Lagrangian Investigation of Wave-Driven Turbulence in the Ocean Surface Boundary Layer

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ABSTRACT

Turbulent processes in the ocean surface boundary layer (OSBL) play a key role in weather and climate systems. This study explores a Lagrangian analysis of wave-driven OSBL turbulence, based on a large-eddy simulation (LES) model coupled to a Lagrangian stochastic model (LSM). Langmuir turbulence (LT) is captured by Craik-Leibovich wave forcing that generates LT through the Craik-Leibovich type 2 (CL2) mechanism. Breaking wave (BW) effects are modeled by a surface turbulent kinetic energy flux that is constrained by wind energy input to surface waves. Unresolved LES subgrid-scale (SGS) motions are simulated with the LSM to be energetically consistent with the SGS model of the LES. With LT, Lagrangian autocorrelations of velocities reveal three distinct turbulent time scales: an integral, a dispersive mixing, and a coherent structure time. Coherent structures due to LT result in relatively narrow peaks of Lagrangian frequency velocity spectra. With and without waves, the highfrequency spectral tail is consistent with expectations for the inertial subrange, but BWs substantially increase spectral levels at high frequencies. Consistently, over short times, particle-pair dispersion results agree with the Richardson-Obukhov law, and near-surface dispersion is significantly enhanced because of BWs. Over longer times, our dispersion results are consistent with Taylor dispersion. In this case, turbulent diffusivities are substantially larger with LT in the crosswind direction, but reduced in the along-wind direction because of enhanced turbulent transport by LT that reduces mean Eulerian shear. Our results indicate that the Lagrangian analysis framework is effective and physically intuitive to characterize OSBL turbulence.

1. Introduction

Turbulent processes in the ocean surface boundary layer (OSBL) play a key role in weather and climate systems by coupling the ocean and atmosphere through air-sea fluxes of heat, momentum, and mass (Jähne and Haußecker 1998; Melville 1996; Thorpe 2004; Wanninkhof et al. 2009; Sullivan and McWilliams 2010; D'Asaro 2014). Upper-ocean turbulence also distributes nutrients and plankton (Denman and Gargett 1995), pollutants (Brunner et al. 2015; Yang et al. 2014), bubbles (Thorpe 1982; Liang et al. 2017), and radiatively important gases, such as CO₂, influencing biogeochemical cycles (Sarmiento and Gruber 2002) and ocean acidification processes (Doney et al. 2009). The goals of this study are to introduce a rational model for turbulent three-dimensional (3D) fluid particle paths in the OSBL and, based on those paths, to conduct a systematic Lagrangian analysis to determine turbulent time scales, dispersion characteristics, and effects of surface gravity waves on OSBL turbulence. turbulence is the influence of surface gravity waves. The Stokes drift due to nonbreaking surface gravity waves interacts with the turbulent currents to drive Langmuir turbulence (LT). Such wave-current interactions are described by the Craik-Leibovich equations that include Craik-Leibovich wave forcing generating LT through the so-called Craik–Leibovich type 2 (CL2) mechanism (Craik and Leibovich 1976). Enhancing turbulent transport, LT is recognized as one key OSBL process (Thorpe 2004; Sullivan and McWilliams 2010; Belcher et al. 2012; D'Asaro 2014). Breaking waves (BWs) are a source of enhanced turbulence intensities and turbulent kinetic energy (TKE; Agrawal et al. 1992; Craig and Banner 1994; Terray et al. 1996; Melville 1996), which contribute significantly to mixing processes close to the surface. Together, LT and the stochastically BW field lead to complicated nonlocal and intermittent transport (Noh et al. 2004; Sullivan et al. 2007; Kukulka and Brunner 2015).

One challenge in modeling and understanding OSBL

Computational, turbulence-resolving LT models are commonly based on large-eddy simulation (LES) models

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adopting the systematic mathematical theory by Craik and Leibovich (1976) (Skyllingstad and Denbo 1995; McWilliams et al. 1997; Li et al. 2005; Grant and Belcher 2009). LES models capture qualitatively and quantitatively many of the observed LT characteristics, such as coherent near-surface convergences zones, strong downwelling jets, relatively large vertical velocity variances, and spatial turbulent scales (Skyllingstad et al. 1999; Gargett et al. 2004; Li et al. 2009; Kukulka et al. 2009, 2011; Harcourt and D'Asaro 2010; D'Asaro et al. 2014).

BWs have been incorporated in an LES with LT by a random surface forcing to imitate TKE injection (Noh et al. 2004; Li et al. 2013) and by stochastic breaking wave events that simulate the evolution of individual breakers (Sullivan et al. 2004, 2007). These previous LES studies are consistent with observed TKE dissipation rates (Terray et al. 1996) and indicate that BW effects are mainly confined to a relatively thin surface layer close to the air–sea interface, approximately one significant wave height deep. Kukulka and Brunner (2015) implemented a relatively simple wave-breaking scheme in an LES based on the Craig and Banner (1994) model that is energetically constrained, captures enhanced near-surface mixing, and agrees with more complete LES approaches.

OSBL turbulence statistics is commonly determined at fixed locations, in the Eulerian reference framework, although previous studies employing LES approaches indicate the effectiveness of tracing particles that follow the fluid motion. Lagrangian particles have been tracked in two-dimensional models (Colbo and Li 1999) and 3D models at a fixed vertical level (e.g., McWilliams et al. 1997). LT significantly affects the 3D distribution of buoyant and neutrally buoyant particles (Skyllingstad 2003; Noh et al. 2006; Noh and Nakada 2010; Liang et al. 2017). Harcourt and D'Asaro (2010) showed that LES particle paths agree with OSBL float observations. These studies provide valuable guidance for the systematic Lagrangian analysis conducted in this study.

The close connection of single, pair, and group particle dispersion with turbulent mixing and transport processes and the unique physical advantages of the Lagrangian descriptions have been established in the fluid dynamics turbulence community (e.g., Sawford 2001; Yeung 2002; Salazar and Collins 2009). In the oceanic context, Lagrangian analyses have been successfully applied to larger-scale current systems based on float observations (e.g., Davis 1991; Rossby 2007) and numerical models with time scales larger than the mixed layer turbulent time scale (Özgökmen et al. 2001; Poje et al. 2010; Özgökmen et al. 2011). Lagrangian frequency spectra of vertical velocity have been determined in the field by Lien et al. (1998) using autonomous Lagrangian floats

(D'Asaro 2003). In addition, a Lagrangian approach is practical and physically intuitive when evaluating the dispersion of nutrients, pollutants, or other neutrally buoyant fluid characteristics.

