Baroclinic Frontal Instabilities and Turbulent Mixing in the Surface Boundary Layer, Part II: Forced Simulations

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Abstract

Generation of ocean surface boundary layer turbulence and coherent roll structures is examined in the context of wind-driven and geostrophic shear associated with horizontal density gradients using a large-eddy simulation model. Numerical experiments over a range of surface wind forcing and horizontal density gradient strengths, combined with linear stability analysis, indicate that the dominant instability mechanism supporting coherent roll development in these simulations is a mixed instability combining shear instability of the ageostrophic, wind-driven flow with symmetric instability of the frontal geostrophic shear. Disruption of geostrophic balance by vertical mixing induces an inertially rotating ageostrophic current, not forced directly by the wind, that initially strengthens the stratification, damps the instabilities and reduces vertical mixing, but instability and mixing return when the inertial buoyancy advection reverses. The resulting rolls and instabilities are not aligned with the frontal zone, with an oblique orientation controlled by the Ekman-like instability. Mean turbulence is enhanced when the winds are destabilizing relative to the frontal orientation, but mean Ekman buoyancy advection is found to be relatively unimportant in these simulations. Instead, the mean turbulent kinetic energy balance is dominated by mechanical shear production that is enhanced when the wind-driven shear augments the geostrophic shear, while the resulting vertical mixing nearly eliminates any effective surface buoyancy flux from near-surface, cold-to-warm, Ekman buoyancy advection.
1. **Introduction**

Mixing in the surface ocean boundary layer is typically produced by a combination of processes related to surface fluxes and the interaction of surface waves with upper ocean currents (Phillips, 1966). In addition to surface-forced turbulent mixing in the ocean, differential buoyancy advection by wind-forced Ekman transport at surface fronts has been recognized as a potential source of mechanically-driven convection in both the coastal (e.g., Foo, 1981; Samelson and de Szoeke, 1988) and open-ocean environments (e.g., Samelson and Paulson, 1988; Thomas and Lee, 2005). Ekman velocities are concentrated at the surface and directed to the right of the wind in the northern hemisphere. If winds are aligned with a front such that denser water is to the left of the wind direction, then (in the northern hemisphere) Ekman current shear will be destabilizing, as it will transport denser water over less dense water, toward a convectively unstable state. The resulting wind-driven advective buoyancy flux divergence is sometimes characterized as an effective surface, or “Ekman,” buoyancy flux (“EBF”; Thomas and Lee, 2005; Thomas and Taylor, 2010); for strong fronts and destabilizing winds, the effective surface cooling fluxes would, in principle, be sufficient to cause vigorous convective mixing.

Surface fronts are also prone to baroclinic instability and the formation of submesoscale features that stir the ocean as frontal zones restratify (e.g., Samelson and Chapman, 1995, Capet, et al., 2008). In Part I of this study (Skyllingstad and Samelson, 2012), the evolution of a small-scale baroclinic instability in the surface boundary layer was studied in the absence of surface forcing. The baroclinic development caused frontogenesis and a transition to turbulence through Kelvin-Helmholtz instability at the intensified front (Skyllingstad and Samelson, 2012; Samelson and Skyllingstad, 2016). The original intent of the present study was to revisit this development...
in the presence of wind forcing, and this is the initial case analyzed below. It is found that when the wind was aligned along the frontal axis, so that the steady wind-driven Ekman transport would be directed across the front, the baroclinic development was strongly affected by the wind-driven turbulent and mean advective responses. In addition, coherent roll structures with horizontal scales 3-5 times the mixed layer depth form within the turbulent surface layer when the Ekman transport is directed toward the warm side of the front.

Evidence of similar coherent structures in the ocean boundary layer has been previously reported, for example, by Sundermeyer et al. (2015) from observations of dye releases in a mixed layer front along with related LES modeling experiments. Strong frontal mixing events along the Gulf Stream and Kuroshio fronts have recently been interpreted in terms of coherent roll instabilities within the boundary layer that are promoted by Ekman buoyancy transport that reduces stratification and potential vorticity (D’Asaro et al., 2011; Thomas et al. 2013; Thomas et al. 2016). Several recent modeling studies have argued for the importance of symmetric instability (Eliassen and Kleinschmidt, 1957) when surface wind forcing affects the frontal dynamics. Taylor and Ferrari (2010) and Thomas and Taylor (2010) addressed this problem using a large-eddy simulation (LES) model for a growing boundary layer and found instances of disturbance growth consistent with symmetric instability of the geostrophic flow. Simulations by Thomas et al. (2016) for a strong storm system acting on the Gulf Stream front suggest that forced symmetric instabilities can drive strong mixing. Hamlington et al. (2014) examined the interaction of Langmuir cells with frontal spin-down, suggesting instead that Langmuir turbulence greatly enhances mixing at surface fronts. Wind forcing in their experiments was relatively weak (e.g. wind stress of 0.025 N m⁻², equivalent to wind speeds of ~ 4 m s⁻¹), but was still strong enough for Langmuir instability to dominate over symmetric instability in some
cases. However, field observations of coherent boundary layer structures are very sparse, and the role that symmetric and other instabilities may have in mixing at fronts when surface fluxes are large is not well understood.

We address this frontal turbulence problem through a modeling study spanning a range of surface forcing and frontal strengths. We employ a high-resolution large-eddy simulation model with a constant background horizontal density gradient. Our experiments assume an existing mixed surface boundary layer and apply moderate to strong wind and wave forcing with relatively short spin up periods, to represent the onset of storm conditions. In previous, similar LES experiments, Taylor and Ferrari (2010) examined the slow boundary layer growth for a weakly wind forced front, focusing on the growth of symmetric instability with generally small buoyancy flux boundary conditions, while Thomas and Taylor (2010), Thomas et al. (2013) and Thomas et al. (2016) examined cases with more vigorous wind forcing, but only for a limited set of cases or with forcing conditions based on observations. We expand on these previous experiments by considering a wider range of forcing conditions, and by using a domain with a larger along-front extent that allows more complete development of three-dimensional disturbance structure. Most of the simulations and analysis focus on the turbulent response and the coherent roll structures, but we also consider the time-mean turbulent dynamics and its dependence on the strengths and relative alignment of the frontal gradients, the associated geostrophic shear, and the wind forcing.

