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Numerical and experimental modelization of the two-phase mixing in a small scale stirred vessel

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ABSTRACT

The numerical prediction of mass transfer rates of gas components within the liquid phase in a stirred two-phase flow reactor is presented. Experiments have been conducted to determine the flow regime and the number and sizes of the bubbles formed under different conditions. The dynamic field of the two-phase flow was obtained through numerical simulations. Bubbles with the experimentally measured diameter were released from the free surface and tracked numerically to compute the particle Reynolds number, which is used to determine the mass transfer rates. The unbaffled reactor provides mass transfer rates 30% larger than the baffled reactor for the bubbly flow. Mass transfer rates drop about 65% when the emulsion is formed. Therefore, above the critical rotation rate at which the emulsion forms for the unbaffled reactor, the baffled configuration provides larger mass transfer rates. The results indicate that even for the most unfavorable case mass transfer is not the limiting step, as 90% of the equilibrium concentration is reached in 10 s.

Introduction

Stirred tanks are widely used in the chemical and petrochemical industries for different types of processes. Frequently these stirred tanks include one or more baffles in order to avoid the formation of a vortex in the free surface. The turbulent flow generated by the interaction of the impeller blades and the other elements present in the tank (like the baffles) is certainly complex, and its topology depends on the shape and size of the different components in the tank.

Different experimental studies have been performed for this type of systems. The influence of the gas flow rate on the structure of the trailing vortices formed behind the blades of a Rushton turbine was studied with Particle Image Velocimetry (PIV) measurements in a baffled stirred vessel with a flat bottom [1]. Gas accumulation behind the impeller blades was shown in the PIV results. The locations of those gas cavities were coinciding with the location of trailing vortices in one-phase liquid flows. A two-camera PIV technique was used on a laboratory scale stirred tank equipped with a Rushton turbine to obtain turbulence data of the flow and angle resolved velocity [2]. Both single phase and two-phase flows were studied. In the two-phase flow, it was observed that the radial velocity of the liquid jet and its trailing vortices were diminished by the presence of the gas. Gas cavities surrounding the back of the impeller blades were also observed in the visualizations. Digital image analysis was coupled with a shadowgraphy-based technique to investigate, for unbaffled tanks, the shape of the free surface vortex [3]. Tank filling level and impeller clearance from the vessel bottom were varied to determine how they influenced the shape of the vortex. A correlation was proposed describing the vortex shape. The oxygen transfer in an unbaffled vessel used as a biochemical reactor for animal cell growth was studied in [4]. The experimental results showed that this kind of bioreactors could provide enough mass transfer for animal cell growth, being that way a valid alternative to sparged reactors.

Several researchers have carried out numerical simulations of gas–liquid stirred vessels over the years using different numerical techniques. Some authors have performed Large Eddy Simulations (LES) [5]. In that computational approach, the large scales of the

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Nomenclature

A	surface where mass transfer takes place, m^2
C	concentration, kg/m^3
$C_{1\varepsilon}$	model constant
$C_{2\varepsilon}$	model constant
$C_{3\varepsilon}$	model constant
D	molecular diffusivity, m^2/s
d_b	bubble diameter, m
g	gravitational acceleration, m/s^2
G_b	turbulent kinetic energy generation due to buoyancy, kg/ms^3
G_k	turbulent kinetic energy generation due to mean velocity gradients, kg/ms^3
k	turbulent kinetic energy, m^2/s^2
k_b	mass transfer coefficient on the surface of the bubbles, m/s
k_e	mass transfer coefficient within the emulsion, m/s
k_T	overall mass transfer coefficient, m/s
p	pressure, Pa
Pe	Peclet number
Re_p	particle Reynolds number
Sc	Schmidt number
Sh	Sherwood number
u	velocity, m/s
V_s	gas slip velocity, m/s
x	spatial coordinate, m
α_k	inverse effective Prandtl number for k
α_ε	inverse effective Prandtl number for ε
δ_{ij}	Kronecker delta
ε	turbulent dissipation rate, m^2/s^3
θ	volume fraction
μ	dynamic viscosity, Pa·s
ν	kinematic viscosity, m^2/s
ρ	density, kg/m^3

flow are solved, while the smaller scales are modeled. Although not as computationally expensive as performing Direct Numerical Simulations (DNS), where all the flow scales are solved, it is still an expensive method. A key feature in LES is the choice of the SubGrid Scale model (SGS), since the accuracy of the results on the smaller scales will depend on it. LES with an implicit SGS model was performed to study a gas–liquid Rushton stirred reactor [6]. To solve the multiphase flow, a combination of Volume of Solid (VOS) and Lagrangian Particle Tracking (LPT) was used [7]. Air was entered at the bottom of the reactor and, under the assumption of bubbly flow the bubbles were tracked in the three-dimensional time-dependent flow field generated by LES. Another study using LES can be found at [8], although in that work there was a single-phase flow. The Smagorinsky SGS model [9] was used in the simulations, performed with the commercial software CFX. As an example of the computational cost of LES, the authors needed 33 days to solve the flow field for the time corresponding to 22 impeller revolutions at 200 rpm, using a 3 GHz processor.