In section 2, we introduce a rational 3D particle path model based on an LES model coupled to a Lagrangian stochastic model (LSM). The LSM is essential for higherfrequency particle motion that cannot be resolved by the LES model. Particle motions at such high frequencies play a key role in many turbulent processes, such as the initial dispersion of point sources. The LSM model shall be designed so that the particle energy is consistent with the energetics of the LES model. The Lagrangian analysis presented in section 3 reveals that Lagrangian autocorrelations, velocity frequency spectra, and particlepair dispersion statistics are effective for characterizing OSBL turbulence. Our conclusions (section 4) highlight that 1) LT is characterized not only by a turbulent relaxation time scale, but also a coherent structure time scale; 2) LT enhances crosswind dispersion, but reduces along-wind dispersion; and 3) BWs play a critical role in rapidly dispersing material near the surface over relatively short time scales.

2. Methods

a. Overview of approach

We consider the trajectory $\mathbf{X}(t, \mathbf{X}_0)$ of a particle at time *t* that is initially t = 0 located at position \mathbf{X}_0 . The particle shall move through a 3D turbulent ocean with Cartesian coordinates $x = x_1$ along the wind direction, $y = x_2$ along the horizontal crosswind direction, and vertical coordinate $z = x_3$, which is defined positive upward with z = 0 at the air-sea interface. The position vector in the Eulerian reference frame is $\mathbf{x} = (x_1, x_2, x_3)$ and the particle position vector is written as $\mathbf{X} = (X_1, X_2, X_3)$. The Lagrangian particle velocity $\mathbf{U}(t, \mathbf{X}_0)$, where $\mathbf{U} = (U_1, U_2, U_3) = (U, V, W)$, is the time derivative of the particle trajectory

$$\frac{d\mathbf{X}}{dt} = \mathbf{U}.$$
 (1)

In this study, we follow common approaches to approximate the turbulent velocity for the wave-driven ocean surface boundary layer, which is highly challenging to model (Leibovich 1983; Thorpe 2004; Sullivan and McWilliams 2010). Based on the wave-phase-averaged framework of Craik and Leibovich (1976), we introduce the Eulerian wave-phase-averaged velocity $\mathbf{u}(t, \mathbf{x})$, where $\mathbf{u} = (u_1, u_2, u_3) = (u, v, w)$, and Stokes drift vector $\mathbf{u}_s(z)$, so that the (now wave-phase-averaged) particle trajectory is governed by

$$\frac{d\mathbf{X}}{dt} = \mathbf{u}(t, \mathbf{X}) + \mathbf{u}_s(X_3), \qquad (2)$$

with the initial condition $\mathbf{X} = \mathbf{X}_0$ at t = 0. For the wavephase-averaged approach, irrotational wave-orbital motions are averaged out, whereas rotational turbulent motions are contained in **u**. Despite such averaging, the irrotational wave motion still influences the flow through the Stokes drift and the Craik-Leibovich wave forcing.

Employing the LES formulation from Moeng (1984), McWilliams et al. (1997) decompose the Eulerian velocity into the subgrid-scale (SGS)-filtered velocity $\overline{\mathbf{u}}$ and its deviation, the unresolved SGS velocity \mathbf{u}^{sgs} , so that

$$\mathbf{u} = \overline{\mathbf{u}} + \mathbf{u}^{\text{sgs}}.$$
 (3)

By design, the LES model only resolves $\overline{\mathbf{u}}$ and does not resolve \mathbf{u}^{sgs} . Turbulent SGS fluxes, for example, related to terms like $\overline{u^{\text{sgs}}w^{\text{sgs}}}$, are parameterized in the LES, while SGS TKE $0.5\mathbf{u}^{\text{sgs}} \cdot \mathbf{u}^{\text{sgs}}$ is modeled by a prognostic equation (section 2b). We estimate $\overline{\mathbf{u}}$ at \mathbf{X} based on spatial linear interpolation of the LES solution. We employ a stochastic model to determine \mathbf{u}^{sgs} (section 2d).

b. LES model for Langmuir turbulence

Following the LES approach from McWilliams et al. (1997) with the modifications for a depth-limited ocean proposed by Kukulka et al. (2011, 2012), the resolved, SGS-filtered velocity field for a nonrotating, constant density ocean is obtained by solving the wave-averaged and spatially filtered Navier–Stokes equation

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_i} = -\frac{\partial \overline{\pi}}{\partial x_i} + \varepsilon_{ikm} u_{s,k} \overline{\omega}_m + \frac{\partial \tau_{ij}^{\text{SGS}}}{\partial x_i}, \qquad (4)$$

where $\overline{\pi}$ is a generalized pressure (divided by density), ε_{ikm} is the Levi–Civita permutation tensor, and $\overline{\omega}_i = \varepsilon_{ikm} \partial \overline{u}_m / \partial x_k$ is the resolved *i*th component of the vorticity vector. The cross-product between Stokes drift and vorticity vector, called Craik–Leibovich vortex force, tilts vertical vorticity into the direction of wave propagation and gives rise to LT. Without waves, the Stokes drift is zero, so that the LES model (4) solves only for shear-driven turbulence (ST).

Unresolved turbulent SGS fluxes are parameterized via an SGS eddy viscosity (e.g., K_M for momentum)

$$\tau_{ij}^{\text{SGS}} = -K_M \left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i} \right), \tag{5}$$

where τ_{ij}^{SGS} is the turbulent SGS momentum flux tensor; K_M depends on the SGS TKE *e* and an SGS length scale *l* determined by the spatial resolution

$$K_M = le^{1/2},$$
 (6)

where *e* is the SGS TKE and $l = (\Delta x \Delta y \Delta z)^{1/3}$ [see Moeng (1984) for details]. The SGS TKE, in turn, is determined from the prognostic equation

$$\frac{\partial e}{\partial t} + \overline{u}_{j} \frac{\partial e}{\partial x_{j}} = \tau_{ij}^{\text{SGS}} \left(\frac{\partial \overline{u}_{i}}{\partial x_{j}} + \frac{\partial u_{s,i}}{\partial x_{j}} \right) + \frac{\partial}{\partial x_{i}} \left(2K_{M} \frac{\partial e}{\partial x_{i}} \right) - \varepsilon + I_{b}, \qquad (7)$$

where the TKE dissipation rate ε is

$$\varepsilon = C e^{3/2} l^{-1}, \tag{8}$$

with C = 0.71. The last term in (7) is a work term because of breaking waves that will be discussed next.

c. Breaking waves

To simulate enhanced near-surface TKE and TKE dissipation rates due to BWs, we follow the approach of Kukulka and Brunner (2015) and impose a BW TKE surface flux F as surface boundary condition for the SGS TKE in (7). This approach is an extension of the work by Craig and Banner (1994), who specified a TKE surface flux F due to BW in a Reynolds-averaged Navier–Stokes equation model, but simplifies the stochastic BW model from Sullivan et al. (2007), which attempts to resolve BW events in an LES model.