2. Model description and Experimental design

a) LES formulation and configuration

Experiments are conducted using a three-dimensional large-eddy simulation (LES) model based on the Deardorff (1980) equation set with subgrid scale turbulence parameterization from
Ducros et al. (1996). The model configuration is similar to that described in Skyllingstad et al. (2000) and Skyllingstad and Samelson (2012). Two configurations are discussed, the first essentially identical to that of the warm-filament simulations of Skyllingstad and Samelson (2012), but with along-front wind forcing, and the second with an imposed uniform horizontal temperature gradient, to focus on the local response within the frontal zones.

b) Warm-filament simulation

The warm-filament simulation used the initial temperature distribution described in Skyllingstad and Samelson (2012), with a temperature anomaly of 0.08 °C relative to the ambient fluid, in a filament with depth of 80 m, zonal width of order 5 km, a north-south extent that was effectively infinite in the doubly-periodic domain, and frontal zones of order 1200 m width on each side of the filament. A northerly (southward) wind stress was applied, which under steady conditions would drive warm-to-cold (stabilizing) Ekman transport across the western front, and cold-to-warm (destabilizing) Ekman transport across the eastern front. The wind stress increased linearly from zero to the fixed prescribed value over the first 12 simulation hours with a constant value through the end of the simulation at hour 60.

c) Frontal-zone simulations

The frontal-zone simulations have instead a uniform, imposed, horizontal temperature gradient, $\Gamma = \frac{\partial T}{\partial x} < 0$, and an initial geostrophic current, $V_G$, that is in thermal-wind balance with the thermal gradient, so that

$$\frac{\partial V_G}{\partial z} = \frac{g \alpha}{f} \Gamma < 0,$$

(1)
where $f = 1 \times 10^{-4}$ s$^{-1}$ is the Coriolis parameter, $g = 9.81$ m s$^{-2}$ is gravitational acceleration, and $\alpha = 2 \times 10^{-4}$ is the approximate expansion coefficient for sea water. The corresponding horizontal buoyancy gradient is denoted

$$M^2 = \frac{\partial b}{\partial x} = g\alpha \frac{\partial T}{\partial x} < 0.$$  

These simulations were initialized with this geostrophically balanced, westward thermal gradient superimposed on a surface mixed-layer thermal structure that varies only in the vertical (Figure 1). The domain size was 2,560 m in both $x$ and $y$, and 150 m in the vertical with grid spacing of 2.5 m in all directions and periodic lateral boundaries. Rigid upper and lower boundary conditions were applied with a Rayleigh damping “sponge” layer over the bottom 12 levels.

For the frontal-zone simulations, we explored a range of temperature gradients and wind forcing. Experiment names (Table 1) indicate, in order, the frontal strength (SF, MF, WF, NF, denoting Strong, Medium, Weak, and No Front) and the wind direction (N, S, E, W, with the meteorological convention) and strength (S, M, W). With winds from the north (cases xxNx), the classical steady Ekman transport would tend to advect cold water from the east over warm, leading to static instability or mechanically forced convection, or to related instabilities. An additional simulation is considered with weak surface cooling and no wind forcing (case SFC20). The frontal-zone simulations each covered 36-hour periods, with wind forcing increasing linearly from zero to the fixed prescribed value over the first 12 simulation hours.

For the northerly wind cases, the eastward Ekman transport from the cold (dense) side of the thermal gradient toward the warm (less dense) side causes a destabilizing horizontal buoyancy flux divergence proportional to the meridional wind stress $\tau^y$ and the horizontal buoyancy gradient $M^2$. 
\[ EBF = -\frac{\tau^y M^2}{\rho_o f} = -\frac{\tau^y}{\rho_o f} g \alpha \frac{\partial T}{\partial x} < 0 \] (2a)

where \( \rho_o \) is the mean density, and the depth-independence of \( M^2 \) has been used to compute the vertical integral (Thomas and Taylor 2010). It has been argued that if this “Ekman buoyancy flux” divergence \( EBF \) is confined close to the surface, then \( EBF \times (\rho_o C_p / g \alpha) \) may be interpreted locally as an effective surface buoyancy flux (e.g., Thomas and Lee 2005). For the medium wind (xxNM) cases here, this effective surface flux would be -400 W m\(^{-2}\). Southerly winds, \( \tau^y < 0 \), will instead generate a stabilizing effective surface flux, \( EBF > 0 \), that promotes restratification of the ocean boundary layer.

An alternative physical interpretation of the role of the wind forcing in frontal zones is, however, also possible. While the \( EBF \) may, for destabilizing winds, contribute to TKE generation through mechanically forced convection, the presence of geostrophic shear that is aligned with the wind-driven shear can also be anticipated to augment the wind-driven TKE generation that occurs through mechanical shear production, in which wind-driven turbulent velocity fluctuations act on the mean vertical shear. With turbulent velocity fluctuations scaled by the friction velocity, \( u_* \), and mean shear scaled by the geostrophic shear, this wind-driven geostrophic shear production is

\[ SP_{geo} = -u_*^2 \frac{\partial V_g}{\partial z}. \] (2b)

This enhancement of the mechanical shear production would potentially occur for the same destabilizing alignment of wind and frontal gradient as an effective \( EBF \) cooling. Moreover, because of the thermal wind relation and the definition \( u_* = (|\tau^y| / \rho_o)^{1/2} \), the values of \( EBF \) in (2a) and \( SP_{geo} \) in (2b) are identically equal, despite their different physical meanings. [A reviewer has commented that it is this mechanical-shear mechanism that provides the source for
TKE generation in previous studies of symmetric instability at wind-forced fronts that have been interpreted in terms of the effect of EBF on the potential vorticity field. Examination of the turbulent kinetic energy generation process is therefore necessary to distinguish these two mechanisms.

d) TKE budget

Turbulent processes in the boundary layer can be analyzed using the turbulent kinetic energy (TKE) budget equation,

\[
\frac{\partial \text{TKE}}{\partial t} = \alpha g \frac{\partial \text{TKE}}{\partial z} - u_i'w' \frac{\partial V_i}{\partial z} - \frac{\partial}{\partial z} \left( \frac{\partial}{\partial z} \right) \left( \frac{w'TKE}{\rho} - K_m \frac{\partial \text{TKE}}{\partial z} \right) - \varepsilon
\]  

where \(i = 1, 2\) denotes the \(x\) and \(y\) directions, respectively, \(u_i\) are the horizontal velocity components, \(w\) is the vertical velocity, \(V_i^a\) and \(V_i^g\) are the horizontally averaged ageostrophic and geostrophic velocity components, \(K_m\) is the subgrid scale eddy viscosity, the overbar represents horizontal averaging, primes indicate deviations from the mean, and

\[\text{TKE} = \left( u_1'^2 + u_2'^2 + w'^2 \right)/2.\]

Terms in (3) are defined in order as the storage of TKE, buoyancy production, ageostrophic shear production, geostrophic shear production, vertical transport, and dissipation. The ageostrophic velocity in the ageostrophic shear production term is defined as the departure of the velocity from the balanced geostrophic velocity, and includes any wind-driven and near-inertial shear. For the simulations described here, \(V_2^g = V_g\) from (1), and \(V_1^g = 0\), with \(V_2^g = 0\) at a depth of 70 m.

e) Linear instability analysis
Linear instability calculations were carried out for several different basic-state profiles, using standard matrix eigenvalue methods to solve discretized representations of linearized versions of the same equations on which the LES model is based, with the exception that the flow-dependent vertical viscosity and diffusivity in the LES model were replaced in the linear disturbance equations by isotropic three-dimensional Laplacian diffusion operators with constant viscosity and diffusivity. The disturbances were assumed, in the standard way, to have plane-wave (single Fourier component) structure in the horizontal and complex exponential time-dependence. A standard finite-difference representation of the resulting set of ordinary differential equations in the vertical coordinate $z$ then yielded the matrix eigenvalue problem to be solved, with the complex frequency as eigenvalue. The boundary conditions imposed on the disturbances were homogeneous in the vertical velocity and temperature, and in the vertical derivatives of horizontal velocity and pressure. Additional details regarding the formulation and numerical methods are provided by Duncombe (2017) and Samelson and Skyllingstad (2017). The basic-state profiles are described below with the corresponding stability results.

