Large eddy simulation of the bubbly ocean: New insights on subsurface bubble distribution and bubble-mediated gas transfer

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The evolution of bubbles in a turbulent oceanic boundary layer is simulated using a multi-size multi-gas bubble model coupled with a Large Eddy Simulation model. Bubbles injected by breaking waves are brought into the boundary layer by episodic bubble plumes, and they form near-surface streaks in the convergence zone of Langmuir circulations. The equilibrium bubble distribution decays exponentially with depth and is a manifestation of intermittent bubble plumes whose bubble number density is at least one order of magnitude higher than the mean bubble number density. Bubble distribution in the injection zone is influenced by injection, turbulent transport, and dissolution. Bubble distribution below the injection zone is determined by the strength of turbulence and dissolution. For a given sea state, bubble e-folding depth increases linearly with friction velocity. Wave age is an additional governing parameter for bubble e-folding depth. The buoyancy of bubbles weakens both Langmuir circulations and near-surface turbulent kinetic energy dissipation. The buoyancy effect increases with wind speed. Gas flux through bubbles depends on both wind speed and wave age. For a given sea state, the bubble flux increases with wind speed to the fifth power.


1. Introduction

Bubbles are ubiquitous in the near surface ocean and are important in the climate system. They are known to elevate the net air-sea gas transfer rate, enhance the equilibrium gas saturation level [e.g., Woolf, 1997; Hare et al., 2004; D’Asaro and McNeil, 2007; Wanninkhof et al., 2009], and modify the optical and acoustical properties of the near-surface ocean at moderate to high ocean surface wind speeds [e.g., Lamarre and Melville, 1991; Zhang et al., 1998; Terrill et al., 2001; Anguelova and Webster, 2006]. They are also used as passive tracers to study upper ocean dynamics, such as the distribution of breaking waves at the ocean surface [Melville and Matusov, 2002], and the evolution of Langmuir circulations (LCs) [Zedel and Farmer, 1991; Farmer and Li, 1995] as well as tidal fronts [Baschek and Farmer, 2010].

Bubbles near the ocean surface are generated during the breaking of surface gravity waves. A few laboratory studies [e.g., Lamarre and Melville, 1991; Asher and Farley, 1995; Deane and Stokes, 2002] have been carried out to investigate the bubble field during and immediately after the breaking of surface gravity waves. Lamarre and Melville [1991] found that up to 50% of the wave energy lost during wave breaking are used to entrain bubbles. Deane and Stokes [2002] showed that bubbles formed under breaking waves have a well-defined size spectrum. The spectrum implies that bubbles with a radius smaller than the Hinze scale (~1 mm) are generated due to entrainment while larger bubbles are fragmented by the turbulent flows. The evolution of bubbles in a laboratory channel has also been investigated numerically [Shi et al., 2010; Liang et al., 2011; Ma et al., 2011]. Wave breaking generates a vortex in the cross-wave direction [Melville et al., 2002; Sullivan et al., 2004]. This vortex, propagating in the wave direction, advects both the bubbles and the dissolved gases from bubbles.

The evolution of bubbles in a turbulent oceanic boundary layer is different from in a laboratory flume due to the presence of boundary layer turbulence. After injection by breaking surface gravity waves, bubbles move with oceanic boundary layer turbulence, exchange gases with ambient water, and change size. Large bubbles will burst at the ocean surface, and small bubbles will fully dissolve into the ocean (Figure 1). Some early in situ observations show that the mean bubble number density decreases exponentially with depth [e.g., Johnson and Cooke, 1979; Thorpe, 1982; Crawford and Farmer, 1987]. Bubbles of radius between
50 µm and 150 µm are more abundant than smaller and larger bubbles [e.g., Farmer et al., 1998; Garrett et al., 2000]. Recent observations focus on the detailed structure of bubble plumes and the correlation of bubble penetration and surface wind speed [e.g., Trevorrow, 2003; Vagle et al., 2010]. There are very few numerical modeling studies of bubble distribution in the ocean. Thorpe et al. [2003] model bubbles of 70 µm under the influence of idealized Langmuir cells. They conclude that Langmuir cells are effective in subducting bubbles of that size and also note that sophisticated models including the information of boundary layer turbulence are needed for a better understanding of subsurface bubble distributions.

Because of the incomplete knowledge of subsurface bubble evolution, the role of bubbles in upper-ocean dynamics and climate is not well understood. The abundance of near-surface bubbles suggests that their buoyancy may weaken the downward branch of Langmuir circulations [Smith, 1998]. By examining the in situ measurements of subsurface bubble distributions, Thorpe et al. [2003] conclude that the buoyancy effect of bubbles is not important at a wind speed of 11 m/s. Gases pass in and out of the ocean through both the atmosphere-ocean interface as well as bubbles [e.g., Woolf, 1997]. Due to hydrostatic pressure and surface tension exerted on bubbles, the air-sea gas transfer rate is larger and the equilibrium saturation level is higher in the presence than absence of bubbles. Although the conceptual idea of how bubbles contribute to air-sea gas exchange are widely accepted, there has not been a consensus on the functional form of bubble-mediated air-sea gas transfer parameterization [e.g., Woolf and Thorpe, 1991; Asher et al., 1996; Woolf, 2005; McNeil and D’Asaro, 2007; Wanninkhof et al., 2009].

Liang et al. [2011] recently report on a bubble model that calculates the concentrations of bubbles of multiple sizes with multiple gas components. The model successfully simulates essential bubble processes including gas dissolution, size change, buoyant rising and advection by turbulent flows. In this study, the bubble model is coupled with a Large Eddy Simulation (LES) model capable of simulating boundary layer turbulence [Sullivan and McWilliams, 2010]. By analyzing a series of solutions for turbulent bubbly flows, we attempt to address the following questions in this paper: (1) How do bubbles evolve after their injection? (2) What determines subsurface bubble distributions? (3) How important is the buoyancy effect of bubbles on boundary layer turbulence? (4) What does the subsurface bubble distribution imply for bubble-mediated gas transfer?