In equilibrium wind-wave conditions considered in this study, the energy loss by BWs F is balanced by the total wind energy input and can be expressed as (Komen et al. 1996)

$$F = g \int_{0}^{\omega_{\text{max}}} \beta \phi(\omega) \, d\omega, \qquad (9)$$

where ω is the radian wave frequency, g is the acceleration of gravity, and ϕ is the one-dimensional waveheight frequency spectrum, which is estimated based on the empirical spectrum from Donelan et al. (1985). The high ω cutoff ω_{max} is specified as 4 times the frequency at the peak of $\phi(\omega)$. The wave growth rate β is adopted from Plant (1982):

$$\beta = c_{\beta} u_*^2 c^{-2} \omega \tag{10}$$

for $c/u_{*_a} < 35$, and $\beta = 0$ otherwise. The wave phase speed *c* is $c = g/\omega$; the wind stress is $\rho_w u_*^2$; u_* and $u_{*_a} = u_* \sqrt{\rho_w/\rho_a}$ denote the water-side and air-side friction velocity, respectively, and ρ_w and ρ_a are the density of water and air, respectively. The coefficient $c_\beta = (32 \pm 16)$ denotes a nondimensional growth rate coefficient with large uncertainties; here we set $c_\beta = 32$. To implement the energy input due to *F* numerically, we impose a constant, horizontally uniform BW work term $I_B(z)$ in (7) that inputs TKE into the SGS motion, so that $F = \int_{-h}^{0} I_B dz$. Kukulka and Brunner (2015) show that this TKE input is consistent with previous estimates and that their approach yields simulated near-surface TKE dissipation rates that are consistent with observations from Terray et al. (1996) for a wide range of wind and wave conditions.

d. Stochastic model for subgrid-scale motions

The high-frequency SGS velocity u_i^{sgs} is not resolved by the LES but needs to be modeled separately. Our design goals of this SGS model for particle motions are 1) the model shall be simple, rational, and computationally efficient; 2) particle SGS motions shall be consistent with the SGS TKE and TKE dissipation rates that are explicitly modeled by the LES through (7) and (8), respectively; and 3) we shall employ an existing model "as is" without tuning, but critically evaluate the model performance based on the analysis of particle motions. In agreement with common LES assumptions and our design goals, we assume that the turbulent motion below SGS is approximately isotropic and homogeneous.

Clearly, these model design choices bring about limitations. For example, by design, SGS particle motions are generally not consistent with the local, instantaneous SGS momentum fluxes parameterized by (5). However, in well-resolved LES approaches, these SGS stresses are small (Pope 2008). Or, SGS motion close to the boundaries is not isotropic, which is a common challenge in LES models and an active field of research (e.g., Sullivan et al. 1994; Pope 2008) beyond the scope of this study. In spite of these limitations, our approach provides a valuable starting point for modeling particle SGS motions.

LSMs of particle trajectories in turbulent flows can be applied to meet our design criteria. LSMs are not based on first principles, but satisfy certain flow criteria with known limitations (Thomson 1987). In this study, we employ the LSM by Weil et al. (2004), which follows closely Thomson (1987) and was applied in an LES to model SGS motions in convective, atmospheric boundary layers (e.g., Weil et al. 2004; Kim et al. 2005). In this model, du_i^{sgs} is governed by

$$du_i^{\text{sgs}} = -\frac{C_0 \varepsilon}{2\sigma^2} u_i^{\text{sgs}} dt + \frac{1}{2} \left(\frac{1}{\sigma^2} \frac{d\sigma^2}{dt} u_i^{\text{sgs}} + \frac{\partial\sigma^2}{\partial x_i} \right) dt + \left(C_0 \varepsilon dt \right)^{1/2} d\xi_i,$$
(11)

where $d\xi_i$ is a normalized Gaussian random variable and $\sigma^2 = (2/3)e$ is the variance of each SGS velocity component.

The model constant C_0 is closely related to the Kolmogorov constant; however, C_0 is often determined experimentally from relatively low Reynolds number data and should therefore be distinguished from the Kolmogorov constant (Pope 2008). Estimates range between $C_0 = 4 \pm 2$ (Thomson 1987) and $C_0 > 4$ (Pope 2008); we set $C_0 = 6$. The model by Weil et al. (2004) furthermore introduces an empirical factor $f_s \le 1$ in the first and last right-hand-side terms, which we do not include, as explained next.

By design, the model (11) has the following desired properties (Thomson 1987; Sawford 2001; Pope 2008): 1) The last right-hand-side (rhs) term of (11) is a stochastic forcing term that results in particle motions consistent with the expected behavior, such as particle dispersion, in the inertial subrange for small time and spatial scales. In this term, Weil et al. (2004) replace ε with $f_s \varepsilon$, which erroneously decreases TKE in the inertial subrange for $f_s < 1.2$) The first rhs term of (11) is a relaxation term that imposes, for stationary and homogeneous turbulence, a Lagrangian SGS time scale $2\sigma^2/C_0\varepsilon$. This ensures that the TKE of the stochastic particle motion is consistent with the SGS TKE of the LES model. In this term, Weil et al. (2004) also replaces ε with $f_s \varepsilon$, thereby moving SGS TKE to lower frequencies, which is inconsistent with the expected turbulent time scale of the SGS scheme obtained from TKE dissipation rates and SGS TKE. 3) The second rhs term of (11) imposes a well-mixed condition, so that already-mixed tracers remain mixed. For strongly nonstationary or inhomogeneous turbulence, this term may modify the Lagrangian SGS time scale imposed by the first term, resulting in TKE due to stochastic particle motion that differs from the SGS TKE of the LES model. This will be assessed below.

e. Experimental design

Our default model setup follows closely our previous approach to simulate a depth-limited ocean that has been analyzed and assessed in detail (Kukulka et al. 2011, 2012). This approach yields also results consistent with the shallow ocean LES from Tejada-Martinez and Grosch (2007). Note that this idealized depthlimited ocean setup greatly facilitates the conceptual understanding and interpretation of results, but more general applications should include the Coriolis force and stratification. The computational domain is h =16-m deep and extends $L_x = L_y = 64$ m in each horizontal direction. The number of horizontal grid points, $n_x = n_y = 128$, and vertical grid points, $n_z = 100$, is sufficient to resolve well energy-containing and fluxcarrying turbulent eddies (Pope 2008). The specific size of streamwise coherent structures (Langmuir cells or "Couette cells" for shear-driven turbulence; e.g., Papavassiliou and Hanratty 1997) depends on the finite horizontal domain size. However, the specific size of such structures is not critical for the conclusions and major findings presented in this paper. This is because the principal differences between Langmuir turbulence and shear-driven turbulence are independent of the specific domain size (see appendix). Note also that our LES flow field is based on previous work with similar domain sizes (e.g., Tejada-Martinez and Grosch 2007; Kukulka et al. 2011, 2012). These previous studies clearly demonstrate that approaches with limited domain size provide a valuable starting point for investigating depth-limited Langmuir turbulence.

