Final Report

Bubble Motion, Deformation, and Breakup, 2000-2003, $199,899

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The P.I. was supported by DOE grant DE-FG02-88ER13919 during the period 7/1/88-7/31/03. He worked on five projects under the above grant:

- "Droplet Motion in Numerically Simulated Turbulence," 1988-1991, $183,000.
- "Lift and Drag Forces on Droplets and Particles in Wall-Bounded Shear Flows," 1991-1994, $186,000.
- "Gas and Solids Holdup in Three Phase Bioreactors," 1994-1997, $199,334.
- "Surfactant Effects on Mass Transfer for Bubbles at Large Reynolds Numbers (with Prof. R.J. Nunge), 1997-2000, $220,212.
- Bubble Motion, Deformation, and Breakup, 2000-2003, $199,899

The results of the research were published in 30 papers in archival journals and 3 papers that are currently under review. The journals include International Journal of Multiphase Flow (8), Physics of Fluids (4), Journal of Colloid and Interface Science (3 published, 1 under review), Journal of Fluid Mechanics (3), Chemical Engineering Science (3 published, 1 under review), International Journal of Heat and Mass Transfer (2), Journal of Computational Physics (2), AIChE Journal (1 published, 1 under review), ASME FED (1), Chemical Engineering Communications (1), International Journal for Numerical Methods in Fluids (1), and Theoretical and Computational Fluid Dynamics (1). In addition, 12 contributions to books or conference proceedings have resulted from the grant.

A total of 5 Ph.D. students and 8 M.S. students have been supported in whole or in part under the grant.

While working on the projects, the P.I. collaborated with a number of researchers at other institutions. These include: Dr. E. S. Asmolov, Zhukosky Central Aero-Hydrodynamics Institute, Russia; Prof. D. Dandy, Colorado State University; Prof. J. J. Derksen, Technical University of Delft, The Netherlands; Dr. Alan Graham, Los Alamos National Laboratory (now at Texas A&M); Prof. T. J. Hanratty, University of Illinois at Urbana-Champaign; Dr. K. Kontomaris, DuPont Central Research & Development; Prof. S. Sundaresan, Princeton University; and Prof. H. E. A. van den Akker, Technical University of Delft, The Netherlands.

Although all of the projects involve aspects of fluid mechanics, they cover a large scope. The first two projects dealt with the behavior of fluid or solid particles in high Reynolds number flows. The first of these projects dealt with the motion and deposition of aerosols in wall bounded turbulent shear flows. The results were obtained by tracking the aerosols through a numerically simulated turbulent channel flow. The project resulted in several findings that have had a significant impact on research on two phase flows. First, it was found that fluid or solid particles with finite inertia tend to accumulate near the walls of a vertical channel flow. This phenomenon is closely related to the notion of "turbophoresis" that was suggested independently by Reeks (1983) and Caporaloni, Tampieri, Trombetti, & Vittori (1975). The P.I.'s results were

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the first confirmation of the above ideas with a direct numerical simulation (DNS). The same DNS of turbulent channel flow provided insights into the roles of various forces in the deposition of aerosols on walls bounding a turbulent shear flow. In particular, it was found that a lift force suggested by Saffman could increase the rate of deposition from a vertical flow by an order magnitude for aerosols in a certain size range. However, it was also found that the assumptions on which Saffman's result for the lift force were based were seriously violated by many particles as they passed through the viscous sublayer on their way to the wall.

The above findings formed part of the motivation for the second project in which a number of new results were obtained for lift forces on small particles. In particular, Saffman's result for the lift on a small particle in an unbounded linear shear flow was generalized to include cases in which the shear rate is weak. In addition, the effects of a distant wall on the lift force were determined. These results bridged the gap between the results for unbounded flows and results obtained by Brenner & Cox for particles that are sufficiently close to a wall that the leading order results for the lift force could be obtained by regular perturbation methods. The latter results were based on the assumption that the distance from the wall was much larger than the particle radius. In modeling deposition or re-suspension of particles, one must deal with situations in which the distance from the wall is comparable to the particle radius. This motivated the P.I. and his Ph.D. student, P. Cherukat to develop asymptotic results that were valid for particle separations between near-touching and the regime where the Cox-Brenner analysis is valid. The above results for the lift force have been widely used by researchers in modeling dilute suspensions of fluid or solid particles.