The paper is organized as follows: Section 2 briefly describes the coupled model and the way we configure it for a bubbly turbulent boundary layer, section 3 presents a set of solutions and discusses the implication of bubble buoyancy effects and bubble-mediated gas transfer, and section 4 is a summary.

2. A Large Eddy Simulation Model for Turbulent Bubbly Flow

The solutions presented in this study are computed with a coupled LES-Bubble-Dissolved-Gas model [Liang et al., 2011]. It comprises a LES turbulence model, a size-resolving bubble model, and a dissolved gas model.

2.1. LES Dynamic Model

The LES dynamic model solves the wave-phase-averaged incompressible Boussinesq equations with a single-point second-moment turbulent kinetic energy (TKE) closure subgrid-scale (SGS) parameterization and a flat top ocean surface. The effect of faster travelling gravity waves on the relatively slower boundary layer currents is represented by the vortex force [Craik and Leibovich, 1976], the Lagrangian advection by Stokes drift (u_o) [McWilliams and Restrepo, 1999], and the wave-averaged increment to the pressure that arises through conservative wave-current interaction [McWilliams et al., 1997]. Following the notation of Sullivan et al. [2007], the momentum and the subgrid-scale TKE equation can be written as

\[
\frac{\partial \vec{v}}{\partial t} = -\delta_{i3} \frac{g \rho_o}{\rho_w} \vec{z} + \cdots \quad (1)
\]

\[
\frac{\partial \varepsilon_{SGS}}{\partial t} = -\delta_{i3} \frac{g \varepsilon_{SGS}}{\rho_w} + \vec{W} + \cdots \quad (2)
\]

where \( \vec{v} \) is flow velocity; \( \delta_{i3} \) is the Kronecher delta (\( \delta_{i3} = 1 \) when \( i = 3 \) and \( \delta_{i3} = 0 \) when \( i \neq 3 \)); \( g \) is the gravity; \( \varepsilon_{SGS} \) is the SGS TKE; \( \vec{W} \) is the subgrid-scale density flux; \( \vec{A} \) and \( \vec{W} \) are the ensemble-averaged momentum and SGS TKE input due to wave-breaking; and \( \varepsilon_{SGS} \) is the density of the mixture of liquid water and bubbles, i.e.,

\[
\varepsilon_{SGS} = (1 - \alpha_b) \rho_o + \alpha_b \rho_w, \quad (3)
\]

where \( \rho_a \) is the density of air, \( \rho_w \) is the density of water, and \( \alpha_b \) is the bubble void fraction. The Boussinesq approximation is valid for dilute bubbly flow when \( \alpha_b \) is much smaller than unity [Buscaglia et al., 2002]. Bubble void fractions in the oceanic boundary layer are typically a few orders of magnitude smaller than unity except right under breaking surface gravity waves where bubble void fraction can be larger than 0.1. In the current study, only the averaged impact of breaking waves is modeled and individual breaking waves
are not resolved. The bubble void ratio is everywhere smaller
than 0.1 and thus the Boussinesq approximation applies. The
dots in equation (1) denote other terms in the momentum
equations, namely, advection, diffusion, pressure, vortex
force, and Stokes-Coriolis terms. The dots in equation (2)
represent other terms in the SGS TKE equation, i.e., advec-
tion, production, and dissipation [Sullivan et al., 2007].

[10] We modify the first two terms on the right hand side
of equations (1) and (2). The buoyancy of bubbles weakens
vertical mixing when they are sufficiently abundant, and this
buoyancy effect is modeled by the first term at the right hand
side of equations (1) and (2). Momentum and energy injec-
tions are parameterized as a horizontally uniform and verti-
cally decaying source function, i.e., $\mathcal{A}(z)$ in equation (1) and
$\overline{W}(z)$ in equation (2). The estimation of $\mathcal{A}(z)$ and $\overline{W}(z)$
will be discussed in section 2.3.

2.2. Bubble Model

[11] The bubble model solves a set of concentration equa-
tions for bubbles of different sizes with different gases
[Liang et al., 2011]. Let $n_m^o(\vec{x},r,t)$ be the concentra-
tion of a gas $m$ ($m = 1$ for $O_2$, $m = 2$ for $N_2$, and $m = 3$ for $CO_2$)
in bubbles of radius increments $[r - \frac{dr}{2}, r + \frac{dr}{2}]$ in a unit
volume centered at location $\vec{x}$, and time $t$. The evolution of
$n_m^o(\vec{x},r,t)$ can be described as

$$\frac{\partial n_m^o}{\partial t} = \frac{Q(r,z)}{4\pi r^3/(3RT)} \chi_m^{um} + \ldots, \quad (4)$$

where $Q(r,z)$ is the volume injection rate of radius $r$ bub-
bles; $P$ is pressure; $R$ is the universal gas constant; $T$ is
temperature; and $\chi_m^{um}$ is the ratio of gas $m$ in the atmos-
phere. Similar to $\mathcal{A}(z)$ and $\overline{W}(z)$, $Q(r,z)$ represents the integral
impact of a spectrum of breaking waves and will be dis-
cussed in detail in section 2.3. The dots in equation (4)
represent advection, diffusion, bubble buoyant rising, bub-
ble size change, and gas exchange with the ambient water.

Parameters and formulas for bubble related processes such as
buoyant rising and dissolution from bubbles are those
proposed by Thorpe [1982] and Woolf and Thorpe [1991].
Liang et al. [2011, section 2] give details of the model for-
mulation and implementation. The consistency of the for-
mulation and the accuracy of the numerical implementation
are shown by validating the model against a Lagrangian
bubble model and laboratory measurements [Liang et al.,
2011; B. Baschek et al., Direct laboratory seawater mea-
surements of the dissolved CO$_2$ signature of individual
breaking waves, unpublished manuscript, 2011].