The wind and wave forcing is specified based on typical observed conditions described in Kukulka et al. (2012). The wind speed at 10-m height is $U_{10} = 7 \text{ m s}^{-1}$, corresponding to $u_* = 0.0083 \,\mathrm{m \, s^{-1}}$. The Stokes drift profile is estimated for a monochromatic depth-limited surface gravity wave with wavelength $\lambda = 40 \text{ m}$ and significant wave height $H_s = 0.75 \,\mathrm{m}$ (or amplitude $a = H_s/\sqrt{8}$, resulting in a turbulent Langmuir number of $La_t = 0.8$. This Langmuir number is relatively large for open ocean Langmuir turbulence but is consistent with previous coastal LES studies that provide a valuable reference point for investigating Langmuir turbulence in a depth-limited ocean (Tejada-Martinez and Grosch 2007; Kukulka et al. 2011, 2012). The BW TKE flux F is determined from (9) for a fully developed sea with $c/u_{*_a} = 35$ and the prescribed U_{10} .

To clearly identify and contrast simulation results for different wave effects, we only present results for three different cases: Case S denotes simulations without any wave effects (shear-driven turbulence), case L includes only Langmuir turbulence, and case LB includes both Langmuir turbulence and breaking wave effects. Case S is characterized by relatively small-scale and less coherent motions (Fig. 1, top panels), whereas the L simulations reveal coherent roll vortices in the OSBL characterized by strong surface convergence regions with organized downwelling jets underneath (Fig. 1, bottom panels).

By default we release 5000 particles on an evenly spaced grid in the domain and track them over a period of 10^5 s (about 28 h), which is much larger than the traditional estimate of a turbulent time scale of $h/u_* = 1930$ s. Particles are perfectly reflected by the surface and bottom boundaries.

3. Results

In section 3a, we will first illustrate that, by design, particle energetics are consistent with the energetics of

the LES model. Section 3b provides an intuitive overview of 3D particle paths and velocities, before analyzing in-depth Lagrangian velocity autocorrelations in section 3c and spectra in section 3d. Fundamental differences due to wave effects in turbulent transport are further highlighted by the investigation of particle cloud dispersion, discussed in section 3e.

a. Energetic consistency of particles and Eulerian fields

To test whether the Lagrangian particle model is energetically consistent with the Eulerian flow field, we compare vertical profiles of horizontally averaged mean velocity and velocity variances (Fig. 2). Profiles from particle trajectories are computed from depth-dependent probability density functions $P(U_i|z)$, which are estimated for depth bins consistent with the vertical resolution of the LES model. For example, the mean along-wind velocity at z is $\int U_1 P(U_1|z) dU_1$ and the along-wind velocity variance is $\int [U_1 - (\int U'_1 P(U'_1|z) dU'_1)]^2 P(U_1|z) dU_1$. The along-wind velocity profile obtained from the particles and Eulerian fields $\langle u \rangle$ (angle brackets denote horizontal averages) agree well (profiles are on top of each other, Fig. 2a).

Since the particle motion includes SGS contributions, the Eulerian velocity variance profiles are estimated based on the resolved flow field and the SGS TKE, assuming isotropic turbulence, so that $\langle u_i^{\prime 2} \rangle = \langle \overline{u}_i^{\prime 2} \rangle + 2/3e$ (prime denotes the deviation from the horizontal average). Velocity variances $\langle u_i^{\prime 2} \rangle$ are only consistent if the LES SGS contribution is included in the Eulerian field, indicating that the model (11) reasonably constrains SGS TKE (Fig. 2c). The profiles of $\langle u_i^{\prime 2} \rangle$ for the S and L cases are in close agreement to those previously simulated for similar shallow-water conditions (Tejada-Martinez and Grosch 2007). For the LB case, BWs enhance nearsurface velocity variances by over an order of magnitude (bottom panels in Fig. 2). In spite of strongly inhomogeneous TKE profiles, the simple model (11) captures reasonably well near-surface TKE and its vertical decay. This comparison indicates that particle energetics agree with the energetics of the Eulerian LES fields, consistent with our particle SGS motion design goals.

b. Example particle trajectories

Example particle trajectories and their corresponding velocities provide an intuitive overview of the Lagrangian fluid motion (Fig. 3). Without LT, the vertical motion is more local with particles moving gradually throughout the OSBL, indicating relatively small energetic OSBL eddies (gray line in Fig. 3a). With LT, energy-carrying eddies are larger and particles move



FIG. 1. Normalized velocity fields (top) without and (bottom) with LT. Horizontal cross section of (a) near-surface v, (b) middepth w, and (c) near-bottom v, and (d) depth–crosswind cross section of w. Particle release locations for point source dispersion experiments are indicated by crosses (section 3e).

more regularly between the OSBL bottom and surface (black lines in Fig. 3a), which is a signature of large-scale coherent vortices extending throughout the whole OSBL. In both cases, higher-frequency motion is found close to the boundaries because of relatively small eddies near the surface. Although differences between L and LB simulations appear to be small at greater depths (cf. thin and thick black lines), BWs drive energetic high-frequency motions near the surface with periods of about a few seconds due to the BW TKE flux at the surface (Fig. 4).

Consistently, particle velocities (Figs. 3d-f) in the LB case are much larger, often exceeding $10u_*$, and rapidly oscillate once particles are sufficiently close to the surface (cf. with vertical trajectories, Fig. 3a). In the S case, variations of U are partially due to particles changing Z because of the vertically sheared along-wind current. This is different with LT, because shear is reduced (Fig. 2). With LT, enhanced U is related to Y as enhanced along-wind jets are found in downwelling regions whose locations depend on Y. The L and LB crosswind trajectories also show that the particles are initially circulating in a roll vortex, moving first in the crosswind direction and then back (Fig. 3b). At about $tu_*/h = 3.8$, Y trajectories for the L and LB cases diverge

because the LB particle moves to a neighboring vortex to continue its motion in the crosswind direction.

This brief overview of Lagrangian time series illustrates that particle trajectories compactly and effectively describe the 3D turbulent flow structure.

c. Lagrangian velocity autocorrelations

Let us next explore more systematically the turbulence structure of energy-containing eddies through Lagrangian velocity autocorrelations

$$R_i(\tau) = \{ U_i'(t) U_i'(t+\tau) \},$$
(12)

where the curly brackets indicate the combined ensemble and time average, and the prime denotes the deviation from the mean, so that $U'_i = U_i - \{U_i\}$. The normalized autocorrelation is defined by

$$r_i(\tau) = R_i(\tau)/R_i(0).$$
 (13)

1) EDDY TURNOVER AND COHERENT STRUCTURES

A common characteristic of r_i is a relatively rapid decorrelation for smaller τ , the presence of at least one zero crossing, and a relatively slow decorrelation for



FIG. 2. Comparison of horizontally averaged along-wind velocity and velocity variances obtained from Lagrangian particle trajectories (thick line) and Eulerian fields (thin lines) with SGS (gray) and without SGS (black) contributions for the (a) S, (b) L, and (c) LB cases. The normalized Stokes drift profile is shown in the top panels of (b) and (c) as a thick dashed line.