3. **Warm filament**

The warm-filament results are summarized here mainly as motivation for the constant-gradient frontal zone experiments that comprise the bulk of this investigation. A similar simulation, with weaker wind forcing, is presented by Hamlington et al. (2014). The evolution of the warm filament simulation with northerly wind forcing is fundamentally different than that of the unforced warm filament considered by Skyllingstad and Samelson (2012). The strength and rapid development of both vertical and lateral mixing generated by the wind-forced processes prevents the formation of the baroclinic waves and eddies that dominated the unforced evolution (Figure 2). Significant baroclinic eddy transport and turbulence mixing takes roughly 3.5 days to
develop in the unforced case, whereas disturbance growth in wind-forced case requires only 1 day to generate significant turbulent mixing. This mixing in the wind-forced case is sufficiently strong to change completely the filament dynamics, as the coherent baroclinic eddy structure is damped and replaced by a more chaotic, smaller-scale development after 3 days (Fig. 2c). The domain-averaged TKE dissipation terms are about 2 orders of magnitude greater for the forced case than for the collapsed, unforced baroclinic fronts in Part I (Skyllingstad and Samelson, 2012, their Fig. 12). Thus, in the presence of wind forcing, the wind-forced turbulence and Ekman transport of the background front completely dominates the boundary layer development, while the weak, downscale transfer of energy from the baroclinic waves through frontal collapse and K-H transition to turbulence can only be detected in the model in the absence of wind forcing (Skyllingstad and Samelson, 2012).

In the forced warm-filament simulation, the structures of the turbulent responses in the two frontal zones also differ fundamentally. At the western front, the northerly wind is stabilizing, as the wind-driven currents strengthen the stratification, oppose the geostrophic shear, and damp the turbulence, leading to a diffuse, uniform frontal gradient. At the eastern front, the northerly wind is destabilizing, as the wind-driven currents weaken the stratification, augment the geostrophic shear, and induce a strong turbulent response. Of particular interest is the characteristic banded structure at the eastern front (Figure 2b). These structures can be neither Langmuir circulations, because no wave or vortex forcing is present in these simulations, nor can they be pure symmetric instabilities, because they are oriented at an angle away from the frontal axis. Additional northerly-wind-forced warm-filament simulations with different wind magnitudes indicated that these structures are formed robustly at the eastern front. The constant horizontal gradient, frontal-zone simulations described in the next section were designed specifically to
explore and address the dynamics of the coherent roll structures of which these bands are the surface manifestation.

4. Frontal zones: strong front, destabilizing winds

a) SFNM simulation

In the warm filament simulation, obliquely-aligned coherent roll structures developed on the eastern front, where the northerly winds were destabilizing (Figs. 2b, c). The SFNM frontal-zone case, with moderate northerly winds over a strong, uniform, westward thermal gradient, was one of 8 cases designed to reproduce this behavior, and indeed develops similar, obliquely aligned, coherent roll structures after a similar integration period. These roll structures are visible, for example, in the surface meridional velocity at simulation hour 17 (Fig. 3b). Before proceeding with analysis of their structure and dynamics, it is useful to summarize the overall evolution of the SFNM simulation fields.

The horizontal domain average of the meridional (alongfront) velocity $v$ remains relatively constant through the first 5 hours of the SFNM simulation, but is then rapidly homogenized vertically by an energetic turbulent mixing event around hour 6, which extends from the surface to the boundary-layer base at 80 m depth (Figs. 4a, b). This transient mixing event ends by hour 8, and the initial $v$ profile is approximately re-established by hour 12. Mixing during the first event primarily affects momentum, as temperature is initially uniform in the vertical. A second energetic vertical mixing event occurs around hour 18, followed again by re-establishment of the meridional vertical shear, and then by a third mixing event around hour 30. This sequence of mixing events can be understood to arise from a combination of instability of the initial geostrophic flow, inertial response to instability-induced mixing, and wind-forcing. The combination of these factors results in a recurrence time of the mixing events that, at roughly 12
hours between events, is 5 hours shorter than the inertial period $2\pi/f = 17.4$ hr. A brief summary of the dynamics of the sequence is given here; a detailed analysis of the near-inertial dynamics will be provided elsewhere (Skyllingstad and Samelson, 2017).

Linear stability analysis of the initial geostrophic flow (Fig. 1), which is a steady solution of the model equations in the absence of wind forcing and viscous-diffusive effects, shows that this flow is unstable to two sets of modes: symmetric instabilities with wavelengths of order 100-300 m and growth rates of order 0.5-1.0 hr, and baroclinic instabilities with much longer wavelengths and slower growth rates (Duncombe, 2017; see also Fig. 7 below). The hour-6 mixing event primarily reflects the growth of the symmetric instabilities of the initial geostrophic flow, from small, random perturbations to finite-amplitude symmetric roll structures that extend through the full depth of the boundary layer at hour 6 (Fig. 3a, Fig. 4b). When they reach finite amplitude near hour 6, these coherent structures efficiently transport meridional momentum vertically, erasing the geostrophic vertical shear and disrupting the geostrophic balance. This is shown by plotting the boxed terms from the momentum budget (Fig. 4c,d),

$$\frac{\partial \Pi}{\partial t} = f(u_{geo} - v) - \frac{\partial (u\omega)}{\partial z} - \frac{\partial (u\omega)_sg}{\partial z}$$

$$\frac{\partial \sigma}{\partial t} = -f(u_{geo} - u) - \frac{\partial (v\omega)}{\partial z} - \frac{\partial (v\omega)_sg}{\partial z}$$

where the first term on the right-hand side of each equation represents the balance between the horizontal pressure gradient and the Coriolis term, and the second and third terms are the resolved and subgrid scale vertical momentum transports (here $u_{geo} = 0.0$). The wind forcing, which is increasing with time but still weak, plays only a small role in the momentum balance during this period. The TKE budget at hour 6 shows dominant production from the geostrophic shear, consistent with symmetric instability dynamics (Figs. 5d, 6ac).
The zero-vertical-shear state induced by the hour-6 mixing event can be understood as the superposition of the initial, negative geostrophic shear and an opposite, positive ageostrophic shear. The subsequent inertial rotation of the positive ageostrophic meridional shear component causes positive vertical shear of the zonal velocity, advecting warm water eastward over cold, which stabilizes the boundary layer and shuts down the instability, rapidly damping out the rolls and the vertical mixing. The rapid decline of the large pulse of geostrophic-shear TKE generation after hour 6 is followed by steady growth of wind-driven, ageostrophic-shear TKE generation (Fig. 5d). The continued rotation of the ageostrophic flow, which eventually reverses its effect on the stratification, coupled with the growing influence of the wind, results in the onset of the second mixing event around hour 18 (Figs. 4a, b, 6bd).