[12] After each time step, the number concentration of
radius $r$ bubbles is diagnosed according to the ideal gas law
as $c_b(r,\vec{x},t) = \sum n_m^o RT/(PV_b(r))$ with $V_b(r)$ the volume
of a bubble with radius $r$. The number density of all bubbles is
calculated as $c_b(\vec{x},t) = \int c_b d\vec{r}$, and the bubble volume
fraction can be calculated as $\alpha_b = \int \sum m n_m^o RT/P dr$.

2.3. Momentum, Energy and Bubble Injection
Due to Breaking Waves

[13] We simulate the open ocean covered by a spectrum of
breaking waves of different wave lengths. In most ocean
models, the momentum and TKE deposited by breaking
waves are modelled as a surface flux calculated by the bulk
formula. The momentum flux is calculated as

$$\overline{\tau}_a = \rho_b C_d \overline{U}_{10} \overline{U}_{10}, \quad (5)$$

where $C_d$ the drag coefficient calculated by the parameteri-
ization proposed by Liu et al. [1979]. The energy flux is
estimated as [Terray et al., 1996]

$$\mathcal{E} = \overline{\tau}_a \bar{c}, \quad (6)$$

where $\bar{c}$ is a wave age dependent quantity as parameterized
by Terray et al. [1996]. Recently, Sullivan et al. [2007]
developed a stochastic breaker model and incorporated it
into a LES model to study boundary layer turbulence
beneath breaking waves. In the model, momentum and
energy impulses of individual breakers are resolved and
stochastically added to the near surface ocean with the
ensemble-averaged momentum and energy injection con-
strained by bulk formulas described above and the prob-
bility density function (PDF) of breaking waves [Melville
and Matusov, 2002; Sullivan et al., 2007]

$$\mathcal{P}(c) = b_1 \exp(-b_2 c/u_*), \quad (7)$$

where $c$ is the speed of the breaking front, $u_* = \sqrt{\frac{\nu}{\rho}}$ is the
friction velocity with $\rho$, the atmospheric density, $b_1$ ensures
the unity of the PDF ($\int \mathcal{P}(c) dc = 1$), and $b_2$ is constrained by
momentum and energy conservation.

[14] In the current study, we calculate a horizontally uni-
formly, vertically decaying, ensemble-averaged breaker
impulse from the breaker model developed by Sullivan et al.
[2007]. Assuming a breaking wave of speed $c$ at location
$(x, y)$ and time $t$, the momentum, energy and bubble injection
rates are $M_b(\vec{x}, c, t)$, $E_b(\vec{x}, c, t)$, and $Q_b(\vec{x}, c, t, r)$, respec-
tively. $\mathcal{A}(z)$ in equation (1), $\overline{W}(z)$ in equation (2), and $Q(r,z)$
in equation (4) are respectively calculated as

$$\mathcal{A}(z) = \frac{1}{L_x L_y} \int \int \int M_b(\vec{x}, c, t) \mathcal{P}(c) dc dx dy dt$$

$$\overline{W}(z) = \frac{1}{L_x L_y} \int \int \int E_b(\vec{x}, c, t) \mathcal{P}(c) dc dx dy dt$$

$$Q(r,z) = \frac{1}{L_x L_y} \int \int \int Q_b(\vec{x}, c, t, r) \mathcal{P}(c) dc dx dy dt,$$

where the formulas for $M_b$, $E_b$, and $Q_b$ follow the functional
forms proposed by Sullivan et al. [2004, section 3] and
Liang et al. [2011, section 4.1]. The vertically integrated
momentum and energy injection rates are constrained by the
bulk formulas, i.e., $\int \mathcal{A}(z) dz = \overline{\tau}_a$ with $\overline{\tau}_a$ calculated by
equation (5) and $\int \overline{W}(z) dz = \mathcal{E}$ with $\mathcal{E}$ calculated by
equation (6). The injected bubble number distribution
follows that measured by Deane and Stokes [2002] in the
laboratory and it is assumed that total energy required
to inject bubbles equals half the energy from breaking
waves, i.e., $\int -\rho_b Q(r,z) dz dr = \frac{1}{2} \mathcal{E}$. This is the upper
limit of total bubble injection amount measured by Lamarre
and Melville [1991].

2.4. Posing the Bubbly Flow Problem

by different combinations of winds and waves (Table 1)
because the importance of Langmuir turbulence varies with the wind and wave fields [e.g., McWilliams et al., 1997; Li et al., 2005; Harcourt and D’Asaro, 2008; Grant and Belcher, 2009]; and we aim to identify the generic behavior of subsurface bubbles and the dynamic effect of gas bubbles on boundary layer turbulence. In the model, the Stokes drift ($u_{st}$) is calculated as [Kenyon, 1969; Sullivan et al., 2007]

$$u_{st}^q(z) = \frac{2}{g} \int_0^\infty F(f)f^3 \exp\left[\frac{2f^2z}{g}\right] df,$$