The last three projects considered various aspects of the behavior of bubbles in high Reynolds number flows. One common theme of these studies has been on the effects of surfactants on bubble motion. The P.I. published the first DNS of bubble motion in water in which the effects of surfactants were included with a stagnant cap model. The results were in good agreement with published experimental results and demonstrated the ability of the stagnant cap model to quantitatively account for the reduction of bubble speed. In a subsequent publication, the P.I. and his M.S. student, S. Ponoth, determined the effect of a stagnant cap on the rate of dissolution of a bubble. The above studies ignored the effects of unsteadiness. The P.I. and his Ph.D. student, Y. Liao, developed DNS methods that enabled them to simulate unsteady motion of both insoluble and soluble bubbles. The simulations included computations of the surfactant concentration field and, in the case of dissolving bubbles, the concentration of the gas solute in the liquid phase, as well as the fluid velocity field, bubble acceleration and deformation. For very dilute surfactant concentrations, the adsorption of surfactant on the bubble is sufficiently slow that the bubble achieves a maximum velocity that may be close to the value for pure water before beginning to slow down. Recently, the P.I. and his former student, Y. Liao, have demonstrated that one can determine the sorption rate constants for surfactants by comparing DNS results with experimental measurements of bubble velocity versus time in the dilute regime. The results have been submitted for publication.

No unexpended funds remain in the grant.

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LETTER TO THE EDITOR

Comments on "Unsteady Bubble Motion and Surfactant Kinetics"

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The numerical simulations of bubble motion in dilute surfactant solutions reported previously by two of the authors contained a serious numerical inaccuracy. In agreement with experiments, single bubbles released from rest were predicted to reach a maximum speed before slowing to a terminal speed. However, subsequent experiments demonstrated that the simulations predicted that the bubbles should reach their terminal speed too quickly. The source of the discrepancy is an inaccuracy associated with the numerical algorithm used to solve the surfactant transport equation on the bubble surface. After correcting the problem, the simulations agree much better with the experiments.

Key Words: bubble; simulation; surfactant adsorption

Liao and McLaughlin (1) presented the results of numerical simulations of bubbles in dilute surfactant solutions. They considered the buoyancy-driven motion of a single bubble in an unbounded liquid that was at rest except for the disturbance created by the motion of the bubble. Simulations were performed for bubbles with equivalent spherical diameters between 0.72 and 1.5 mm since bubbles in this size range rise along rectilinear paths in dilute aqueous surfactant solutions.

Several experimental studies have shown that, in sufficiently dilute surfactant solutions, bubbles in the size range considered by Liao and McLaughlin reach a maximum speed before slowing to a terminal speed. References to these papers may be found in Zhang *et al.* (2). If the solution is sufficiently dilute, the maximum velocity is close to the steady-state velocity in pure water. Zhang et al. (2) measured the velocity of 0.8 mm bubbles in aqueous solutions of Triton X-100; the concentration ranged from $2.5\times10^{-5}\,\mathrm{mol/m^3}$ to $74.9\times10^{-5}\,\mathrm{mol/m^3}$. Liao (3) performed similar experiments over a range of concentrations that overlapped the range considered by Zhang et al., and found that the bubble rise velocity increased monotonically to its steady-state value in a solution containing $0.01\,\mathrm{mol/m^3}$ of Triton X-100. Liao used slightly smaller bubbles (0.69 mm) in her experiment, and her experiments were conducted in a shorter column (1.22 m instead of 3 m) than the one used by Zhang et al (1). The use of a shorter column was possible since, in the concentration range considered by Liao, the bubble reached its terminal velocity more quickly. Wang (4) used the same system to perform experiments for bubbles in dilute solutions of decanoic acid and sodium do-decylsulfate ("SDS"). The experiments showed that the bubbles reached a terminal velocity too quickly in the simulations.