FIG. 3. Examples of (a)–(c) turbulent trajectories and (d)–(f) velocities for the S (thick black line), L (gray line), and LB (thin black line) cases. Normalized velocities are offset by -10 and 10 for the S and L cases, respectively. The box in the top-left corner of (a) is enlarged in Fig. 4.

larger τ , so that r_i converges to zero with greater τ (Fig. 5). (Taylor 1922, p. 210) commented on the possibility of zero crossings "due to some sort of regularity in the eddies of which the turbulent motion consists." For w, the first zero crossing at $\tau = T_e$ defines an eddy turnover time scale as half of the particles reverse their vertical direction of motion. Without LT, eddies break up more quickly after T_e , resulting in a more random field of motion and in a more rapid convergence of r_3 to zero (Fig. 5a, thick black line). With LT, r_i is more negative and multiple zero crossings can be observed because of the presence of larger-scale coherent structures

(Fig. 5, gray line). The TKE input due to BWs appears to disrupt such coherent structures because velocities are less correlated (Fig. 5a, thin black line), but the effect is relatively small for the larger-scale turbulent motion that is highlighted by r_i .

2) U' and V' decorrelate more slowly

The autocorrelation r_2 converges more slowly to zero than r_3 (cf. Fig. 5b with Fig. 5a), and r_1 even more slowly than either r_3 and r_2 (cf. Fig. 5c with Figs. 5a and 5b). This is because particles that move in the crosswind direction may move to a neighboring eddy, thereby not



FIG. 4. Closeup of the Z trajectory for the LB case shown in Fig. 3a.

turning over but maintaining the previous direction of motion. In addition, the along-wind velocity is vertically sheared, introducing a depth-dependent component of U', so that the velocity variance is related to $\langle u \rangle$ and u_s by

$$R_1(0) = \overline{\overline{\langle u'^2 \rangle}} + \overline{\left(\langle u \rangle + u_s - \overline{\langle u \rangle + u_s}\right)^2}, \qquad (14)$$

where the double overbar indicate depth averages. This equation shows how particle velocity variance partitions into turbulent and mean shear parts. The last term on the rhs is not a turbulent term in the Eulerian framework based on horizontal averages, but describes a turbulent deviation from the Lagrangian mean due to particles moving in a sheared flow. This term is enhanced without LT because of the enhanced vertical shear (Fig. 2). With LT, we find $R_1(0) = 7.8u_*^2$ and determine the sheared component (last term on the rhs) as $2.4u_*^2$ based on the results shown in Fig. 2. Without LT, we find $R_1(0) = 14.5u_*^2$ and the sheared component (last term on the rhs) is $8.2u_*^2$, so that the sheared component is dominant for shear-driven turbulence. At the same time, the U' component due to shear can only decorrelate because of relatively weak vertical motion, leading to the slow velocity decorrelation shown by r_1 (Fig. 5c).

3) LAGRANGIAN INTEGRAL TIME SCALES

We estimate the Lagrangian velocity integral time scale (Yeung 2002)

$$T_i = \int_0^\infty r_i(\tau) \, d\tau \tag{15}$$

for different velocity components U'_i and different wave cases (Table 1).

As expected from the foregoing discussion of $r_i(\tau)$, we find that $T_3 < T_2 < T_1$. With and without wave effects, T_3 takes similarly small values. Note that it is challenging to



FIG. 5. Normalized velocity autocorrelation r_i for the S (thick black line), L (gray line), and LB (thin black line) cases. Dashed lines show r_i only for LES-resolved scales without SGS model (11) for the S (black) and L (gray) cases.

estimate T_3 with high confidence, and its physical interpretation is not obvious because the magnitude of positive and negative contributions to the integral (15)are much larger than T_3 and approximately cancel. For the crosswind direction, T_2 is greater with LT because of coherent roll vortices. Conversely, T_1 is greater without LT because of enhanced shear. BWs do not significantly affect T_i values, indicating that they do not strongly influence the larger-scale turbulent eddies. For exponentially decaying r_i , T_i is the exponential decay time, providing a physically intuitive interpretation for T_2 without LT. For turbulence characterized by coherent structures, this interpretation is obscured because positive and negative r_i cancel to reduce T_i . For example, it is not clear how T_3 with LT is related to T_e or the decay or oscillations of $r_i(\tau)$. The will be addressed in the following subsection.

Without SGS contributions, the autocorrelation $r_i(\tau)$ decreases more slowly and T_i typically increases by 10%–20% (dashed lines in Fig. 5). These T_i values are greater than expected for the real flow field because of the missing SGS contributions. To estimate by how much T_i may increase without SGS contributions, we consider that the energy-containing low-frequency contributions to TKE are only weakly influenced by SGS motions, so that $R_i(0)T_i$ approximately equals $\overline{R}_i(0)\overline{T}_i$, where $\overline{R}_i(\tau)$ and \overline{T}_i denote the dimensional autocorrelation and integral time, respectively, obtained from the LES-resolved flow without SGS contributions. Thus, T_i is expected to increase by a factor $R_i(0)/R_i(0)$ relative to T_i . Our simulated increase in \overline{T}_i is consistent with our LES that resolves between 10% and 20% of TKE.

4) BEYOND LAGRANGIAN INTEGRAL TIME SCALES

Let us next explore two physically intuitive time scales that take into account a relaxation time T_r due to eddy breakup and a time scale T_c of coherent structures that characterizes their periodicity. The normalized autocorrelation for an idealized model of the breakup process is $r(\tau) = \exp(-\tau/T_r)$ (e.g., Pope 2008) and for an idealized coherent structure model is $r(\tau) = \cos(2\pi\tau/T_c)$. With both processes combined, one may expect

$$r(\tau) = \exp(-\tau/T_r)\cos(2\pi\tau/T_c), \qquad (16)$$

that is, *r* is a sinusoidally oscillating function with an exponentially decaying envelope. For $T_r = T_c$, the integral time scale of (16) is $T = T_r/[1 + (2\pi)^2] \approx 0.025T_r$, which is much smaller than T_r or T_c and, therefore, challenging to interpret physically.

TABLE 1. Normalized T_i and normalized A_i for the horizontal directions.