where $F(f)$ is the Donelan-Banner spectrum [Donelan et al., 1985; Banner, 1990] that is dependent on both wind speed ($U_{10}$) and wave age ($C_p/U_{10}$), with $f$ the frequency and $C_p$ the peak phase speed. A larger wave age implies a stronger Stokes drift and subsequently stronger Langmuir turbulence. In cases 1, 6, and 11, wave and wind are in equilibrium ($C_p/U_{10} = 1.2$), and $u_{st} = u_{st}^q$. In tests 2, 3, 7, 8, 12, and 13, wave age $C_p/U_{10} = 1.07$ and 2.97, for different $U_{10}$ respectively. When $C_p/U_{10} = 1.07$, the wave is developing and $u_{st} < u_{st}^q$. At $C_p/U_{10} = 2.97$, swell is important and $u_{st} > u_{st}^q$. These two values are the lower and upper limits of wave age in ocean station Papa (http://www.pmel.noaa.gov/stnP/) between June 2010 and December 2010 when $U_{10} > 7.5$ m/s (Data downloaded from http://www.pmel.noaa.gov/stnP/data.html). In tests 4, 5, 9, 10, 14, 15, $u_{st}$ is equal to $u_{st}^q$ multiplied by a factor of 2 and 4 for different $U_{10}$ respectively. The bubble volume injection profiles for the three different wind speeds are shown in Figure 2a. This is the integral injection profile of a spectrum of breaking waves from the stochastic breaker model by Sullivan et al. [2007]. The injected bubble volume decreases gradually with depth (Figure 2b) for a single breaking wave, while the injected bubble volume decreases exponentially with depth when the ocean surface breaking wave distribution follows equation (7). There are $300 \times 300 \times 96$ spatial grids. Vertical grids are stretched and surface intensified. We simulate bubbles of 17 sizes with the smallest bubbles of 35 $\mu$m and the largest of around 10 mm. In these simulations, injected bubbles contain 22% O$_2$ and 78% N$_2$. More gases can be added at the expense of computational time. Dissolved gas saturations are set to 100% throughout the simulations. For each case, a spin-up run is first carried out and bubbles are injected after boundary layer turbulence is fully developed. Further grid refinement does not change the results.

### 3. Results and Discussion

#### 3.1. The Evolution of Subsurface Bubbles

[16] The evolution of bubbles after their injection is studied in this subsection. Figure 3 shows an instantaneous vertical cross-section of vertical velocity, the total bubble number concentration ($C_b$) and the bubble void fraction ($\alpha_b$) for case 11 ($U_{10} = 20$ m/s, $u_{st} = u_{st}^q$). Alternating positive and negative velocities in Figure 3a indicate downward and upward plumes of Langmuir cells [Leibovich, 1983; Thorpe, 2004]. The downward branches of LCs bring bubbles from the upper few meters down to a depth of more than ten meters, forming episodic bubble plumes penetrating into the boundary layer. Below the upper few meters where bubbles are injected by breaking surface gravity waves, there are very few bubbles outside bubble plumes (Figures 3b and 3c). The bubble volume density is less than 1% everywhere (Figure 3c). This confirms that the use of concentration approach to simulate bubbles (section 2.2) and the Boussinesq

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**Table 1.** Meteorological Conditions for Different Test Cases

<table>
<thead>
<tr>
<th>Test Case</th>
<th>Wind, $U_{10}$ (m/s)</th>
<th>Wave: $C_p/U_{10}$</th>
<th>$u_{st}/u_{st}^q$</th>
<th>$\Delta z_{min}$ (m)</th>
<th>$\Delta x$, $\Delta y$ (m)</th>
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<tr>
<td>4</td>
<td>1.07</td>
<td>&gt;1</td>
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<td>2.97</td>
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</table>
approximation in calculating the buoyancy impact of bubbles (section 2.1) are valid. Figure 4 shows the instantaneous snapshots of vertical velocity and total bubble number concentration at a horizontal cross-section at \( z = -3.15 \) m. The downward branches of LCs extend along the wind and wave direction and form near-surface bubble streaks. Both the episodic bubble plumes and the surface bubble streaks have been observed in the ocean by acoustical measurements and visual images [e.g., Zedel and Farmer, 1991; Smith, 1992; Farmer and Li, 1995], while bubbles were used as flow tracers to investigate the structure of LCs in those studies. The co-occurrence of bubble plumes and downward branches of LCs also corroborates the use of bubbles as tracers of LCs.

Figures 5a–5c show the mean subsurface bubble distribution for case 11 \((U_{10} = 20 \text{ m/s}, u_{st} = u_{st}^{eq})\). The average manifestation of episodic bubble plumes is an exponentially decaying mean bubble number density (Figure 5a) and bubble void fraction (Figure 5b) in the vertical direction. The exponential decay of the mean bubble number concentration has been observed in the open ocean [e.g., Crawford and Farmer, 1987], and the mean bubble number concentration can be expressed as

\[
\langle C_b(z) \rangle = C_0 \exp \left( \frac{z}{z_0} \right),
\]

where the angle bracket indicates ensemble averages; and \( z_0 \) is the e-folding depth. The decay of bubble density is larger in the injection zone and smaller below it. The decay of bubbles is size dependent: it is faster for larger bubbles and slower for smaller (Figure 5c). The ratio \( c_b(z = -10 \text{ m})/c_b(z = 0 \text{ m}) = 9 \times 10^{-4} \) for 114 \( \mu \)m bubbles, and is \( 6 \times 10^{-6} \) for 1222 \( \mu \)m bubbles. Figure 5d shows the vertical profile of the mean \( O_2 \) to \((O_2 + N_2)\) ratio inside bubbles. Since \( O_2 \) dissolves faster than \( N_2 \), the \( O_2 \) to \( N_2 \) ratio decreases with depth. Figure 6 shows the bubble size spectrum at different
depths for case 1 ($U_{10} = 10$ m/s, $u_0 = u_{10}'$). Spectral peaks are at 114 $\mu$m at all depths and the tails at both ends sharpen with depth. These features are also observed in the open ocean under similar wind speeds [see Garrett et al., 2000, Figure 4; Vagle et al., 2010, Figure 4]. In the study of Vagle et al. [2010], the spectral peaks are between around 100 $\mu$m to around 160 $\mu$m at different depths. Size class centering at 114 $\mu$m spans between 70 $\mu$m to 158 $\mu$m. A better resolution in the size direction is required in the model to capture the change in different observed spectral peaks at different depths. Larger bubbles have less of a chance to get drawn down by turbulence and gases in smaller bubbles dissolve faster.