The simulation program developed by Liao and McLaughlin used the streamfunction-vorticity formulation of the Navier-Stokes equation since, in the bubble size range that they considered, the motion of the liquid was axisymmetric. The bubble was treated as a void in the simulations. The governing equations were formulated in the frame of reference of the bubble. The governing equations were solved with a finite difference method using an adaptive boundary fitted

coordinate system that was an extension of a technique described by Ryskin and Leal (5-7) and Kang and Leal (8).

The Reynolds number, Re, was order (10^2) for the simulations discussed by Liao and McLaughlin, but the Weber number was much smaller than unity. Thus, the maximum deviation from a spherical shape was of order 1% of the equivalent spherical radius.

Liao and McLaughlin used the Langmuir model to describe the surfactant sorption kinetics:

$$j = \beta c_s(\Gamma_\infty - \Gamma) - \alpha\Gamma, \qquad [1]$$

where j is the net flux of surfactant to the interface from the liquid, c_s is the concentration of surfactant in the liquid adjacent to the interface, Γ is the surface concentration of surfactant, α is a desorption rate parameter, and β is an adsorption rate parameter. Chang and Franses (9) discussed techniques for determining the sorption rate parameters and tabulated their values for several surfactants.

Stone (10) showed that the transport equation for the surface concentration of surfactant may be written as follows:

$$\frac{\partial\Gamma}{\partial t} + \nabla_s\cdot(\mathbf{v}_s\Gamma) + (\nabla_s\cdot\mathbf{n})(\mathbf{v}\cdot\mathbf{n})\Gamma = D_s\nabla_s^2\Gamma + j. \qquad [2]$$

In Eq, [9], ∇_s is the surface gradient operator, $\mathbf{v}_s$ is the surface fluid velocity, $\mathbf{n}$ is the unit normal vector, $\mathbf{v}$ is the fluid velocity, and D_s is the surface diffusivity. Liao and McLaughlin took the surface diffusivity to be the bulk diffusivity.

Liao and McLaughlin used Newton's method to determine the bubble acceleration on each time step. On each Newton step, it was necessary to solve the streamfunction-vorticity equations, the transport equation for the surfactant concentration in the liquid, and the transport equation for the surface concentration of surfactant. Using Γ, the surface tension was obtained from the Frumkin equation. An upwind difference method was used to compute the convective terms in Eq. [2]. This method did not conserve the total number of moles of surfactant and, after many time steps, lead to a serious error in the bubble velocity. Specifically, the bubble reached a terminal velocity too quickly in the simulations. This was caused by a spurious accumulation of surfactant on the bubble surface. To fix this problem, on each time step, the correct increase in the moles of adsorbed surfactant was computed by integrating j over the bubble surface. Then, the values of Γ were normalized to obtain the correct number of adsorbed moles. Figure 1 compares the bubble velocity with and without the above correction for a 0.69 mm bubble in an aqueous solution containing $4.3\times10^{-4}\,\mathrm{mol/m^3}$ of Triton X-100. The same figure also shows the experimental results (see below) for the bubble velocity versus time obtained by Liao (3). The simulations were done for $\alpha = 0.033\mathrm{s}^{-1}$, $\beta = 50\,\mathrm{m^3/mole\cdot s}$, which are the lower bounds given by Lin et al. (11). It may be seen that the corrected simulation agrees better with the experiments although, for large times, the bubble velocity decreases more slowly in the simulation than in the experiments.