	T_3u_*/h	T_2u_*/h	T_1u_*/h	$A_2/(hu_*)$	$A_1/(hu_*)$
S	0.0037	0.076	0.44	0.15	6.47
L	0.0037	0.157	0.30	0.43	2.33
LB	0.0031	0.148	0.30	0.47	2.68

With LT, r_3 is relatively narrow-banded with an apparent envelop, conceptually similar to (16). To estimate the envelop and phase of $r_3(\tau)$, we apply the Hilbert transform (Bendat and Piersol 2000)

$$\tilde{r}(\tau) = \int_{-\infty}^{\infty} [-j \operatorname{sign}(f)] \mathscr{F}[r] \exp(j2\pi f\tau) \, df \,, \quad (17)$$

where $\mathscr{F}[r] = \int_{-\infty}^{\infty} r(\tau) \exp(-j2\pi f\tau) d\tau$ denotes the Fourier transform of *r* and $j = \sqrt{-1}$. After defining the analytic signal

$$\hat{r}(\tau) = r(\tau) + j\tilde{r}(\tau) = |\hat{r}| \exp[j\theta(\tau)], \qquad (18)$$

the envelop is retrieved by $|\hat{r}| = (r^2 + \tilde{r}^2)^{1/2}$ and the phase θ by $\theta = \tan^{-1}(r/\tilde{r})$ (Fig. 6). This procedure allows us to objectively estimate T_r by fitting $|\hat{r}| \propto \exp(-\tau/T_r)$ for $\tau/T_e > 0.25$ (Fig. 6, thin black line). We find $T_r u_*/h = 0.63$ and 1.31 without and with LT, respectively, indicating that for shear-driven turbulence, larger-scale eddies break up significantly faster. This was not clear from the T_3 estimates alone. Furthermore, with LT, the Hilbert transform reveals the oscillating sinusoidal part of $r(\tau)$ through the real part of $\hat{r}/|\hat{r}|$, which is $\cos(\theta)$, with an approximate period of $T_c u_*/h = 2.78$ [determined from the slope of $\theta(t)$]. For the S case, T_c cannot be determined with high confidence; and for the LB case, results of T_r and T_c are similar to the L case.

5) TURBULENT DIFFUSIVITIES

For long time lags, with $R_i(\tau)$ approaching zero, $R_i(\tau)$ is a useful mathematical construct to understand singleparticle dispersion over time scales much longer than some integral time (see next subsection), that is, when particle motion is equivalent to a random walk (Taylor 1922). In this case, the turbulent diffusion coefficient along *i* is

$$A_{i} = \int_{0}^{\infty} R_{i}(\tau) \, d\tau = R_{i}(0)T_{i}, \qquad (19)$$

which is determined here only for the horizontal directions because particles are already well mixed in the vertical over long times. With LT, crosswind dispersion is substantially enhanced because of coherent roll vortices (e.g., Majda and Kramer 1999), whereas along-wind dispersion is significantly



FIG. 6. Normalized autocorrelation r_3 (thick black line) for the (a) L and (b) S cases with its envelope $|\hat{r}|$ (thin black line) and $0.2 \cos(\theta)$ (gray line); see (16).

reduced relative to the S case because LT reduces the vertical shear in the along-wind flow (Table 1). In both cases, horizontal dispersion is strongly anisotropic with greater dispersion in the along-wind than crosswind direction. This anisotropy is much enhanced for the S case, so that a point source disperses much more along a line in the wind direction without LT, whereas dispersion is more radially symmetric with LT.

A simple conceptual model of A_1 for the S case is derived by assuming that differential advection in the along-wind direction and small-scale vertical mixing predominantly govern A_1 (Taylor 1953; Saffman 1962; Fischer 1973), so that A_1 can be estimated by an "effective" eddy diffusivity (e.g., Esler and Ramli 2017)

$$A_{\rm eff} = \overline{\left(\frac{Q^2}{A_v}\right)},\tag{20}$$

where $A_{\nu}(z)$ is the depth-dependent vertical turbulent <u>diff</u>usivity and Q(z) is defined by $Q(z) = \int_{-h}^{z} (\langle u \rangle - \overline{\langle u \rangle}) dz$. The mean profile $\langle u \rangle$ is approximated by a log-profile $\langle u \rangle = u_* \kappa^{-1} \log(z/z_0)$ from the bottom to middepth and by a corresponding log-profile that is symmetric with respect to point z = -h/2 in the upper half of the water column (Kukulka et al. 2011, 2012). Here, $\kappa = 0.4$ denotes the von Kármán constant and $z_0 = 0.001$ m is a roughness length consistent with the LES model (Kukulka et al. 2011). Assuming furthermore that $A_{\nu}(z)$ is equal to the eddy viscosity $u_*^2/(d\langle u \rangle/dz)$, we find $A_{\text{eff}} = 10.1u_*h$. If the dominant contribution to $R_1(0)$ is due to shear, the idealized model also yields $A_{\text{eff}}/R_1(0) = T_1 = 0.77h/u_*$. Both estimates agree within an order of magnitude with our solutions and illustrate the importance of shear dispersion dynamics. With LT, (20) suggests that A_1 is reduced because of weaker shear and enhanced A_v ; however, application of (20) to the L case is too oversimplified because of the substantial nonshear contribution to $R_1(0)$ and nonlocal vertical transport due to LT (Kukulka et al. 2012).

d. Lagrangian velocity frequency spectra

To examine the TKE content of all time scales much larger than the dissipation range, we introduce the onesided velocity frequency spectrum for U'_i

$$S_i(f) = 2\hat{S}_i(f)$$
 for $f > 0$ and $S_i(0) = \hat{S}_i(0)$, (21)

where $\hat{S}(f)$ is the two-sided spectrum defined by

$$\hat{S}_i(f) = \mathscr{F}[R_i(\tau)] = \int_{-\infty}^{\infty} R_i(\tau) \exp(-j2\pi f\tau) \, d\tau.$$
(22)

1) LOW-F SPECTRAL PEAK

With LT, S_2 and S_3 peak at about $fh/u_* = 0.35 \approx h/(u_*T_c)$, corresponding to a period of about 5000s, which is consistent with the T_c for the coherent part of $r_3(\tau)$ determined in section 3c(4) (Fig. 7). As expected for coherent LT roll vortices that are aligned with the wind, the peak of the crosswind S_2 and vertical S_3 exceeds the spectra without LT. Without LT, a peak is still



FIG. 7. Normalized Lagrangian velocity spectra S_i .

evident for S_3 , which is, however, relatively broad and due to eddy turnover in the vertical direction, discussed in section 3c(1). This is qualitatively consistent with the fact that T_c could not be determined with high confidence for the S case. Note that peaks in S_3 are challenging to observe in the ocean because of uncertainties in low-frequency spectral estimates (Lien et al. 1998). Without LT, S_1 and S_2 level off at low frequencies without a pronounced peak. The energy-containing part of S_1 at lower frequencies significantly exceeds the one with LT because of along-wind shear contributions [see section 3c(2)]. Our results indicate that BWs do not significantly affect the energy-containing range of motion. Similarly, without SGS contribution (dotted lines in Fig. 7), the energy-containing range is, as expected, not significantly affected by the SGS model (11).

2) HIGH-F SPECTRAL TAIL

Without SGS contribution, the frequency spectrum rapidly decreases at higher frequencies because high-frequency content is not resolved by the LES (dotted lines in Fig. 7). Thus, SGS contributions modeled by (11) are critical at higher frequencies.