[18] Figure 7a shows the vertical profile of the mean total subsurface bubble number concentration ($C_b$) at three different wind speeds under wind-wave equilibrium (cases 1, 6, and 11). Consistent with conclusion drawn from previous in situ observations, $z_0$ increases with $U_{10}$. Figure 7b displays vertical profiles of $C_b$ for cases 11, 12, and 13 ($U_{10}$=20 m/s; while $u_0 = u_{10}'$, 2$u_{10}'$, 4$u_{10}'$). The bubble e-folding depth $z_0$ is larger when $u_0$ is larger. The bubble e-folding depth forced by 2$u_{10}'$ is 7%, 16% and 17% larger than forced by $u_{10}'$ at a surface wind speed of 10 m/s, 15 m/s, and 20 m/s, respectively. Previous studies have attempted to identify the correlation between the bubble e-folding depth $z_0$ and subsurface flow structures such as the downwelling plume depth [e.g., Trevorrow, 2003] as well as the surface meteorological conditions such as wind speed $U_{10}$ [e.g., Vagle et al., 2010]. These studies find that $z_0$ increases with bubble plume depth and $U_{10}$. From the bubble field under wind up to 25 m/s, Vagle et al. [2010] fit a linear relation between $z_0$ and $U_{10}$: $z_0 = 0.018 + 0.434U_{10}$ when $U_{10} < 25$ (m/s). Figure 7c shows $z_0$ against $U_{10}$ from the data and the linear relation from Vagle et al. [2010]. The scatter in the data is attributed to the fact that NCEP reanalysis wind cannot represent local wind variability [Vagle et al., 2010]. Computed solutions for the case of wind-wave equilibrium are also shown in Figure 7c. They are within the observed range of Vagle et al. [2010]. It should be noticed that $z_0$ increases with $U_{10}$ faster than linear. This will be explained in the next subsection. The error bars indicate bubble penetration when $C_b/U_{10}$ =1.07 and 2.97 (runs 4, 5, 9, 10, 14 and 15). These are the wave age at Ocean Station Papa at moderate wind speed ($U_{10} > 7.5$ m/s) between June and December 2010. There is 10% to 15% variability with respect to $z_0$ at wind-wave equilibrium. This indicates that sea state is a governing parameter for bubble penetration in addition to wind magnitude. The modeled $z_0$ variability due to wave age at $U_{10}$ = 10 m/s explains little observed scatter at the same wind speed. At higher wind speed ($U_{10}$ = 20 m/s), nearly 40% of the scatter in $z_0$ can be explained by the variability of wave forcing.

3.2. Control on Subsurface Bubble Distribution

[19] To gain more insight into the processes responsible for the mean subsurface bubble distribution, we construct the budget for the mean bubble number concentration from the solutions. Three processes govern the mean subsurface bubble number concentration, i.e., transport ($T_b$), dissolution ($D_b$), and injection ($I_b$). In statistical equilibrium, the balance of these three processes can be expressed as

$$\frac{\partial \langle C_b \rangle}{\partial t} = 0 = T_b + D_b + I_b,$$

(11)

where

$$T_b = \sum \left( \frac{\partial F_{SWS}}{\partial z} + \frac{\partial w_{vm}}{\partial z} \right) \frac{\partial}{\partial z} \left( \frac{dr}{dt} n_{tot} \right) \frac{RT}{PV(r)}$$

$$D_b = \sum \left( \frac{d n_r}{d t} + \frac{\partial}{\partial z} \left( \frac{dr}{dt} \right) n_{tot} \right) \frac{RT}{PV(r)}$$

$$I_b = \langle Q \rangle,$$

(12)

with the angle brackets indicating ensemble averages;

$$\frac{\partial}{\partial t} \frac{w_r}{c_z} = \frac{1}{r} \frac{d r}{d t} \langle C_b \rangle,$$

(13)

where $w_r$ is the average velocity of bubbles; and $\frac{1}{r} \frac{d r}{d t}$ can be written as [Thorpe et al., 2003]

$$\frac{1}{r} \frac{d r}{d t} = RTD_n \left( S_{\omega \omega x} + S_{\omega \omega x} / r^2 \right) (z + H_0),$$

(14)
where \( Nu \) is the Nusselt number defined as the ratio between the total gas flux and the molecular diffusive flux across the bubble surface; \( D \) is the diffusivity; \( S \) is the Bunsen solubility; and \( H_0 \approx 10 \) m is the height of water column with hydrostatic pressure equal to one standard atmospheric pressure. \( Nu, S, \) and \( D \) are all calculated with formulas from Woolf and Thorpe [1991]. Integration of equation (13) together with equation (14) gives

\[
\langle C_s(z) \rangle = c_1(z + H_0)\exp \left( \frac{C_2 z}{w_t} \right), \tag{15}
\]

where \( c_1 \) and \( c_2 \) are integration constants. It is obvious from equation (15) that \( z_0 \propto w_t \). Since bubbles are transported into the boundary layer by the downward branches of LCs, \( w_t \) should represent the strength of LCs. We therefore assume that \( w_t \) is proportional to the mean standard deviation of vertical velocity below the injection zone \( \left\langle (w^2)_{\text{mean}} \right\rangle = \frac{1}{z_0-z_a} \int_{z_a}^{z_0} \left\langle (w^2) \right\rangle dz \) with \( z_a \) the depth to which bubble plumes penetrate and \( z_0 \) the bottom of the injection zone. Figure 9a shows the relationship between \( z_0 \) and \( \left\langle w^2 \right\rangle_{\text{mean}} \) for runs 1, 2, 3, 6, 7, 8, 11, 12, and 13. Results from runs forced by the same wind speed but different Stokes drift are displayed by the same symbol. It can be seen that \( z_0 \) depends almost linearly on \( \left\langle w^2 \right\rangle_{\text{mean}} \) for cases with different wind and wave forcing.