The experimental system was similar to that used by Sam et al. (12) and Zhang et al. (2). Therefore, the description of the system will be brief with emphasis on the differences between the system and that used by the above investigators. The column was a 1.3 m high glass cylinder with an inner diameter equal to 12.7 cm. The base of the column was made of stainless steel. A square Plexiglas view box enclosed the column except for the top and bottom. In all experiments, the view box was filled with water to reduce the optical distortion caused by the cylinder. A

transparent measuring scale was attached to one side of the view box to determine the position of the moving bubble.

Sam et al. (12) described the bubble generation system It consisted of a gas source, pressure gauge, stainless steel tubes, needle valve, flex connect tube, and a glass capillary tube. A glass capillary tube produced by Friedrich & Dimmoch Inc., with an outer diameter equal to 3 mm and a nominal inner diameter equal to 0.025 mm, was used to produce bubbles.

The camera system was designed to track the bubble along the column. Since one camera could not focus on both the bubble and the scale, two CCD cameras were used in the experiments. One camera was placed on top of the platform and focused on the bubble, and the other camera was underneath the platform and focused on the scale attached to the back of the view box. A variable speed motor driving a chain belt over a pulley with a counterweight was used to move the platform on which the two cameras were mounted. The signals from the video cameras were synchronized by a distributor. The shutter time of the cameras was set to 1 ms to avoid blurring of the bubble image; the camera speed was 30 frames per second. By introducing a splitter, pictures of the bubble and the scale could be simultaneously displayed on the monitor. A time code (frame number) was placed on the upper right corner of the screen. The bubble images were recorded by a VCR.

Electronics grade water was used to make solutions to minimize the effect of unknown surface-active impurities. All experiments were performed at $25 \pm 0.5^{\circ}C$. Helium bubbles were used in the experiments. The dissolution of the helium bubbles was negligible over the rise distances considered in the experiments.

The surfactants used in the experiments were Triton X-100, decanoic acid, and SDS. Some published results were available for the sorption rate constants of the surfactants (although not in the concentration range considered in the experiments.) The choice of Triton X-100 also made it possible to make comparisons with the experiments reported by Zhang et al. (2).

Figures 2 and 3 compare bubble rise velocities predicted by the simulations with the experimental results for Triton X-100 and decanoic acid. In each case, the results of two experiments are shown to provide some indication of the reproducibility of the results. For values of the sorption rate constants used in the simulations, reasonable agreement with the experimental results is obtained. The ratio α / β was fixed since it is known from equilibrium measurements of surface tension. If one uses a least squares fit to the experimental results for t>0.1s, one can identify the sorption parameters that produce the best agreement with the slope of the line through the experimental points. For Triton X-100, the results for $\alpha = 0.132\,\mathrm{s}^{-1}$, $\beta = 200\,\mathrm{m}^3/\mathrm{mole}\cdot\mathrm{s}$ provide the best agreement with the experiments; these values are four times larger than the lower bounds determined by Lin et al. (12). For decanoic acid, the best agreement is obtained for $\alpha = 3.57\,\mathrm{s}^{-1}$, $\beta = 40\,\mathrm{m}^3/\mathrm{mole}\cdot\mathrm{s}$, which are the values given by Borwankar and Wasan (13). The results obtained for SDS are not shown since, over the time period covered by the simulations, the bubble velocity changed very little after reaching its maximum value in both the simulations and the experiments.

The simulations predict a maximum velocity that is larger than the experimental maximum velocity. It is plausible that this is caused by initial contamination of the bubbles in the experiments since each bubble resided on the end of the capillary tube for approximately 0.8 s. However, it would be difficult to test this idea since it would be difficult to simulate a growing bubble on the end of the capillary in the surfactant solution.