It is the coherent rolls driving this second mixing event (Fig. 3b), which arise under the combined influence of the wind forcing and the geostrophic shear, that are of primary interest here. These well-defined circulations develop with separation length of ~300-500 m, somewhat larger than the symmetric-instability rolls that form around hour 6 (Fig. 3a), before the wind influence is significant. Moreover, the band axis of these larger-scale rolls is oriented 20-25 degrees clockwise from the wind stress and the frontal symmetry axis. Because of their lack of along-front symmetry, these roll structures cannot be understood to arise simply from symmetric instability of the geostrophic flow field. Decomposing the shear production into the \( u \) and \( v \) components,

\[
-\overline{v'w'} \frac{\partial \overline{\sigma}}{\partial z} \text{ and } -\overline{u'w'} \frac{\partial \overline{\sigma}}{\partial z}
\]

where \( \overline{u} \) and \( \overline{v} \) represent the horizontally averaged velocity, provides further evidence that these coherent structures arise in part from instability of the ageostrophic shear (Figs. 6bd): there is significant shear production, peaking near the bottom of the boundary layer at 60 m, from the
purely ageostrophic zonal flow. Dynamical explanations for the coherent roll structures that develop at around hour 16 in case SFNM are sought here in linear instability theory and in more qualitative, parcel-based analysis of instability dynamics, both of which include and address the roles of the wind-driven and other ageostrophic components of the flow field.

b) Dynamics of coherent roll structures – stability analysis

The linear instability approach takes the perspective that the hour-16 SFNM roll features may be understood as quasi-equilibrated, nonlinear states that develop from the underlying mean flow as spontaneously growing disturbance modes, initially excited by random, small-amplitude fluctuations. Following this approach, linear instability calculations were conducted for a variety of different mean-flow states, from the combination of which a physical interpretation of the source of the roll structures can be extracted. Two main results follow from these linear instability calculations. First, the SFNM hour-16 state supports growing linear disturbance modes that correspond closely in structure and alignment to the coherent roll structures identified in the SFNM simulation. This is consistent with the general interpretation that the roll structures arise spontaneously as instabilities of the mean SFNM circulation. Second, the instability of the SFNM hour-16 state is seen to be best understood as a mixed instability, to which both symmetric and Ekman-layer instability dynamics contribute.

The first mean-flow state considered was constructed by horizontally averaging the SFNM temperature, lateral temperature gradient, and horizontal vector velocity fields at simulation hour 16, yielding vertical profiles of these quantities (Fig. 1). The linear instability calculation using this hour-16 profile implicitly makes a “frozen-field” approximation, in which the timescale for growth of the resulting linear instabilities is assumed to be sufficiently short that the mean-flow
profile can be considered approximately in steady state. The second mean-flow state retains only
the geostrophic component of the hour-16 velocity profile, along with the hour-16 mean
temperature profile and the constant mean lateral temperature gradient; except for small changes
in the stratification, this basic state is the same as the initial geostrophic basic state (Fig. 1), for
which the linear instability characteristics were summarized above. A third mean-flow state was
specified as a classical Ekman profile in a neutrally stratified fluid, with no lateral gradients and
constant eddy viscosity. A family of additional basic states for the stability analysis were
constructed by linearly interpolating between the hour-16 SFNM state and either the second or
the third states. The linear instability modes are obtained as a function of wavelength $\lambda$ and
orientation angle $\phi$, where $\phi = 0$ corresponds to a zonal wavenumber vector, with meridional
band (symmetry) axis parallel to the frontal-symmetry and wind-direction axis.

At wavelengths $\lambda \approx 300$ m, the SFNM hour-16 state is linearly unstable to a range of
growing modes, the most rapidly growing of which have symmetry axis aligned roughly $20^\circ$
clockwise from the surface geostrophic flow (Fig. 7). This orientation coincides with that of the
SFNM coherent roll structures (e.g., Fig. 3b). The growth rates of these linear modes are of order
$1.6 f$, corresponding to an $e$-folding time scale of roughly 1.5 hours, sufficiently short relative to
the overall flow evolution (timescales of 6-12 hr, excluding the instability-driven mixing events
themselves; Fig. 4a) to support at least a qualitative interpretation based on the frozen-field
approximation. The SFNM hour-16 state also supports an Eady-type baroclinic instability (Fig.
7), which may explain some of the along-axis distortions of the LES rolls (e.g., Fig. 3b), but
these modes are only the most rapidly growing at longer wavelengths, and their influence is
limited in the LES model by the relatively small (2560 m) domain size. The growth rates of the
roll instability modes – especially their high wavenumber extent – are affected by the value of
the specified constant eddy viscosity and diffusivity; the relatively small value 0.005 m² s⁻¹ (e.g., Fig. 7) gives a particular clear illustration of the intrinsic characteristics of the underlying instabilities.

It can be further discerned that the growing modes near 20° clockwise orientation resolve into two distinct neighboring growth-rate maxima between wavelengths 50 m and 400 m, with symmetry axes aligned, respectively, 16° and 24° clockwise from the surface geostrophic flow (Fig. 7). The associated mode structures at 300-m wavelength are generally similar, with both dominated by a baroclinic mode-1 structure with phase lines slanting upward toward the east, but the 16° mode has a stronger surface signature than the 24° mode (Fig. 8). At mid-depth, both modes show motion that is downward, toward the warm side (westward), and in the direction of surface geostrophic flow (southward) at one phase extreme, and upward, toward the cold side (eastward), and against the surface geostrophic flow (northward) at the opposite phase extreme. The 16° and 24° modes become more distinct toward shorter wavelength, with the 16° mode becoming more surface trapped.

The 25° clockwise orientation of the SFNM roll structures and the similar orientation of hour-16 linear modes, relative to the geostrophic flow direction, suggests that the underlying instability cannot be understood as a pure symmetric instability, for which the axis of the symmetry of the growing disturbance and the geostrophic flow would be aligned. The apparent presence of two distinct sets of growing roll instability modes, with similar growth rates, is consistent with this suggestion. In order to gain insight into the mechanisms supporting these modes and the evidently related SFNM roll structures, the linear instability calculation was repeated for the two additional, idealized profiles, both of which support sets of growing modes with e-folding timescales similar to those in the hour-16 profile.
The linear instability calculation for the modified, pure-geostrophic SFNM hour-16 profile, with ageostrophic velocities removed, reproduces the classical small-scale symmetric instability of the geostrophic frontal shear (Fig. 7). At larger scales, the pure geostrophic flow state, like the full hour-16 state, also supports Eady-type baroclinic instability modes. When the linear instability calculation is repeated for a sequence of basic states that linearly interpolate between the modified, pure-geostrophic state and the full SFNM hour-16 state, the symmetric instability modes are found to transform continuously into the hour-16 growing modes near 20° clockwise orientation. Thus, the addition of the ageostrophic shear modifies the roll instability, and causes the rotation of the disturbance axis of symmetry away from the geostrophic flow direction.

To understand this roll orientation, it is useful to consider the third profile, the classical neutral Ekman spiral, and its instabilities. For this calculation, the Ekman-spiral surface velocity was set equal to three times the SFNM hour-16 mean ageostrophic surface velocity, with Ekman depth $\delta_E = (2 \times 0.005 \text{ m}^2 \text{s}^{-1}/f)^{1/2} = 10 \text{ m}$. The resulting linear instability of the Ekman spiral manifests as roll disturbances with symmetry axes rotated 30°–50° clockwise from the geostrophic flow direction, approximately twice the rotation angle for the SFNM roll structures (Fig. 7). The tendency of the Ekman-spiral instability is thus to produce roll structures that are rotated away from the geostrophic flow in the same sense as the SFNM roll structures, suggesting that the SFNM roll structures are partly supported by an instability of the ageostrophic velocity shear that is analogous to the instability of the Ekman spiral. When this linear instability calculation is repeated for a sequence of basic states that interpolate between the neutral Ekman-spiral state and the full SFNM hour-16 state, the Ekman instability mode is also found to transform continuously into the hour-16 growing modes near 20° clockwise orientation. Thus, the addition of the geostrophic shear modifies the Ekman instability, and causes the
rotation of the disturbance axis of symmetry toward from the geostrophic flow direction. Note that the Ekman-spiral ageostrophic flow differs substantially from the SFNM hour-16 ageostrophic flow, with the former being surface-trapped, and the latter stronger at mid-depth. The mode structure transforms through the interpolated sequence to match the changing shear depth, so that the hour-16 growing modes (Fig. 8) are less surface trapped than the neutral Ekman-spiral instability.

