of the rotational impeller speed (N), which is valid for laminar regime [16]. In turbulent flow, the power number is constant [13,14]. Therefore, by substituting the value of P/V (which is proportional to N³) in the Eq. (4), we get:

$$\gamma = \beta N^{1.5} \tag{11}$$

where β is a constant for a Newtonian fluid because the power number and viscosity are constants. In the present study, flow is in fully turbulent condition.

MEASUREMENTS

An experimental and numerical scheme has been adopted to calculate mass transfer rate and shear rate, respectively, in a baffled circular surface aerator. The cross-sectional areas of the circular tanks tested are $A=1 \text{ m}^2$ and 0.5184 m^2 . A schematic diagram of the baffled aerator is shown in the Fig. 1.



Fig. 1. Schematic diagram of a baffled bioreactor.

Where, A is the cross-sectional area of the tank, H is the depth of water in the tank, D is tank diameter, B is the width of baffle, N_b is the number of baffles, d is the diameter of the rotor and the distance between the top of the blades and the horizontal floor of the tank is h and b, *l* are the linear dimensions of the blade. A six-blade Rushton rotor has been used in the experiments [17]. The Rushton disk turbine, due to its high local shear, suitable for dispersion processes, is one of the most commonly used mixers for gas-liquid mass transfer in the processes of chemical industries [18,19]. The Rushton turbine produces radial flow and high shear rates near the impeller, which is important for air dispersion. Conditions of geometric similarity, i.e., $\sqrt{A/d=2.88}$, H/d=1.0, *l*/d=0.3, B/D=0.5, N_b=4, b/d=0.24 and h/d=0.94, as suggested by Rao and Jyothish [20] were maintained in all the surface aerators.

According to two-film theory [21], the mass transfer coefficient at T^oC, $K_L a_T$ may be expressed as follows:

$$K_{L}a_{T} = [\ln(C_{s} - C_{0}) - \ln(C_{s} - C_{t})]/t$$
(12)

where, In represents natural logarithm and C_s , C_0 and C_t are dissolved concentrations in parts per million (ppm), C_s =the saturation concentrations at time tending to very large values, C_0 is at the beginning of time t=0 and C_t is at time t=t. The value of K_ta_T can be obtained as the slope of the linear plot between $\ln(C_s-C_t)$ and time t. The value of K_ta_T can be corrected for a temperature other than the standard temperature of 20 °C as K_ta_{20} , using the Van't-Hoff Arrhenius equation:

$$K_{L}a_{T} = K_{L}a_{20} \ \theta^{(T-20)}$$
(13)

Where θ is the temperature coefficient equal to 1.024 for pure water [22]. Once the rotor starts rotating, the DO meter reading is noted at regular intervals up to the point when the DO values reaches 80% of the saturation value or above. Thus with the known values of DO measurements in terms of C_t at regular intervals of time t (including the known value of C₀ at t=0) a line is fitted, by linear regression analysis of Eq. (12), between the logarithm of (C_s-C_t) and t, by assuming different but appropriate values of C_s such that the regression that gives the minimum "standard error of estimate" is taken and thus the values of K_t ar and C_s are obtained simultaneously. Oxygen transfer modeling by two-film theory assumes that a single and constant value of C_s is adequately representative of the equilibrium



Fig. 2. Determination of $K_L a_T$

DO for the liquid phase oxygen mass transfer for the entire aeration systems and the transfer process is predominately liquid phase mass transfer controlled, and the gas phase resistance to transfer can be ignored. Now by fixing the value of C_s , the value of $K_I a_T$ has been determined by the best fit straight line, semi-logarithmic plot of $(C_s - C_t)$ and t. The value of C_s used in the log-deficit approach can be based on field measurement, published value, or simple assumption. It is a common practice to fix the value of C_s around the maximum DO value with some increment in it, as long as it gives the best fit. The slope of such a straight line is equal to - $K_{I}a_{T}$. It is worth noting that selection of a particular value for C_s will influence the resultant value for $K_{I}a_{T}$ determined by this approach. This is illustrated in Fig. 2. The mass transfer coefficient calculated using this method may have errors, because the method used requires a straight line to fit the data; the error could be reduced if the linear regression coefficient of the chosen line is high. In that case the slope of the line would accurately represent the oxygen transferred to the water. The values $K_{L}a_{20}$ are computed using Eq. (13) with θ =1.024 as per the standards for pure water [22]. Thus, the values of $K_L a_{20}$ were determined for different rotor speeds N of the rotor in all of the geometrically similar tanks.