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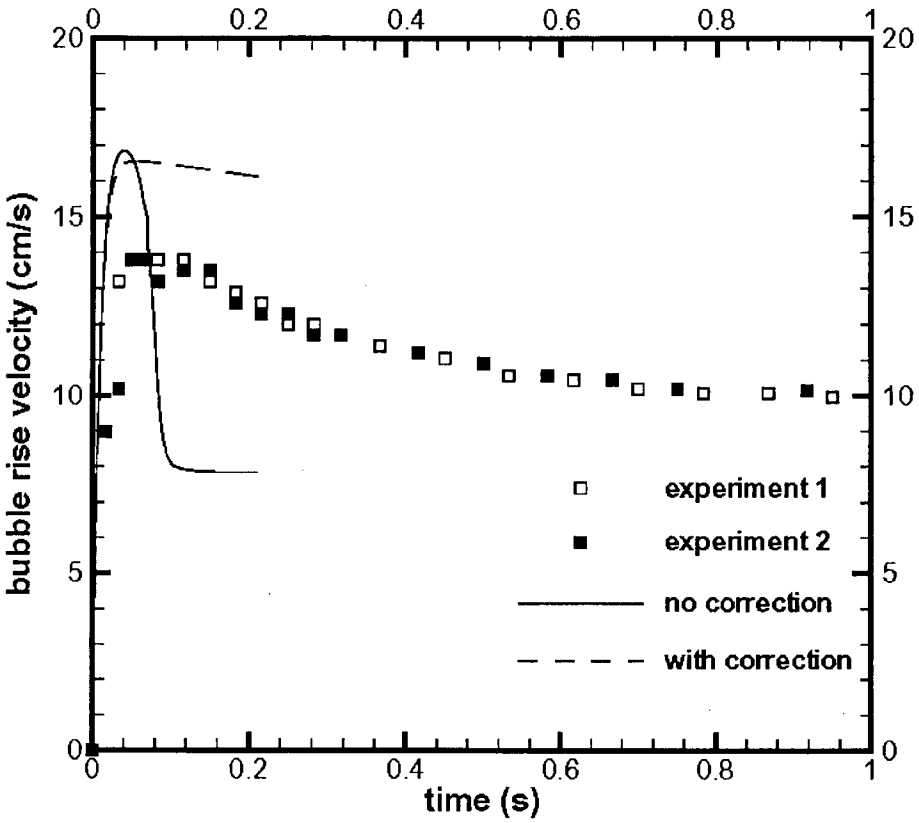

FIG. 1. Bubble rise velocity versus time for an aqueous solution containing $2.3\times10^{-4}\,mole/m^3$ of Triton X-100. Simulations with and without the correction to the algorithm for the surfactant transport equation are shown.