The hour-16 structures are therefore best understood as the result of a mixed instability, in which two distinct dynamical mechanisms – Ekman-spiral and symmetric instabilities – jointly support the growth of the disturbance. In this context, it is important to recall that the instability of the Ekman spiral can be understood in terms of the inflection-point instabilities of the velocity profile normal to the mode axis of symmetry (Barcilon 1964, 1965). This is essentially different than the symmetric instability, in which the mean-flow velocity is aligned along the mode axis of symmetry, and vanishes normal to that axis. The two instability mechanisms contributing to the hour-16 linear disturbance growth are thus explicitly distinct. The hour-16 ageostrophic velocity profile is not a classical Ekman spiral, and contains a large, deep shear component, but the continuity of the respective interpolated-state results indicates that the instability of the full hour-16 profile is partly supported by dynamics that are essentially similar to those of the Ekman-spiral instability. The vertical structure of the SFNM TKE (Fig. 4b) is consistent with these two modes, showing a maximum in the middle of the boundary layer at hour ~6 corresponding to the symmetric mode and a maximum near the surface at hour ~18 corresponding to the Ekman mode. The energy-production balance computed from the linear-instability modes also shows this mixed character: while the kinetic energy source for the Ekman-spiral instability is entirely the ageostrophic shear, and that for the symmetric instability of the pure geostrophic profile is
entirely the geostrophic shear, the SFNM hour-16 modes at 300-m wavelength derive roughly one-quarter of their energy from the ageostrophic shear.

c) Dynamics of coherent roll structures – parcel theory

Analysis of the vertical structure of the coherent rolls indicates that the horizontal orientation of the roll circulations does not vary significantly with depth during the strong mixing event at hour 17. In addition, the vertical temperature structure is nearly uniform, with only weak vertical gradients in isolated regions (Fig. 9a). Symmetric instability (“slantwise convection”) is often described in terms of a parcel theory combining vertical static stability with horizontal inertial stability (Emanuel 1994, Haines and Marshall 1998). In general, for two-dimensional flow, if surfaces of absolute momentum, defined here as $M_{abs} = f x + v$, have a shallower slope than potential temperature surfaces, then the flow is potentially unstable to symmetric instability. Perturbed parcels that are unstable will accelerate toward their respective $M_{abs}$ and potential temperature surfaces and away from their original location. An unstable configuration is indicated at hour 17 of the SFNM simulation (Fig. 9b), with steep isentropic surfaces that are consistent with the nearly vertical circulations shown in the top panel. By hour 24 (Fig. 9c), surfaces of $M_{abs}$ and potential temperature are very nearly aligned below 30 m depth, indicating near-neutral rather than symmetrically unstable conditions, consistent with weaker roll circulations and lower TKE during this period. This parcel analysis is strictly valid only for two-dimensional flow, where there are no along front variations. Nevertheless, the orientations of the $M_{abs}$ and potential temperature surfaces are consistent with a symmetric-instability contribution to roll generation.
Further insight on the possible role of symmetric instability is provided by the average potential vorticity,

\[ q = (f \hat{k} + \omega) \cdot \nabla b \]  

(5)

and Richardson number defined as

\[ Ri = \frac{N^2}{(\partial v/\partial z)^2}, \]  

(6)

where \( \omega = \nabla \times v \) is the relative vorticity, \( \hat{k} \) is a vertical unit vector, \( N^2 = -\frac{g}{\rho_0} \frac{d\rho}{dz} \) and \( v \) is the three-dimensional velocity. Potential vorticity was calculated every model time step and averaged horizontally and over a 30 second time period. Disturbance growth dominated by symmetric instability generally occurs only for average \( q < 0 \) and \( Ri \) between 0.25 and 1.0 (or 0.95) over a sufficient period of time to allow instability growth (e.g., Stone 1966; Arobone and Sarkar, 2015), with smaller \( Ri \) perhaps relevant for exactly linear geostrophic shear (Vanneste 1993). For Case SFNM, the initial value of the potential vorticity in the boundary layer for this case is equal to the geostrophic value,

\[ q_{geo} = f N^2 - \frac{M^4}{f} = -\frac{M^4}{f} = -3.85 \times 10^{-10} \text{ s}^{-3}, \]

because \( N = 0 \) in the boundary layer. For almost all of the simulation, the mean value of \( q \) is negative in the upper water column above \( \sim 50 \) m (Fig. 10). However, \( Ri < 0.25 \) over most of the water depth at hours 14-18, indicating near neutrally stratified conditions that are susceptible to shear instabilities whenever there is curvature in the shear profile.

Strong mixing shown in figure 3-4 at hour 14-18 could result from either buoyancy forcing, shear instability, symmetric instability, or through the mixed instability discussed above. The mixed layer scaling of Taylor and Ferrari (2010) may be used to estimate the relative importance
of surface buoyancy forcing by comparing a convective layer depth, \( h \) and the depth of the low PV layer, \( H \). This scaling results in the balance

\[
\frac{M^4}{f^2} (B_o + B_{wind})^{1/3} h^{4/3} = c (B_o + B_{wind}) \left( 1 - \frac{h}{H} \right)
\]  

where \( B_o \) is imposed surface buoyancy flux, \( B_{wind} \) is either \( EBF \) or the integrated inertial buoyancy flux, \( B_{int} \), defined below in our analysis, and \( c \approx 14 \) is a constant. Equation (7) neglects terms associated with entrainment at the boundary layer base that were originally considered in Taylor and Ferrari (2010), and we note that they only considered \( B_{wind} = EBF \). The terms in (7) may be estimated by \( B_o = 0 \) and

\[
B_{int} = \overline{u \frac{\partial b}{\partial x}} dz
\]

where the overbar represents averaging in the horizontal and through the boundary layer depth and the full zonal velocity is used. The derivation of (7) assumes that the boundary layer buoyancy fluxes are nearly in steady state, which is clearly not the case in this experiment with rotating currents, hence our use of the integrated advective buoyancy. Nevertheless, the estimate \( h \) obtained from (7) shows that convective forcing from the wind driven buoyancy flux is dominant only in the upper 25 m of the boundary layer, and only when the inertially rotating ageostrophic current reverses to remove its stabilizing effect (Figure 11). Interestingly, the maximum depth of the oscillating convective depth is roughly equal to the steady-state solution obtained from (7) using \( EBF \) in place of \( B_{wind} \). Both estimates indicate that shear production is the dominant source of turbulence over the lower portion of the mixed layer.
5. Frontal zone – additional cases

a) Strong or vanishing destabilizing winds

Additional insight can be gained by comparing SFNM to two other northerly wind cases: SFNS, with the same frontal gradient as SFNM but stronger destabilizing winds, and NFNM, with no frontal gradient but the same northerly wind forcing as SFNM. Similar coherent structures (not shown) are produced in case SFNS, but with stronger velocity variations in response to the larger wind stress. Circulations in case NFNM (no horizontal temperature gradient) are also oriented to the right of the wind (Fig. 12), but have a reduced separation of about 100 m and weaker intensity. These circulations in case NFNM, unlike those for SFNM, do not evolve significantly after the initial 16 hours, and presumably result from Ekman-spiral instabilities.