In the real ocean, it is difficult to have information about \( \left\langle w^2 \right\rangle_{\text{mean}} \) inside the boundary layer, and we thus attempt to find a relationship between \( z_0 \) and surface meteorological conditions. It has been found that vertical velocity variances and other turbulence statistics in the boundary layer can be scaled by \( u_* La_{t,2/3} \) [Li et al., 2005; Grant and Belcher, 2009]. The turbulent Langmuir number \( La_t \) is the ratio of wind stress to Stokes forcing and is calculated as \( La_t = \frac{\nu_{st}}{U_{10}^2} \) [McWilliams et al., 1997]. Figure 9b shows \( z_0 \) versus \( u_* La_{t,2/3} \). Harcourt and D’Asaro [2008] show that turbulent intensities scale better with \( u_* La_{SL,2/3} \), where \( La_{SL} = \frac{\nu_{st}}{U_{10,SL}} \) with \( \langle u_{st} \rangle_{SL} \) the averaged \( u_{st} \) within the surface layer. Since \( u_{st} \) are multiples of \( u_{st}^* \) in the runs shown in Figure 9, i.e., the shape of \( u_{st} \) does not change among different cases forced by different \( u_{st} \), a scaling using \( u_* La_{SL,2/3} \) will not change the results shown in the figure. Although the profile of \( \left\langle (w^2) \right\rangle \) is scaled by \( u_* La_{t,2/3,0} \), \( z_0 \) is not perfectly scaled by \( u_* La_{SL,2/3} \). For the same \( u_{st} \), \( z_0 \) increases almost linearly with \( u_* \). Since the drag coefficient \( C_d \) parameterized as Liu et al. [1979] increases linearly with \( U_{10} \) when \( U_{10} \) is between 10 m/s to 20 m/s, \( u_* \propto (C_d U_{10})^{1/2} \propto U_{10} \). This explains the result in Figure 7c that \( z_0 \) increases with \( U_{10} \) faster than linear at wind-wave equilibrium. The increase of \( z_0 \) with \( u_* La_{t,2/3} \) is faster for different wind speed than for different sea state. The reason is that the bubble injection depth changes (Figure 2) and subsequently the depths that \( w^2 \) averages over to obtain \( \left\langle w^2 \right\rangle_{\text{mean}} \) changes when wind speed changes.

### 3.3. Dynamic Impact of Bubble Buoyancy

Because bubbles are buoyant in liquid water, their existence can alter the stratification in the near surface...
ocean. It has been speculated that the buoyancy can weaken vertical turbulence when bubbles are sufficiently abundant [Smith, 1998; Sullivan et al., 2004].

Figure 10a compares the mean total TKE \( E(z) = e_R + e_{SGS} \) with the resolved TKE \( e_R = \frac{1}{2} (u'^2 + v'^2 + w'^2) \) (here the prime denoting deviation from a horizontal mean) for runs with and without bubbles. The mean total TKE is largest at the surface and decreases significantly with depth for both runs. It is noticeably smaller for the run with bubbles than without bubbles in the bubble-rich near surface region. Figure 10b displays the SGS TKE for both cases. The magnitude of the near-surface \( e_{SGS} \) is close to \( E \) and it is noticeably smaller for the case with bubbles than without bubbles. Figure 10c shows the vertical distribution of resolved velocity variances for both runs. Langmuir circulations are counter-rotating cells in the direction of wind and waves. Therefore, \( \langle v'^2 \rangle \) is largest at the surface and \( \langle w'^2 \rangle \) is largest near the surface. Both \( \langle v'^2 \rangle \) and \( \langle w'^2 \rangle \) are larger than \( \langle u'^2 \rangle \). It can be seen in Figure 10c that both the surface \( \langle v'^2 \rangle \) and the near-surface \( \langle w'^2 \rangle \) are smaller with bubbles than without bubbles. The maximum \( \langle w'^2 \rangle \) for the bubble run is about 8% smaller than for the non-bubble run. If \( \langle w'^2 \rangle_{\text{max}} \) is used to measure the strength of Langmuir circulations, the result indicates that LCs are about 4% weaker with bubbles than without bubbles. The weakening of LCs due to bubbles decreases when wind speed decreases. It is 2.8% when \( U_{10} = 15 \) m/s (case 6) and less than 1% difference when \( U_{10} = 10 \) m/s (case 1). Downward branches of LCs are narrower but stronger than upward branches of LCs, and the third moment of vertical velocity \( \langle w'^3 \rangle \) is negative. Since LCs are weaker with bubbles than without bubbles, \( \langle w'^3 \rangle \) is smaller (by absolute value) with bubbles than without bubbles.

Figure 11 compares the mean velocities \( \langle u \rangle \) and \( \langle v \rangle \) for the runs with and without bubbles when \( U_{10} = 20 \) m/s under wind-wave equilibrium. It can be seen that the mean velocity profiles are essentially the same except very near the surface where \( \langle u \rangle \) is slightly more positive and \( \langle v \rangle \) is slightly more negative. The slightly larger gradient near the surface indicates slightly weaker mixing when bubbles are included.

In the presence of bubbles, it can be anticipated that a certain amount of TKE is consumed to counteract the buoyancy of bubbles to push down into the boundary layer. We compare the TKE budgets of runs with and without bubbles. The mean balance relations for the profile of \( e(z) \) in statistical equilibrium are (J. C. McWilliams et al., The wavy Ekman

\[
\frac{\partial e_R(z)}{\partial t} = T_R - \epsilon_R + P^\mu_R + P^\nu_R + B_R = 0 \tag{16}
\]

\[
\frac{\partial E(z)}{\partial t} = T - \epsilon + I + P^\mu + P^\nu + B = 0, \tag{17}
\]

where

\[
T_R = -\bar{c}_e \left( \langle w' e \rangle_R + \langle w' p / \rho_w \rangle + \frac{2}{3} \langle w' e_{SGS} \rangle_R + \langle w' \tau \rangle_R \right)
\]

\[
\epsilon_R = -(\tau_{ij} S_{ij})
\]