BWs enhance the high-frequency spectral tail by over an order of magnitude for $fh/u_* > 50$. Recall that BW motions are simulated with the stochastic model (11) and the TKE surface flux (9). A transition from the energy-containing turbulent scales due to BW to the inertial subrange is expected near $fh/u_* = h/u_* \{C_0 \varepsilon/(2\sigma^2)\} \approx 50$, which agrees with our simulations. In interpreting these

BW results, it is important to keep in mind that the length scale of BW motion is determined from the SGS model. More realistic modeling approaches should estimate this length scale directly from wave dynamics, which is beyond the scope of this study.

With and without wave effects, S_i is proportional to f^{-2} for high f (Fig. 7). In the inertial subrange, dimensional analysis suggests that $S_i = B\varepsilon f^{-2}$ (Corrsin 1963; Tennekes and Lumley 1972), where B is a universal constant coefficient here taken as $B = C_0/(2\pi^2)$, which is mathematically consistent with the stochastic model (11) for $f \to \infty$. In this study, turbulence is inhomogeneous so that ε needs to be replaced by the average $\{\varepsilon\}$ and $S_i = B\{\varepsilon\}f^{-2}$. We find $\{\varepsilon\}u_*^{-3}h = 24, 17,$ and 220 for the S, L, and LB cases, respectively, which is consistent with the simulated spectra at high frequencies in the inertial subrange (Fig. 7). Note that simulated spectra for vertical velocities S_3 are slightly larger than what is expected for the inertial subrange because the bounce condition at the surface and bottom boundaries introduces high-frequency energy.

e. Point-source dispersion

To examine in detail particle dispersion dynamics, we analyze particle-pair statistics of evolving clouds of particles due to point sources. We release point sources at t = 0 with 1000 particles at 12 different locations, including three depth levels (at the surface, at middepth, and near the bottom) and four horizontal locations near downwelling, upwelling, and roll vortex center regions (Fig. 1).



FIG. 8. Particle locations after the release of point sources at 12 locations after (a), (c) $tu_*/h = 0.05$ (t = 100 s) and (b), (d) $tu_*/h = 0.11$ (t = 400 s) (a), (b) in 3D and (c), (d) projected into a plane orthogonal to the x direction.

Figure 8 shows the evolution of particle clouds for the LB case after $tu_*/h = 0.05$ (t = 100 s) and $tu_*/h = 0.11$ (t = 400 s). Initially, breaking waves near the surface rapidly disperse the cloud. The dispersion is smallest at middepth, where the mean Lagrangian shear is smallest (Fig. 2, top panels). At the surface, particle clouds are transported into convergence zones, where they are rapidly advected downward. Particle clouds in the center of Langmuir cells (cf. with Fig. 1) disperse much more slowly. These results suggest that the initial particle dispersion strongly depends on release location.

The mean squared particle-pair distance is effective in describing the evolution of such clouds (Sawford 2001; Salazar and Collins 2009), which is defined here for each direction

$$d_i^2 = \{ (X_i - X_i')^2 \}, \qquad (23)$$

where $(X_i - X'_i)^2$ is the squared distance along *i* of two particles, one located at $X_i(t)$ and the other at $X'_i(t)$. Our results reveal three distinct dispersion regimes: for small times (say, $t \ll T_r$, see discussion below), d_i^2 rapidly increases; for intermediate times $(t \sim T_r)$, d_i^2 increases irregularly at different, sometimes negative, rates; finally, for long times $(t \gg T_r) d_i^2$ is a linear function of *t* (Figs. 9 and 10).

1) **DISPERSION FOR SHORT TIMES**

In our study, we do not resolve the TKE dissipation range, so that the inertial subrange extends to arbitrarily large f, which can be interpreted as an infinite Reynolds



FIG. 9. Evolution of normalized mean squared particle-pair distance d_i^2 initially located at y/h = 1.6, coinciding with downwelling locations (cf. Fig. 1): S (thick black line), L (gray line), and LB (thin solid black line) cases. For d_3 , the dashed line shows the expected value for vertically well-mixed particles. Solutions of d_2 and d_1 converge to the theoretical asymptotic limits for long times (dashed line) and short times (dotted line).

number limit. Therefore, the initial dispersion is isotropic and independent of the initial separation distance of particles (Richardson 1926; Batchelor 1950), and is expected to follow the Richardson–Obukhov law in the inertial subrange (Sawford 2001; Salazar and Collins 2009)

$$d_i^2 = \frac{G}{3}\varepsilon t^3,\tag{24}$$

where G is the nondimensional Richardson constant, which is twice the Lagrangian velocity structure function



FIG. 10. Evolution of normalized mean squared particle-pair distance d_i^2 initially located at four different crosswind locations and at middepth z/h = -0.5 (cf. Fig. 1): S (thick black line), L (gray line), and LB (thin solid black line) cases. For d_3 , the dashed line shows the expected value for vertically well-mixed particles. Solutions of d_2 and d_1 converge to the theoretical asymptotic limits for long times (dashed line) and short times (dotted line).

constant, often referred to as the Kolmogorov constant (Pope 2008). Consistent with the stochastic model (11), we take $G = 2C_0$ [see above for assumptions and discussions in Pope (2008)].

The dispersion law, (24), is overall consistent with our simulations (Figs. 9 and 10). Deviations from (24) are partially due to inhomogeneous turbulence, as in particular ε increases toward the boundaries (Fig. 11). Consistent with (24), the initial dispersion strongly depends on the initial value of $\varepsilon(x, y, z)$ at the particle release locations, which is not only enhanced at the boundaries but also greater in up- and downwelling regions because ε is advected from the boundaries into the interior by Langmuir cells. Relatively small ε are thus found in Langmuir cell vortex centers (cf. with Fig. 11). TKE input by BWs enhance ε by more than one order of magnitude (Fig. 11) and, consequently, controls initial dispersion rates close to the surface, which also increase



FIG. 11. Instantaneous snapshots of normalized ε cross sections where particles have been released initially; see Fig. 1.

by an order of magnitude in the presence of BWs. Furthermore, our results suggests that short-term dispersion rates are locally substantially enhanced under surface convergence regions because downwelling BW TKE is advected to greater depth.

2) DISPERSION FOR INTERMEDIATE TIMES

The inertial subrange regime transitions around $tu_*/h = 0.01-0.1$ to the energy-containing regime for intermediate times before d_i^2 converges to the long time regime at about $tu_*/h = 1-10$. One striking feature of the dispersion at intermediate scales is that d_i^2 increases at varying rates and may even decrease. In particular with LT, this regime is characterized by rapid turbulent transport by larger-scale turbulent structures without necessarily mixing and dispersing particle clouds. For nonisotropic eddies with larger extent in the horizontal than the vertical direction, particle clouds are stretched in the horizontal, so that d_3^2 is relatively small and d_1^2 and d_2^2 are relatively large, whereas clouds are

squeezed in up- and downwelling regions, so that d_3^2 is relatively large and d_1^2 and d_2^2 are relatively small.