Both of these cases show a weaker near-inertial signal than SFNM. Horizontally averaged conditions for case NFNM show a much weaker inertial response with nearly uniform currents and TKE after the initial 12-hour wind spin-up (Fig. 13a). The maximum strength of mixing for NFNM, as suggested by horizontally averaged TKE, is roughly half the value achieved for SFNM, and the NFNM boundary layer temperature remains relatively constant, in contrast to a significant mean cooling for SFNM. The NFNM results are similar to non-resonant wind forced simulations presented in Skyllingstad et al (2000). A consistent inertial response is also absent when the wind stress is increased in case SFNS (Figure 13b), as the inertial restratification is not sufficient to prevent strong turbulence. Instead, the boundary layer takes on a more classically turbulent structure with essentially random pulses of TKE and mixing. The maximum TKE values in this case are about 3 times stronger than in case SFNM, mostly due to the increased momentum flux.
b) Stabilizing winds

For southerly winds, we expect a reduction in turbulence because the vertical flux of momentum reduces the total shear and the Ekman buoyancy transport $EBF$ acts to restratify the upper boundary layer. Mixing in Case SFSM is indeed much weaker than any of the destabilizing wind examples, with TKE about 10 times smaller in comparison with case SFNM (Fig. 14). The boundary layer is stratified throughout the simulation with only small variations in response to the induced inertial current. With the absence of additional ageostrophic shear from wind forcing, the mixing-induced near-inertial response results in a recurrence interval between the first and second mixing events that is nearly equal to the 17-hr inertial period (Fig. 14).

Interestingly, this case presents conditions that are conducive to the formation of symmetric instability near the bottom of the boundary layer, namely, in a region with geostrophic shear and reduced stratification between 30 and 80 m depth. In this region, $q$ is negative and $Ri$ is between 0.25 and 1.0 (Figure 15). Decoupling of this symmetric instability layer from the surface, controlled by the higher $Ri$ between 20 and 30 m depth, allows these deeper instabilities to grow without disruption from surface forced turbulence. The meridional velocity $v$ at 50 m depth from hour 22 shows coherent structures that are aligned with the geostrophic shear, consistent with traditional symmetric instability (Fig. 16).

c) Surface cooling, no winds

When the wind forcing is removed entirely and replaced with a weak surface cooling, in case SFC20, the resulting TKE is about an order of magnitude weaker than for SFNM, which had moderate wind stress and no cooling (Figs. 17, 4a). Horizontally averaged profiles for
SFC20, which has no wind forcing, show a significant near-inertial response that is again generated by vertical mixing of the geostrophic momentum (Figs. 17, 4a). Shear instability, triggered by surface cooling, drives the vertical momentum flux that initially disrupts the geostrophic balance and induces the inertial response. Temperature advection by the inertial current again modulates the boundary layer stratification, damping the instabilities as it restratifies the boundary layer. The much weaker second pulse of turbulence at hour 24 occurs with the boundary layer having $Ri$ between 0.25 and 1.0, and roll structures develop that are aligned with the temperature gradient, consistent with symmetric instability (Fig. 18). Parcel analysis at hours 19 and 22 for this case also indicates conditions that are unstable to symmetric instability, with $M_{abs}$ surfaces less steeply sloped than potential temperature surfaces at these times (Fig. 19). However, TKE generation in case SFC20 is generally weaker than in the wind forced case SFNM.

It is interesting to note that the initial pulse of turbulence in case SFC20 does not immediately develop roll circulations. While this flow is unstable for symmetric instability, it is also unstable for shear instability when the linear shear profile is disrupted. As a test, we conducted an experiment with the same initial shear profile as the imposed geostrophic shear, but without rotation or a frontal temperature gradient (e.g. similar to equatorial flow). The resulting turbulence kinetic energy evolution (not shown) was nearly the same as in Figure 17 through hour 6, suggesting that symmetric instability cannot be uniquely identified by estimating the shear production term.

In contrast to case SFNM, geostrophic shear production is the dominant source of TKE in both SFSM and SFC20, consistent with symmetric instability dynamics (Fig. 20). Buoyancy production also contributes to the disturbance growth, while ageostrophic shear production is
mostly negative, implying that the total shear production is smaller than the inferred geostrophic shear production. These balances differ from those for SFNM also in that both buoyancy production and vertical transport of TKE are relatively small at most depths for SFNM.

6. Turbulent kinetic energy: generation and scaling

a) TKE generation processes

The simulations in Sections 4 and 5 have focused primarily on the development and dynamics of coherent roll structures in the turbulent boundary layer. However, these simulations also reveal a dependence of the temporal and domain mean TKE on the frontal strength and on the strength and relative alignment of the winds. In general, the mean TKE budget is dominated by a balance between shear production and mechanical dissipation, while buoyancy production is typically small and positive (Fig. 5). With fixed, moderate northerly winds, mean TKE production increases with frontal strength (Figs. 5b-d), while for fixed strong frontal gradient, mean TKE production increases with northerly wind amplitude (Figs. 5a, d, e). Further, for the SFNS case, with a strong frontal gradient and strong destabilizing winds, the pulses of turbulence associated with the development of roll structures at hours 5 and 13 contribute only a relatively small fraction of the time-mean TKE production (Fig. 5e), suggesting that nearly all of the TKE in that case is directly wind-driven. For case SFNM, the coherent structure and mixing-pulse development are themselves driven in part by ageostrophic shear production: at hour 17, ageostrophic shear production exceeds geostrophic shear production near the surface and base of the boundary layer (Fig 6b). In contrast, for the case SFC20 with no wind forcing, geostrophic shear dominates, and there is minimal ageostrophic shear production (Figs. 5a, 20b).

The total horizontal and time mean TKE shows direct dependencies on the frontal strength and wind direction (Fig. 21) similar to results of Taylor and Ferrari (2010). In general, the
stronger the frontal gradient, the greater the total integrated TKE and subsequent mixing at the
bottom of the boundary layer, if the wind is in the destabilizing direction (Fig. 21a). For the
strong front case, mean TKE increases by a factor of 5-10 over much of the boundary layer for
northerly, destabilizing winds relative to southerly, easterly, or westerly winds (Fig. 21b). Mean
TKE also decreases for southerly, stabilizing winds over a strong front relative to winds of equal
amplitude with no front (Fig. 21a, SFSM vs. NFNM).

As noted above, the geostrophic relation between the frontal gradient and the geostrophic
shear presents a possible ambiguity in interpretation of the dependence of mean TKE on wind
direction and frontal strength: the Ekman buoyancy transport divergence $EBF$ (2a) may
contribute to TKE generation through mechanically forced convection, or the wind-driven shear
aligned with geostrophic shear may augment turbulence from symmetric instability through
mechanical shear production $SP_{geo}$ (2b). It is clear from the TKE budgets that it is the second of
these interpretations that is correct, and that mechanically forced convection plays at most a
limited role in these simulations; rather, it is the alignment of wind-driven shear with geostrophic
shear that controls TKE production.

