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An adaptive model for gas–liquid mass transfer in a Taylor vortex reactor

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ABSTRACT

Gas–liquid Taylor–Couette flow devices have attracted interest for use as chemical and biological reactors, and consequently the accurate prediction of interphase mass transfer coefficients is crucial for their design and optimization. However, gas–liquid mass transport in these systems depends on many factors such as the local velocity field, turbulent energy dissipation rate, and the spatial distribution and size of bubbles, which in turn have complicated dependencies on process, geometric, and hydrodynamic parameters. Here we overcome these problems by employing a recently developed and validated Eulerian two-phase CFD model to compute local values of the mass transfer coefficient based upon the Higbie theory. This approach requires good estimates for mass transfer exposure times, and these are obtained by using a novel approach that automatically selects the appropriate expression (either the penetration model or eddy cell model) based upon local flow conditions. By comparing the simulation predictions with data from corresponding oxygen mass transfer experiments, it is demonstrated that this adaptive mass transfer model provides an excellent description for both the local and global mass transfer of oxygen in a semibatch gas–liquid Taylor–Couette reactor for a wide range of azimuthal Reynolds numbers and axial gas flow rates.

1. Introduction

Interphase mass transfer plays a crucial role in the design, scale-up and optimization of multiphase chemical and biological reactors. As a result, considerable effort has been expended to develop reliable correlations for estimating interphase mass transfer coefficients. For gas–liquid systems, it is usually assumed that the liquid side mass transfer resistance at gas–liquid interfaces limits interphase mass transport, and therefore gas side mass transfer resistance is neglected [1]. Hence, the liquid side volumetric mass transfer coefficient (k_La) is used to compute the overall mass transfer rate across a gas–liquid interface. However, it can be difficult to estimate k_La because of the many factors affecting this quantity, such as gas holdup and bubble size, slip velocity, and turbulent energy dissipation rate. These factors in turn depend non-trivially on reactor operating conditions, geometry, and physical properties of the gas and liquid phases. Some dependencies of the volumetric mass transfer coefficient on hydrodynamic, operating, and geometric parameters are illustrated in Fig. 1.

Although numerous empirical correlations have been developed for gas–liquid mass transfer in bubble columns [2–5], airlift reactors [6–8], and stirred tanks [9–12], comparatively little is known concerning interphase mass transfer in Taylor–Couette flow cells [13–16], which have recently gained interest for use as bioreactors [17–24]. These devices, which consist of fluids confined in the annular space between two coaxial cylinders (see Fig. 2) with the inner cylinder undergoing rotation, can be used to generate pairs of toroidal vortices with mixing characteristics advantageous for culturing a variety of microorganisms [17–19,21,22]. Specifically, as the inner cylinder rotation speed increases above a critical value that depends upon the reactor geometry and fluid properties, the fluid undergoes transition from laminar Couette flow (circular flow with only an azimuthal component) to laminar Taylor vortex flow. Subsequent increases in cylinder rotation speed lead to higher order instabilities such as wavy vortex flow, modulated wavy vortex flow, and turbulent Taylor vortex flow [25–28].

Although a large literature concerning single phase Taylor vortex flow has been built over many years, far less is understood concerning multiphase Taylor vortex flow, particularly with respect to mass transport in such systems. The addition of a second fluid phase leads to instabilities and flow patterns not observed in single-phase flow (e.g. phase inversions and nonhomogeneous distribution of fluid phases) [29–33]. The available information for interphase mass transport in two-phase Taylor–Couette flow is even more limited, and until now, no computational or theoretical models for interphase mass transfer have been developed for this

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Nomenclature

Notation

a	specific gas–liquid interfacial surface area, m^{-1}
c_l	liquid molar concentration, kmol m^{-3}
c_{l^*}	liquid saturation molar concentration, kmol m^{-3}
C_D	drag coefficient, dimensionless
d_b	sauter mean diameter of bubble, m
D_L	diffusion coefficient gas in liquid, $m^2\ s^{-1}$
Eo	Eötvös number, dimensionless
H	Henry's law constant, Pa m^3 $kmol^{-1}$
F	interphase force, kg $m^{-2}\ s^{-2}$
g	gravitational acceleration, m s^{-2}
G_k	generation of turbulent kinetic energy, kg $m^{-1}\ s^{-3}$
G_ω	generation of specific dissipation rate, kg $m^{-3}\ s^{-2}$
k_l	turbulent kinetic energy of liquid, $m^2\ s^{-2}$
k_L	liquid side mass transfer coefficient, m s^{-1}
L	cylinder height, m
M_w^i	molecular mass, kg $kmol^{-1}$
p	pressure, Pa
r	cylinder radius, m
R_{gl}^i	rate of gas–liquid mass transfer of species *i*, kmol $m^{-3}\ s^{-1}$
Re_b	bubble Reynolds number, dimensionless
Re_a	axial Reynolds number, dimensionless
Re_θ	azimuthal Reynolds number, dimensionless
S	net rate of production/destruction, kg $m^{-3}\ s^{-1}$
Sh	Sherwood number, dimensionless
t_e	exposure time, s
u	velocity, m s^{-1}
Y^i	mass fraction of specie of species *i*, dimensionless
Y_k	dissipation of turbulent kinetic energy, kg $m^{-1}\ s^{-3}$
Y_ω	dissipation of specific dissipation rate, kg $m^{-3}\ s^{-2}$