\[
P^\mu_R = -\langle \bar{u}_i w_j \rangle_{R} \partial_j \bar{u}_i
\]

\[
P^\nu_R = -\langle \bar{u}_i w \partial_j \bar{u}_j \rangle_{R}
\]

\[
B_R = -g / \rho_w (w \bar{p})_R - \gamma_T \langle w T \rangle_R.
\]

\[
T = -\bar{c}_e \left( \langle w' e \rangle_{TOT} + \langle w' p / \rho_w \rangle + \frac{2}{3} \langle w' e_{SGS} \rangle_{TOT} + \langle w' \tau \rangle_{TOT} \right)
\]

\[
I = \langle \mathcal{W} \rangle
\]

\[
P^\mu = -\langle \bar{u}_i w_j \rangle_{TOT} \partial_j \bar{u}_i
\]

\[
P^\nu = -\langle \bar{u}_i w \partial_j \bar{u}_j \rangle_{TOT}
\]

\[
B = -g / \rho_w (w \bar{p})_{TOT} - \gamma_T \langle w T \rangle_{TOT}.
\] \tag{18}

\[
T \text{ is the transport; } \epsilon \text{ is the dissipation; } P^\mu \text{ is the shear production; } P^\nu \text{ is the Stokes production; } B \text{ is the buoyancy due to both temperature and bubble buoyancy with } \gamma_T \text{ the thermo-expansion coefficient; and } S_{ij} \text{ is the resolved flow strain tensor. The subscript } (\cdot)_R \text{ indicates a resolved term and the subscript } (\cdot)_{TOT} \text{ indicates the sum of both resolved and subgrid scale fluxes.}
\]

**Figure 10.** Vertical profiles of (a) mean total turbulent kinetic energy (TKE), (b) subgrid-scale TKE, (c) resolved velocity variances, and (d) the third moment of resolved vertical velocity for runs with and without bubbles for case 11 \(U_{10} = 20 \text{ m/s, } u_{st} = u_{st}^e\).

**Figure 11.** Vertical profiles of mean velocities \(\langle u \rangle\) and \(\langle v \rangle\) for case 11 \(U_{10} = 20 \text{ m/s, } u_{st} = u_{st}^e\).
weakens near-surface dissipation and transport. Near-surface turbulence subducts bubbles. This sink of TKE is balanced by the sink of dissipation. In the run with bubbles, TKE production by shear and Stokes productions is much larger than TKE production by wave breaking, which is much larger for the same runs. The major near-surface source is the energy injection by wave breaking, which is much larger for the same runs. The net gas flux ($F_{net}$) between the atmosphere and the ocean can be formulated as [McNeil and D’Asaro, 2007]

$$F_{net} = F_s + F,$$

where $F_s$ is the gas flux at the ocean surface; $F$ is the gas flux through all bubbles in the boundary layer; generally, for any flux, $F > 0$ means a flux into the water. At low wind speed, $F_s$ is dominant and its functional form is relatively well studied. At moderate to high wind speeds, the bubble-mediated flux $F$ becomes important, yet the determination of $F$ is still controversial. Prevailing bubble-mediated gas flux parameterizations assume that $F \propto U_{10}^2, U_{10}^3, U_{10}^4$ for a given atmosphere-ocean gas concentration difference [e.g., Asher et al., 1996; Wanninkhof et al., 2009; Vagle et al., 2010]. The argument behind the proportionality is that whitecap coverage is parameterized as $U_{10}$ to $U_{10}^{-3}$ [e.g., Wu, 1988; Monahan, 2001] and whitecap coverage indicates the concentration of bubbles at the ocean surface. However, McNeil and D’Asaro [2007] found that $F$ increases with $U_{10}^{-0.35}$ under hurricane winds. Chiba and Baschek [2010] found that $F$ increases with $U_{10}^2$ to $U_{10}^4$ using a single bubble model.

In this subsection, computed bubble fields are used to calculate gas flux through bubbles under different wind and wave conditions. We do not attempt to derive a generalized functional form for air-sea gas transfer, but suggest how current air-sea gas transfer parameterizations can be improved. Given a subsurface bubble field, the gas flux through bubbles can be calculated as

$$F_m = \int_{-\infty}^{0} \int_{0}^{r_z} \frac{dn_m}{dt}(r,z)(c_1(r,z))drdz,$$

where $m$ denotes gas species (in the current study, O$_2$ and N$_2$). The gas flux through an individual bubble and the ambient water is calculated as [Thorpe, 1982]

$$\frac{dn_m}{dt} = -4\pi r D_{m} N u_m \left[ S_m \left( \rho_m - \rho_g + \frac{2\zeta}{r} \right) - c_m \right].$$

Figure 12. Resolved TKE budget (a) near the surface and (b) inside the boundary layer for the runs with and without bubbles for case 11 ($U_{10} = 20$ m/s, $u_{st} = u_{st}^{eq}$).

Figure 13a shows the near-surface total TKE budget for the same runs. The major near-surface source is the energy injection by wave breaking, which is much larger than TKE production by shear and Stokes productions. This source is balanced by the sink of dissipation. In the run with bubbles, TKE is consumed to counteract bubble buoyancy when turbulence subducts bubbles. This sink of TKE weakens near-surface dissipation and transport. Near-surface dissipation is weakened by 27%, 24% and 13% when $U_{10} = 20$, 15, 10 m/s, respectively. Terms in the near-surface total TKE budget (Figure 13a) are more than one-order of magnitude larger than terms in the resolved TKE budget (Figure 12a) as SGS TKE is dominant over resolved TKE (refer to Figures 10a and 10b). Inside the boundary layer, the total TKE budget (Figure 13b) is similar to the resolved TKE budget (Figure 12b) in both the balance and the magnitude of each term. Although the LES model is forced by a horizontally uniform and vertically decaying momentum and energy sources representing the integral impact of a spectrum of breaking waves, the TKE balance without bubbles is similar to the TKE balance forced by a stochastic momentum and energy injection representing a spectrum of breaking waves (McWilliams et al., submitted manuscript, 2012).
where \( c_m \) is the dissolved gas concentration in the water; the other notations are as for equation (12). Figure 14 shows \( F \) versus \( U_{10} \) for \( N_2 \) and \( O_2 \). The gas flux is positive for both gases even though the water is 100% saturated. Under wind-wave equilibrium, \( F \) increases with approximately \( U_{10}^{5} \) for both \( N_2 \) and \( O_2 \). It is slightly larger for \( N_2 \) since the ratio of \( N_2 \) to \( O_2 \) increases with depth (Figure 5d). It is greater than between \( U_{10}^{4} \) and \( U_{10}^{5} \). The \( U_{10}^{5} \) proportionality can be understood upon manipulation of equations (21) and (22).