Moreover, comparison of the no-wind, weak-cooling case SFC20 (Fig. 17) with the basic
moderate-wind case SFNM (Fig. 4) shows that a surface cooling that is much weaker than the
inferred $EBF$ equivalent surface heat flux is sufficient to maintain the stratification near
neutrality. The initial state in both cases is unstable to symmetric instability and only requires a
small perturbation to generate disturbance growth. The SFC20 case has surface cooling of only
20 W m$^{-2}$, while the $EBF$ for SFNM would equate to approximately 400 W m$^{-2}$ cooling. If
SFC20 were repeated with the SFNM $EBF$ cooling of 400 W m$^{-2}$, the boundary layer would be
completely dominated by convective turbulence, with no significant symmetric instability
component. For SFNM, the wind-driven shear turbulence production $SP_{geo}$ is sufficiently strong that the lateral Ekman buoyancy fluxes are rapidly mixed vertically. Consequently, the Ekman buoyancy advection in SFNM does not act as an effective surface heat flux, and a physical interpretation based on the $EBF$ would be essentially misleading. Instead, the wind contribution to the TKE scaling for case SFNM – and the other wind-driven cases considered here - should be understood physically in terms of the $SP_{geo}$ wind-driven shear production.

\textit{b) Simple TKE budget model}

The analysis of TKE generation processes in the preceding section establishes that the dominant source of mean TKE in these simulations is mechanical shear production, and that the efficiency of this mechanical generation depends on the relative alignment of the mean geostrophic and ageostrophic vertical shear. For many mixed layer parameterizations, for example the KPP scheme (Large et al., 1994), estimation of eddy viscosity depends on assumptions about the scale of TKE production terms. For example, the commonly used Obukhov length, $L$, provides a measure of stratification versus shear allowing universal functions of $z/L$. Here we perform a scale analysis of the TKE budget equation and define a new length scale analogous to $L$, but relating ageostrophic and geostrophic shear production. Our intent is to demonstrate that the relative importance of geostrophic shear versus wind-forced shear can be estimated through a simple parameter that is dependent on horizontal temperature (or salinity) gradient and the destabilizing wind component velocity.

Traditional scaling of the TKE budget for the surface layer begins with the definition of a reference velocity (or friction velocity), $u^*$ (see Kaimal and Finnigan 1994). For a wind-forced, neutral boundary layer, average shear near the surface can be scaled using
where, \( \kappa \) is the von Karman constant (\(-0.4\)), and \( z \) is the depth. Turbulence kinetic energy dissipation for the surface layer is roughly equal to shear production, or

\[
\epsilon = u' w' \frac{\partial \bar{u}}{\partial z} = u_* \left( \frac{u_*}{\kappa z} \right) = \frac{u_*^3}{\kappa z} \quad (9)
\]

This scaling for dissipation or shear production can be used to compare various terms in the TKE budget equation for flows near the surface. Here, we apply a similar scaling for the boundary layer following methods presented in Moeng and Sullivan (1994) and Belcher et al. (2012).

For boundary layer mixing in frontal zones where the buoyancy term is relatively small, we would like to know which is more important; TKE production from wind and/or wave mixing through the ageostrophic shear production terms (we ignore Langmuir wave effects here), or TKE growth from geostrophic shear production. Assuming steady state, we express the TKE budget as a balance between shear production from ageostrophic shear, \( SP_{ageo} \), geostrophic shear, \( SP_{geo} \), and dissipation, or

\[
\epsilon = SP_{ageo} + SP_{geo} \quad , \quad (10)
\]

where parameters are assumed to be averaged over time. We ignore the buoyancy term, which is typically small in our simulations. We can replace the shear production terms in this equation using surface layer scaling for turbulence, for example, as used in equation (9),

\[
\epsilon(z) = \left( A \frac{u_*^3}{\kappa z} + u_*^2 \frac{\partial \bar{v}_g}{\partial z} \right) \left( 1 - \frac{z}{h} \right) \quad (11)
\]
where we have scaled \( \overline{u'w} \) with \( u_*^2 \) and applied a simple model for the linear variation of budget terms over the boundary layer depth, \( h \), following Moeng and Sullivan (1994). The second term in this model is the same as the dissipation scaling derived by Thomas and Taylor (2010) in their analysis of wind-work reduction by symmetric instability. We include an empirical constant, \( A = 0.5 \), which accounts for the reduction in shear and subsequent scaled dissipation rate because of the rotating inertial current, and differences between the surface layer and mixed layer scaling.

We can also express (11) in terms of a characteristic length scale,

\[
L_{sp} = \frac{u_* f}{\kappa g \alpha \frac{\partial \theta}{\partial x}} = \frac{u_*}{\kappa \frac{\partial \theta}{\partial z}}, \tag{12}
\]

analogous to the Obukhov length, but with buoyancy production replaced with shear production by geostrophic shear. Equation (11) can be rearranged to yield,

\[
\varepsilon(z) = \frac{u_*^2}{k z} \left( 0.5 + \frac{z}{L_{sp}} \right) \left( 1 - \frac{z}{h} \right). \tag{13}
\]

When \( z = L_{sp} \), shear production from geostrophic shear is roughly equal to shear production from wind stress acting on the ocean surface, consequently, large \( L_{sp} \) implies either strong wind forcing or a weak horizontal temperature gradient. The formula (13) is similar to the TKE budget parameterizations presented in Thomas and Taylor (2010) and applied for a case study on the Gulf stream in Thomas et al. (2016), but we include the surface wind momentum flux shear term and introduce the characteristic length scale, \( L_{sp} \). Ramachandran et al. (2013) also use (12) as a means of comparing the effects of the Ekman buoyancy flux relative to geostrophic shear in a mesoscale model mixed layer parameterization, and find that (12) provides a consistent length scale for determining the depth above which the ageostrophic shear production dominates over the surface forced Ekman buoyancy flux. We reinterpret this scale here, however, as relating to the geostrophic shear rather than the Ekman buoyancy transport.
Plots of the average dissipation rate from the LES model are presented in Figure 22 for both weak and moderate wind forcing cases along with predicted profiles from Eq. (13). Overall, results from the simple model are in good agreement with the LES and indicate how the geostrophic shear contributes to increased turbulence, especially near the base of the boundary layer where geostrophic shear dominates, for example at ~70 m for case SFNM. For moderate winds, even the weakest gradient of 0.2 °C/10 km generates a significant increase (factor of 2-3) in turbulence dissipation rate over the lower half of the boundary layer.

7. Discussion

The present simulations and analysis have points in common with many recent related studies presented in Taylor and Ferrari (2010), Thomas and Taylor (2010), Thomas et al. (2013), and Thomas et al. (2016), but with significant differences in the model spin up procedure, wind stress forcing, and frontal strength. As a result of these differences, classical inflection-point shear instability is found to contribute significantly to the development of coherent roll structures in the wind-driven frontal surface boundary layer, and interpretation of the roll dynamics purely in terms of symmetric instability, as in these previous studies, is not possible. This Ekman-like instability of the wind-driven shear causes the oblique orientation of the rolls that is observed in the LES model simulations.