Given the high computational cost of LES, the Reynolds Averaged Navier-Stokes (RANS) approach [5] has become more popular. In this approach, only the average field is solved and turbulence is modeled. A widely used turbulence model is the two-equation $k-\varepsilon$ model [10], which uses the kinetic turbulent energy (k) and its dissipation rate (ε) to compute the turbulent viscosity. The works from other authors using RANS reported here all except one use the $k-\varepsilon$ model. A gas–liquid stirred tank using CFX and the Sliding Grid (SG) technique [11] was simulated [12]. In the Eulerian–Eulerian multiphase model [13], both phases shared the same values of k and ε. The authors found that including lift and virtual mass forces does not change the results. The SG technique was also used in the study of an aerated Rushton impeller [2]. The authors report that the drag force is the most important one in these systems, and that the bubble induced turbulence should be taken into account, thus making the effective viscosity the sum of the molecular, turbulent and bubble induced turbulent viscosities. The free surface of a Continuous Stirred Tank Reactor (CSTR) was studied at [14]. The authors also employed the SG technique, but this time using the Star CD software and the VOF model [15], instead of the Eulerian–Eulerian multiphase model. The range of rotation rates was between 70 and 280 rpm. The authors reported that macromixing is bad in low velocity regions found at the curved bottom, slightly downstream the baffles and near the free surface, although the one at the curved bottom may be destroyed by gas bubbles. The vortex shape in a partially baffled agitated vessel, with a Eulerian–Eulerian multiphase model and using the Multiple Reference Frame (MRF) technique [16], where a region of the computational domain, placed around the impeller, rotates with the same velocity that the impeller and the rest of the domain is static was studied in [17]. The authors found that extracting an isosurface of liquid volume fraction of 0.9 from the numerical simulations matched experimental data better than the classical value of 0.5. The MRF technique was also used to study the two-phase flow mass transfer in a stirred reactor [18], where Computational Fluid Dynamics (CFD) was coupled with Population Balance Method (PBM). The mass transfer prediction was compared with experimental data, showing reasonable agreement. The MRF technique was also used to study the micromixing of viscous systems with competitive parallel reactions in a stirred-tank reactor [19], but the Reynolds Stress Model (RSM) was used to account for the effects of turbulence. They found that micromixing was improved when the agitation speed was high and the fluid viscosity low. A stirred vessel using a Rushton turbine was studied in [20]. The computational software FLUENT [21] was used with a Eulerian–Eulerian multiphase model, and the Snapshot method [22] was implemented through User Defined Functions (UDF). This method consists in adding a mass source term to the equations solved to model impeller motion. The author reports that there is an accumulation of gas behind the impeller blades, and that the hydrodynamics cannot be determined with a steady state approach.

The aim of the present work is to analyze the two-phase mixing processes that occur in a small-scale batch reactor. A sketch of the stirred tank reactor is shown in Fig. 1, corresponding to the unbaffled (Fig. 1a and c) and baffled (Fig. 1b and d) configurations. The liquid and gas phases are in contact and, due to rotation, the free surface of the liquid changes its shape and gas bubbles are formed around the axis and blades and move within the liquid. The main objective is to determine the mass transfer rates for the different gas components (hydrogen (H_2) and carbon monoxide (CO)) within the liquid phase and whether it is a limiting step in the process or not. A numerical simulation approach was used in this study. Previous to the simulations some flow information was needed. For this reason the work has an initial stage that implies an experimental part. All relevant information about how bubbles inside the liquid phase are formed, the amount and their sizes were extracted from these experiments and used in the numerical simulations, performed with the commercial CFD software FLUENT. However, the actual operating conditions of the reactor could not be reproduced in the laboratory, given that the experimental analysis of the flow requires a transparent vessel to allow the visualization of the fluid within the reactor. Therefore, a dimensional analysis was performed in order to be as close as possible to reality. Table 1 shows the comparison between the