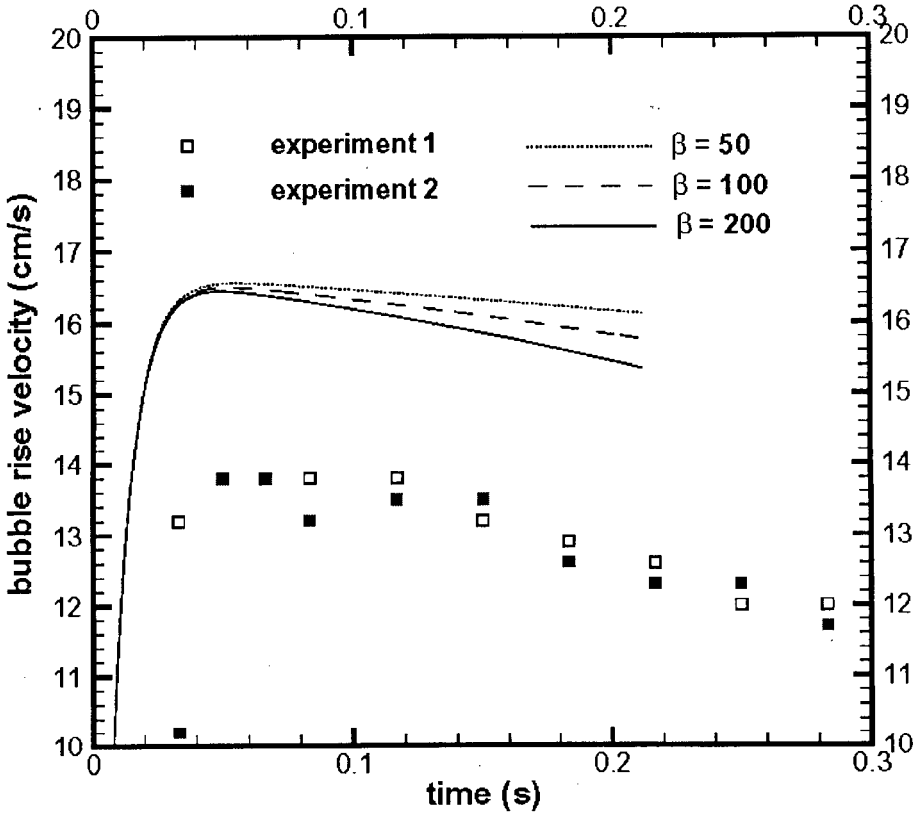

FIG. 2. Bubble rise velocity versus time for an aqueous solution containing $2.3\times10^{-4}\,mole/m^3$ of Triton X-100. The values of α and β in the simulations are: 0.033 s^{-1}, 50 m^3/mole-s; 0.066 s^{-1}, 100 m^3/mole-s; and 0.132 s^{-1}, 200 m^3/mole-s, respectively.

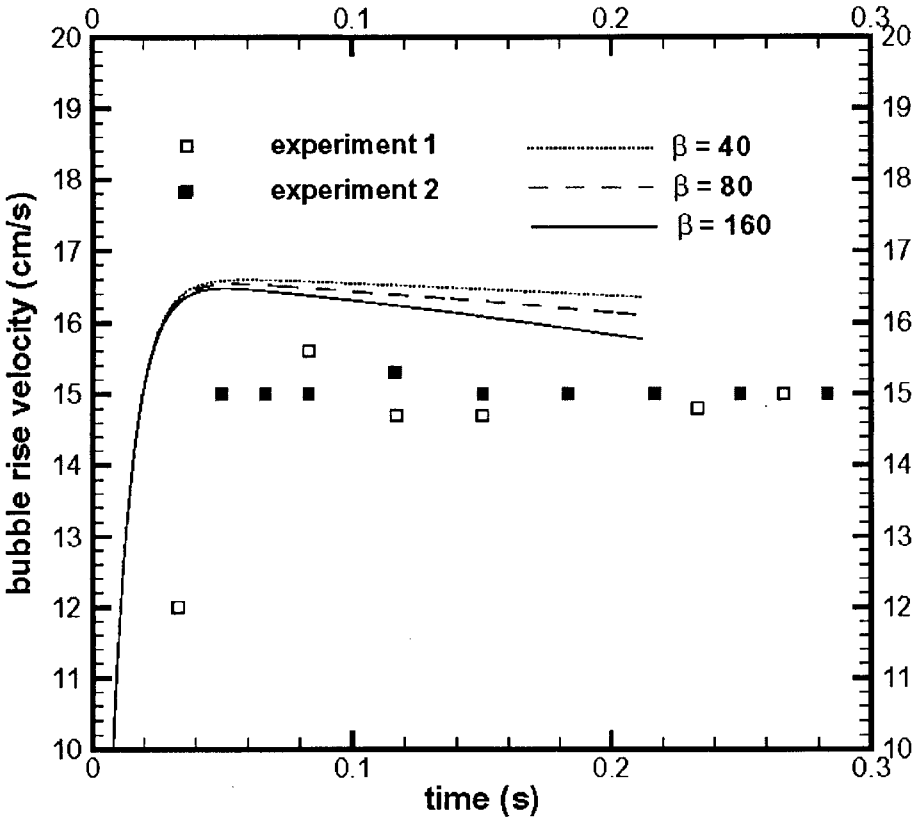

FIG. 3. Bubble rise velocity versus time for an aqueous solution containing $2.3\times10^{-4} mole/m^3$ of decanoic acid. The values of α and β in the simulations are: 3.57 s^{-1}, 40 m^3/mole-s; 7.14 s^{-1}, 80 m^3/mole-s; and 14.28 s^{-1}, 160 m^3/mole-s, respectively.