Greek letters

α	volume fraction, dimensionless
ε	turbulence dissipation rate, $m^2\ s^{-3}$
ω	specific dissipation rate, s^{-1}
ν	kinematic viscosity, Pa s
μ_t	turbulent viscosity, Pa s
ρ	density, kg m^{-3}
$\bar{\bar{\tau}}$	phase stress tensor, N m^{-2}
$\bar{\bar{\tau}}^{Re}$	phase stress tensor, N m^{-2}
Γ	aspect ratio, dimensionless
η	radius ratio, dimensionless

Subscripts and Superscripts

b	bubble phase
l	liquid phase
g	gas or global
i	species index

system. Most of what has previously been reported concerning interphase mass transfer in Taylor–Couette flow is attributable to work performed by Wroński et al. [14] and Dluska et al. [15,16], who carried out experiments in a continuously-fed horizontally-oriented gas–liquid Taylor–Couette reactor and observed volumetric mass transfer coefficients with values on the order of 0.1 s^{-1}. However, the flow patterns generated in a horizontal gas–liquid reactor are significantly different from those that are produced in a vertically oriented reactor, because axial symmetry is destroyed in a horizontal reactor by the vertical gravity field that gives rise to a nonaxisymmetric bouyant force.

In contrast to horizontally oriented gas–liquid Taylor–Couette reactors, the buoyant force acting on gas bubbles is parallel to the cylinder axis in vertically oriented reactors. As a result, effluent gas can easily be separated from the liquid phase by feeding gas through the bottom of the reactor and by providing sufficient head space for bubbles to rupture as they emerge from the liquid free surface at the top of the reactor. Such a configuration is particularly useful for delivery of carbon dioxide and removal of oxygen during the culture of phototrophic microorganisms. Interest in vertically oriented gas–liquid Taylor vortex reactors has also been driven by the discovery of the existence of nontrivial bubble distributions and dramatic drag reduction on the rotating inner cylinder [34–37].

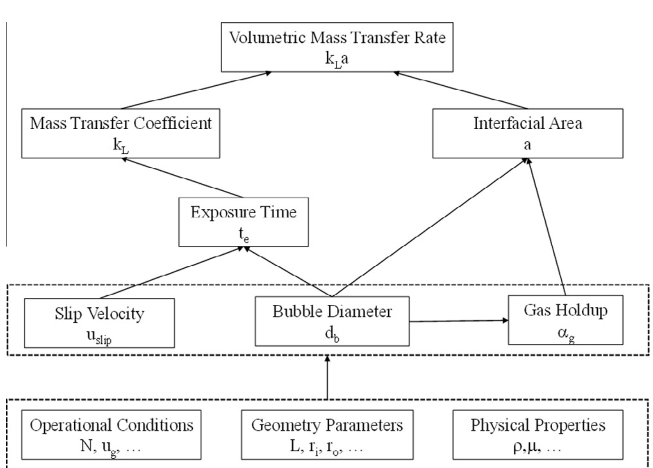

Fig. 1. Illustration of the relationships between volumetric mass transfer coefficient and various geometric, operational, and hydrodynamic parameters.

Recently the authors carried out oxygen transport experiments in a vertical gas–liquid Taylor–Couette reactor [38]. They found that gas–liquid mass transfer coefficients in the vertical reactor were significantly smaller than those reported for horizontal reactors. In addition, the authors developed empirical correlations for the mass transfer coefficient and the mean bubble diameter as functions of the liquid azimuthal Reynolds number and the gas axial Reynolds number. While these correlations are useful for understanding the relative contributions of the azimuthal and axial flows in determining the magnitude of mass transfer coefficients, they cannot easily be generalized because (a) Taylor vortex flow patterns cannot be predicted based solely upon axial and azimuthal Reynolds numbers (they also depend upon reactor geometry) and (b) Taylor vortex flow is known to exhibit flow pattern multiplicity, depending upon flow history [25].

In view of the above discussion, it is evident that the prediction of interphase mass transport coefficients for arbitrary Taylor–Couette reactor geometries and operating conditions requires an approach that incorporates details of the fluid flow. To that end, and by making use of our recently-developed computational fluid dynamics simulations for two-phase Taylor vortex flow [39,40], in this work we compute interphase mass transfer coefficients by integrating local fluid velocity and phase distribution information into well-known theoretical models for interfacial mass transport. This method for computing mass transfer coefficients is then validated by comparing model predictions against our existing experimental data for interphase mass transport in a vertical Taylor–Couette gas–liquid reactor [38]. Indeed, by properly