Neglecting surface tension and the change in \( \chi_m \) with depth, \( \frac{d\chi_m}{dz} \propto -z \). Therefore,

\[
F \propto \int_{0}^{\infty} \int_{-\infty}^{0} z c_0 \exp(z/z_0) dz dr \propto \int_{0}^{\infty} c_0 z_0^2 dr. \tag{23}
\]

Since the bubble e-folding depth \( z_0 \propto U_{10}^{1.5} \) and \( c_0 \propto U_{10}^{2} \) in the current configurations, \( F \propto U_{10}^{5} \). The \( U_{10}^{5} \) increase in bubble-mediated gas transfer rate is the consequence of

**Figure 13.** Total TKE budget (a) near the surface and (b) inside the boundary layer for the runs with and without bubbles for case 11 (\( U_{10} = 20 \) m/s, \( u_{st} = u_{st}^{eq} \)).

**Figure 14.** (a) Nitrogen and (b) oxygen flux through bubbles at different wind speeds and Stokes drifts.
bubble injection near the surface, and bubble penetration due to turbulence. Gas flux through bubbles ($F$) increases slightly faster with wind speed for $N_2$ than for $O_2$. This is because bubbles penetrate deeper at higher wind speeds and the $O_2$ ($N_2$) fraction in bubbles decrease (increase) with depth (Figure 5c). Figure 14 also shows that $F$ increases with $u_{st}$ under the same wind speed, because $F$ increases with $z_0$ and $z_0$ increases with $u_{st}$. Given that sea state changes both whitecap coverage [Woolf, 2005] and bubble penetration, future development of gas-transfer parameterization at high wind speeds should include sea state as a parameter.

4. Summary

[30] We couple a size-resolving bubble model with a Large Eddy Simulation model for a surface oceanic boundary layer. The impact of breaking waves is parameterized as horizontally uniform and depth-decaying momentum, sub-grid-scale turbulent kinetic energy, and bubble injection. The coupled model is used to study the evolution of bubbles and the impact of bubble buoyancy on oceanic boundary layer dynamics. The coupled model qualitatively reproduces observed bubble size spectrum in the oceanic boundary layer. Bubbles are transported into the boundary layer by episodic downward branches of Langmuir circulations and its statistical equilibrium manifestation is a exponentially decaying mean bubble number density profile. Near the surface, the source of bubbles is injection by breaking waves; and both turbulent transport and dissolution are the sink of bubbles. Below the bubble injection zone, transport is the source and dissolution is the sink. The $e$-folding depth of the mean bubble number density $z_0$ is positively linearly correlated with the turbulent intensity at the depth to which the bubbles have penetrated. Bubbles are not only correlated with ocean surface wind speed, but also with Stokes drift, because both parameters determine the strength of Langmuir turbulence. The buoyancy of bubbles weakens both Langmuir circulations and near-surface TKE dissipation. This buoyancy effect increases with wind speed. TKE consumed to draw bubbles into the boundary layer is compensated by the weakening of both the near-surface TKE transport and dissipation. The dependence of the bubble-mediated gas flux $F$ on both the number of bubbles injected at the surface and bubble $e$-folding depth yields strong dependence on wind speed, approximately $U_{st}^2$ for both $O_2$ and $N_2$. Future development of air-sea gas transfer parameterization should include sea state as a parameter.

[31] Our results emphasize the importance of Langmuir turbulence and therefore wind stress and Stokes drift (sea state), on both bubble penetration and bubble-mediated air-sea gas flux. This conclusion offers a possible explanation to inconsistencies in observations under different meteorological conditions. Wang et al. [2011] obtained in situ bubble statistics under hurricane conditions ($U_{10} > 30$ m/s). They found the dependence of $z_0$ on $U_{10}$ is different from data obtained by Vagle et al. [2010] at lower wind speeds ($U_{10} < 25$ m/s). The bubble $e$-folding depth ($z_0$) increases more slowly with $U_{10}$ than at lower wind speed. Vagle et al. [2010] also noticed that the bubble-mediated gas transfer rate estimated by formula derived from data taken in hurricane conditions [McNeil and D’Asaro, 2007] underestimates the bubble-mediated gas transfer rate at a lower wind speed. This also indicates $z_0$ increases more slowly with $U_{10}$ under hurricane conditions than under lower wind speeds. Right beneath a passing hurricane except near the eye, ocean wave is less developed (P. P. Sullivan et al., Signatures of Langmuir turbulence in ocean boundary layers driven by hurricane winds and waves, submitted to Journal of Physical Oceanography, 2012) and the Stokes drift is smaller than that under wind-wave equilibrium ($u_{st} < u_{eq}$). According to our results, bubbles penetrate shallower under the same wind speed when the stokes drift is smaller. Besides the importance of wave age for bubble $e$-folding depth, our results also imply that wave age is an important parameter on air-sea bubble-mediated gas transfer parameterization. We are currently simulating the evolution of bubble and dissolved gases under hurricane conditions.

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References


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