Simulation of bubble breakup dynamics in homogeneous turbulence

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This paper presents numerical simulation results for the deformation and breakup of bubbles in homogeneous turbulence under zero gravity conditions. The lattice Boltzmann method was used in the simulations. Homogeneous turbulence was generated by a random stirring force that acted on the fluid in a three-dimensional periodic box. The grid size was sufficiently small that the smallest scales of motion could be simulated for the underlying bubble-free flow. The minimum Weber number for bubble breakup was found to be about 3. Bubble breakup was stochastic and the average time needed for breakup was much larger for small Weber number numbers than for larger Weber numbers. For small Weber numbers, breakup was preceded by a long period of oscillatory behavior during which the largest linear dimension of the bubble gradually increased. For all Weber numbers, breakup was preceded by a sudden increase in the largest linear dimension of the bubble. When the Weber number exceeded the minimum value, the average surface area increased by as much as 80%.

Keywords: Bubble breakup; Multiphase flow; Numerical simulation; Turbulence

1. Introduction

Gas-liquid turbulent flows occur in industrial systems such as stirred tank biochemical reactors and bubble columns. In these flows, the deformation and breakup of bubbles strongly affect the interfacial area which, in turn, affects the rates of heat, mass, and momentum transfer. It is, therefore, of interest to determine the conditions that lead to bubble deformation and breakup.

Kolmogorov (1949) and Hinze (1955) developed a theory for bubble or drop breakup in turbulent flows. They proposed that a bubble breaks as a result of interactions with turbulent eddies that are of approximately the same size as the bubble. They assumed that the bubble size was in the inertial sub-range of turbulence length scales so that Kolmogorov's universal energy spectrum could be used to estimate the strength of eddies having sizes comparable to the bubble. Hinze formulated a criterion for breakup based on a force balance. He pointed out that, in sufficiently strong turbulence, a bubble would deform and break when the surface tension force was unable to balance the random pressure fluctuations that cause deformation. He defined a Weber number, $We = \rho_l < \delta u^2(d_e) > d_e / \gamma$, where ρ_l is the liquid density, d_e is the equivalent spherical diameter of the bubble, γ is the surface tension, and $<\delta u^2(d)>$ is the mean-square longitudinal velocity difference of the undisturbed flow over a distance d. He proposed that, when the Weber number exceeded a critical value, We_{cr}, the bubble would break. Based on the

Large-eddy simulation of flow dynamics in an industrial crystallizer geometry

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Abstract

Large-eddy simulations (LES) of the single-phase flow in a baffled, industrial crystallizer with a draft tube were performed. They were based on a Smagorinsky subgrid-scale model with c_s=0.12. The flow in the crystallizer was driven by a standard Rushton turbine. A secondary flow was generated by a throughput stream that entered through a nozzle at the bottom and exited through the sidewall. In the simulations, two Reynolds numbers (*viz.* Re=14,000 and Re=82,000), and two spatial resolutions (differing a factor of two in lattice spacing) were considered. The simulation algorithm was implemented on a parallel computer platform using up to 12 processors. It showed good scaling behavior. The simulations showed strongly non-homogeneous turbulent kinetic energy, dissipation rate, and extent of anisotropy. The average flow in the annular region was found to be dependent on the Reynolds number. The baffle configuration strongly affected the overall flow, as was demonstrated by comparing simulations with slightly different baffle layouts.

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