Liquid mixing involves three interdependent processes: bulk flow, turbulence and molecular diffusion. Turbulence plays a key role in many mixing applications, but the measurement of turbulence is difficult and requires specialized equipment not typically available to industrial labs and pilot plants. In the present work, shear rate of surface aeration systems has been calculated by using commercial software Visimix®. The Visimix® program can be helpful in analyzing the mixing parameters in a stirred tank [23,24]. It can be useful in investigating different scenarios for scaleup and changes in agitator and vessel configuration. One of the standard parameters for scale up is shear, rate and one of the simpler ways to calculate shear rate is agitator tip speed over the distance between the tip and the vessel wall:

$$\gamma = N d/(D-d) \tag{14}$$

where, D is the tank diameter. Turbulence consists of eddies which vary in size from a maximum, L_{max} , depending on the scale of the equipment down to a minimum, L_0 , which depends primarily upon

the power input per unit mass and the kinematic viscosity as:

$$L_0 = [(\mu^3 V)/(P \rho^2)]^{0.25}$$
(15)

This is called the Kolmogorov length. L_0 can be also related to shear rate as:

$$L_0 = (\nu)^{0.5} / \gamma$$
 (16)

Visimix®, however, defines shear rate as the ratio of turbulent fluctuation velocity, v_0 , to the Kolmogorov turbulence scale, L_0 as follows:

$$\gamma = v_0 / L_0 \tag{17}$$

 v_0 is defined as = $[\nu e]^{0.25}$.

where ν is kinematic viscosity and e is the turbulent energy dissipation rate, or power per unit mass. L₀ is called the Kolmogorov length and depends primarily upon the power input per unit mass and the kinematic viscosity.

RESULTS AND DISCUSSION

As discussed, understanding the magnitude of shear in a surface aerator has significant implications for design. Values of shear rate calculated at different rotational speeds in both the surface have been plotted with N in the Fig. 3.

In the present case, as said flow is fully turbulent, thus theoretically the shear rate should depend on $N^{1.5}$ as derived in the Eq. (11). As shown in Fig. 3, regression lines have been drawn between shear rate and rotational speed for different-sized surface aerators and regression equations are:

$$\gamma = 1949 N^{1.497}$$
 for A=1 m²
 $\gamma = 1407.2 N^{1.496}$ for A=0.5184 m² (18)

Eq. (18) correlates the data with a regression coefficient of 0.99. The exponent on N-term in Eq. (11) is quite close to the theoretically derived value of 1.5.

The volumetric oxygen mass transfer coefficient is one of the most important parameters in scaling-up surface aeration systems.



Fig. 3. Shear rate with rotational speed.



Fig. 4. Mass transfer rate as a function of function of shear rate.

It is a measure of the gas-liquid mass transfer performance of a given surface aerator. Various correlations [24,26] have been utilized to correlate the mass transfer coefficient ($K_t a_{20}$) with the operation variables (N and P), the geometric parameters of the systems (V and d), and the physical properties of the fluids. Correlations of mass transfer rate with shear rate have been discussed and available in the literature, for example; Deckwer et al. [27], Godbole et al. [28], Merchuk and Ben-Zvi [29] and Nakanoh and Yoshida [30] for bubble column; Pérez et al. [12] for stirred tank bioreactor and bubble column reactors, Campesi et al. [16] for a stirred tank bioreactor. The present work develops the correlation for geometrically similar baffled surface aeration systems. Fig. 4 shows the correlation of mass transfer rate with shear rate. As can be seen, observations corresponding to different sized surface aerators fall on a single curve. The equation representing the curve is:

$$\frac{K_L a_{20}}{\sqrt{\gamma}} = -198.43 e^{\gamma \frac{00007}{0007}} + 198.51 - \frac{61.6}{10^8} e^{0.395 \left(\frac{\gamma - 5480}{1000}\right)^2}$$
(19)

The correlations proposed (Eqs. (18) and (19)) in the present work can be useful in scaling up the surface aeration systems. Now by maintaining the present optimal geometrical similarity condition, one can predict mass transfer rate by knowing the shear rate through the Eq. (19).

CONCLUSIONS

By experimental and numerical approach we have developed scale up and scale down criteria for mass transfer rate of geometrically similar surface aerators. It is found that shear rate in the vicinity of impeller can be used as a scale up or scale down criteria for the process phenomena (mass transfer) in surface aerators. The nonlinearlity of shear rate with rotational speed has been also studied in the present work. Here, it can said that the developed simulation equation for mass transfer rate will be very useful in the field installation.

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NOMENCLATURE

- A : cross-sectional area of an aeration tank
- B : width of the baffle
- b : width of the blade
- C_0 : initial concentration of dissolved oxygen at time t=0
- C_s : saturation value of dissolved oxygen at test conditions
- C_t : concentration of dissolved oxygen at any time t
- d : diameter of the rotor
- e : the turbulent energy dissipation rate
- H : depth of water in an aeration tank
- h : distance between the top of the blades and the horizontal floor of the tank
- $K_L a_T$: overall oxygen transfer coefficient at room temperature T°C of water
- K_La₂₀ : overall oxygen transfer coefficient at 20 °C
- *l* : length of the blade
- N : rotational speed
- N_b : number of baffles
- P : power available to the rotor shaft
- N_P : Power number
- R_e : ND²/n, Reynolds number
- V : volume of water in an aeration tank
- θ : 1.024, constant for pure water
- γ : shear rate
- au : the shear stress
- μ : viscosity
- v₀ : turbulent fluctuation velocity
- L₀ : Kolmogorov turbulence scale

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