The time for particles to move from a squeezing to a stretching region is characterized by the coherent structure time scale T_c from section 3c(4). For example, for coherent transport, a peak in d_3^2 (particles are located mainly in down- or upwelling regions) is expected to follow a local minimum when particles are transported closer to the boundaries after $0.25T_cu_*/h \approx 0.7$, which is consistent with our results (gray lines in Figs. 9 and 10).

Consistent with the previous discussions of T_i and T_r , the details of the transition timing between different regimes depend on the particular wave case and the direction *i*. For example, particles homogenize vertically faster (d_3^2 approaches a constant) without LT, which is anticipated based on our T_r estimates (recall $T_r u_*/h =$ 0.63 and 1.31 without and with LT, respectively). Similarly, the convergence of d_2^2 to the long time regime occurs faster for the S case but d_1^2 converges more slowly than the cases with LT, which is qualitatively consistent with T_1 and T_2 discussed in section 3c(3).

3) DISPERSION FOR LONG TIMES

After long times, the dispersion behavior is governed statistically by the long time limit of single-particle dispersion originally described by Taylor (1922). In the vertical direction, particle distributions simply homogenize and $(d_3/h)^2 = 1/6$ (Figs. 9 and 10), while in the horizontal directions with i = 1, 2, one expects $A_i = (1/4)d(d_i^2)/dt$ (note there is a factor-of-2 difference between single-particle and particle-pair diffusion), so that $d_i^2 = 4A_it$. These predictions agree well with our simulation results (Figs. 9 and 10) and interpretations of these results have been discussed in detail in section 3c(5).

4. Conclusions

Based on a large-eddy simulation (LES) model coupled to a Lagrangian stochastic model (LSM), we have conducted a Lagrangian investigation of wave-driven turbulence in the ocean surface boundary layer (OSBL). Coherent roll vortices due to wave–current interactions, called Langmuir turbulence (LT), are captured by the Craik–Leibovich wave forcing that generates LT through the CL2 mechanism. Breaking surface gravity waves (BWs) are a source of near-surface turbulent kinetic energy (TKE) and are modeled by a surface TKE flux, which is constrained by wind energy input to surface waves. We model particle motions that are not resolved by the LES, that is, subgridscale (SGS) motions, through the LSM, which is by design energetically consistent with the LES SGS model.

Lagrangian autocorrelations of velocities reveal unique differences between shear-driven and Langmuir turbulence. For a case with LT, a turbulent relaxation time scale estimated for vertical velocities is about twice as large as for the case without LT, revealing that Lagrangian time scales cannot be simply scaled by only the traditional parameters of water friction velocity u_* and depth h. In addition, with LT, autocorrelations reveal oscillations because of persistent coherent features, whose period was determined objectively and identified as a coherent structure time scale. The integral of autocorrelations over all time lags determines turbulent diffusion coefficients for times much larger than the relaxation times. We find that LT substantially enhances the crosswind dispersion because of coherent roll vortices. However, LT significantly reduces the alongwind dispersion because LT decreases the vertical shear in the along-wind mean flow. In both cases, horizontal dispersion is strongly anisotropic with greater dispersion in the along-wind than crosswind direction. This anisotropy is enhanced without LT, so that without LT, material



FIG. A1. Horizontal cross section of normalized vertical velocity at middepth (a) without and (b) with LT for the extended horizontal domain. Compare to smaller-domain-size results shown in Fig. 1b.

disperses qualitatively along a line in the wind direction (i.e., elliptical dispersion with much greater major than minor axis), whereas dispersion is more radially symmetric with LT (i.e., minor and major axes of the dispersion ellipse are much closer).

The analysis of Lagrangian frequency velocity spectra reveals pronounced spectral peaks in the presence of LT that are associated with energetic coherent motion and occur at frequencies consistent with the Lagrangian coherent structure time scale. In comparison, spectra are relatively flat at low frequencies without LT. With and without waves, the high-frequency spectral tail is consistent with expectations for the inertial subrange. Furthermore, our results indicate that BWs substantially increase spectral levels at high frequencies.

Consistently, over short times, particle-pair dispersion results agree with the Richardson-Obukhov law for the inertial subrange, and dispersion is significantly enhanced because of BWs near the surface. Dispersion over short time periods is also enhanced close to the surface and bottom boundaries where local TKE dissipation rates are relatively large. With LT, energetic turbulence at the boundaries is advected into the interior by relatively strong down- and upwelling flows due to LT. This increases the dispersion in down- and upwelling regions. On the other hand, in vortex centers TKE dissipation rates are relatively low and the initial dispersion is weakest there. Our results also suggest that short-term dispersion rates with BWs can be locally substantially enhanced under surface convergence regions because high TKE from BW is advected to greater depth. Over longer times, particle-pair dispersion results are consistent with the horizontal turbulent diffusion coefficients obtained from the autocorrelations (Taylor



FIG. A2. Normalized (a),(e) along-wind velocity and (b)–(d),(f)–(h) velocity variance profiles (top) without and (bottom) with Langmuir turbulence. Default study domain size (black) and enlarged domain (gray).

dispersion), confirming the strongly anisotropic dispersion without LT and enhanced dispersion rates in the crosswind direction with LT. Our results suggest that the Lagrangian analysis framework is effective and physically intuitive to characterize OSBL turbulence.

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APPENDIX

Horizontal Domain-Size Sensitivity Experiments

To show that our major findings and conclusions are not sensitive to the particular domain size, we extend the horizontal domain size to $L_x = L_y = 6h = 96$ m, which is identical to the domain size from Kukulka et al. (2011, 2012). The number of grid points is $128 \times 128 \times 100$ in the *x*, *y*, and *z* directions, respectively. Our flow results (Figs. A1 and A2) are very similar to the higherresolution grid with $256 \times 256 \times 100$ grid points from Kukulka et al. (2012). This change in domain size forces a change in Langmuir cell width, so that the extended domain includes two pairs of counterrotating vortices (Fig. A1), rather than the single pair found for the smaller domain (Fig. 1).

In spite of the substantial change in the number of Langmuir cells and cell width, the mean flow and velocity variance profiles still agree very well qualitatively and reasonably well quantitatively (Fig. A2). These results imply that the time scale associated with Langmuir turbulence must be smaller for the extended domain



FIG. A3. Normalized velocity autocorrelation r_i (a)–(c) without and (d)–(f) with Langmuir turbulence. Default study domain size (black) and enlarged domain (gray).

because velocity variances are similar but the Langmuir cell size is smaller. Consistently, normalized autocorrelation functions oscillate faster for the extended-domain case (Fig. A3). Qualitatively, however, r_i for the extended domain captures all physics features discussed in the main text for the smaller domain. This sensitivity study indicates that the details of numeric simulation values depend on the domain size, but that the conclusions and major findings with regard to the principal differences between Langmuir turbulence and shear-driven turbulence are independent of the specific domain size.

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