A more subtle distinction from these previous studies relates to the origin and role of inertial currents. In particular, the near-inertial current generated in our configuration arose not from wind forcing alone but from instability-driven vertical mixing of momentum that disturbed the initial geostrophic balance. This inertial current is distinct from wind-forced inertial oscillations and has a damping effect on the boundary layer instabilities. In Thomas et al. (2016), the primary driver of the inertial current was the wind, whereas here disruption of the
geostrophic balance is the main source of inertial current energy. In addition, their wind
direction rotated inertially (clockwise, which would imply resonance, Crawford and Large 1996)
at the onset of the study period followed by a cross-front direction from cold to warm water. As
a consequence, the wind-forced inertial current shear varied significantly from cases presented
here where we apply constant wind stress direction. In Taylor and Ferrari (2010), wind forcing
was 10 times smaller than in the current cases and the simulations were initialized with constant
vertical stratification throughout the model depth, and consequently the boundary layer required
~20 days to reach a depth of 50 m. This initialization and spin up produced stratification in the
forced symmetric instability region with a near-neutral bulk Richardson number equal to 1. A
stronger wind stress of 0.1 N m$^{-2}$ was applied by Thomas and Taylor (2010) in similar LES
experiments, however inertial effects were removed through averaging. For comparison, we
performed two additional experiments initialized with constant stratification and no predefined
mixed layer, following Taylor and Ferrari (2010). Destabilizing wind forcing of 0.01 N m$^{-2}$ and
0.1 N m$^{-2}$ were applied and simulations were conducted over a 10-day period. In both cases,
inertial currents were greatly reduced in comparison with the prescribed mixed layer depth cases
presented here, and geostrophic shear production dominated the TKE budget in agreement with

The importance of inertial oscillations for boundary layer turbulence and mixing has long
been recognized (e.g., Pollard et al., 1973). The role of near-inertial shear in controlling
stratification and shear production in our simulations is generally consistent with the conceptual
model presented in Thomas et al. (2016) based on observations and LES modeling results.
Thomas et al. (2016) conducted a linear stability analysis for a case in which thermal advection
by inertial shear had a destabilizing effect on boundary layer stratification, and showed
specifically that symmetric instability could result from this inertial destabilization. There is some similarity between that analysis and the conditions found here, for example, Cases SFNM and SFC20. However, there are also significant differences. In the linear stability analysis of Thomas et al. (2016) construction, the frontal gradient is stronger, there is no wind-generated turbulence, and the Richardson number is never below ¼. Moreover, both the geostrophic and the idealized inertial shear in Thomas et al. (2016) are linear in depth, precluding the formation of inflection point instabilities such as Kelvin-Helmholtz or the Ekman instability described above. Further, in the cases examined here, the role of the mixing-induced inertial current is generally opposite: it stabilizes the stratification and damps, rather than strengthening, the instability.

The prescribed mixed-layer initialization used here promotes both the generation of a near-inertial current from geostrophic imbalance and a more direct link between roll instabilities and small-scale turbulence. Turbulence in Taylor and Ferrari (2010), which considered a more stratified system, was generated through shear instabilities (e.g. Kelvin Helmholtz) imbedded in the more uniform, horizontal flow associated with the growing symmetric instability. In our simulations with $Ri < 0.25$, coherent structures behaved much like boundary layer eddies with a range of scales that are part of a turbulence cascade. In two of our cases where $0.25 < Ri < 1.0$, coherent structures formed that were aligned with the temperature gradient consistent with traditional slanted, symmetric instability. Winds in one case were opposed to the surface geostrophic flow, forcing restratification through Ekman transport of warm water over cold. Consequently, the boundary layer developed into two regions; one near the surface dominated by wind-forced shear, and second deeper layer separated from the shear-driven layer by a region of stable stratification. This lower layer had both initial negative potential vorticity and Richardson
number between 0.25 and 1.0, consistent with conditions for symmetric instability. A second case with symmetric circulations did not have wind forcing, but only weak surface cooling. Again, the simulation exhibited Richardson number between 0.25 and 1.0, and negative potential vorticity. In both of these cases, TKE was much lower in comparison with the cases where Ri < ¼.

In previous LES modeling studies of frontal instabilities, the TKE budget was used to argue that symmetric instabilities were the main source of significant boundary layer mixing for cases with negative potential vorticity and Ri < 1.0 (Taylor and Ferrari 2010; Thomas et al. 2013; Thomas et al. 2016). In these studies, the primary source of shear production can be attributed to the geostrophic shear, which is the source of energy for symmetric instability. However, there is nothing unique about geostrophic shear that would prevent other instabilities such as Ekman, Kelvin-Helmholtz or other inflection point instabilities from extracting energy from the mean flow if Ri < 0.25. Here, our analysis indicates that the combination of wind forced and geostrophic shear is the primary source of kinetic energy for the coherent turbulent structures produced in the model. We note that the dissipation parameterization presented in section 6b is based in principle on similarity theory (e.g. see Phillips pg. 284) and would be the same regardless of the source of the shear.

An important question concerns when and where we would expect strong boundary layer mixing in the ocean because of frontal instabilities as modeled here. Using a range of wind forcing and horizontal temperature gradients, we examined how important wind forced shear is relative to geostrophic shear and related this to wind speed and horizontal temperature gradient. We find that enhanced mixing is primarily associated with destabilizing winds that align so that wind-driven shear augments geostrophic shear; other wind directions examined produced
turbulence intensity similar to cases without a horizontal temperature gradient. This wind-
direction dependence agrees with that found by Taylor and Ferrari (2010), but we suggest that a
different interpretation of the underlying physical mechanism is appropriate for our simulations,
in which TKE is seen as scaling with wind-driven geostrophic shear production $SP_{geo}$ (2b) rather
than the numerically equivalent $EBF$ (2a). We showed also that combining a parameterization of
dissipation rate similar to Thomas and Taylor (2010) with boundary layer scaling from Moeng
and Sullivan (1994) leads to a simple model of boundary layer dissipation rate dependent on
wind stress and frontal strength.

Simulations of oblique roll instabilities under conditions generally conducive for
symmetric instability are not unique to this study. Jones and Thorpe (1992) explored the linear
evolution of initially symmetric perturbations for flow with $Ri = 0.4$ and found fast growing
asymmetric modes for large initial perturbations, whereas small-scale perturbations lead to
dominant symmetric modes. Using a direct numerical simulation model, Arobone and Sarkar
(2015) found both symmetric and asymmetric modes during initial growth of frontal disturbances
for flow with $Ri = 0.5$. They determined that the asymmetric mode evolved nonlinearly before
the symmetric mode, leading the transition to turbulence. Neither of these studies examined
cases of forced symmetric instability, so the oblique roll orientations likely arose from viscous or
perhaps nonlinear effects.

8. Summary

The wind-forced warm-filament simulation demonstrates that along-front wind forcing can
dramatically alter the evolution of shallow baroclinic (“mixed-layer”) instabilities, relative to
unforced conditions. The strength and rapid development of both vertical and lateral mixing
generated by the wind-forced processes was seen to prevent the formation of the baroclinic waves and eddies that dominated the unforced evolution. In addition, coherent roll structures that qualitatively resembled recent oceanographic frontal observations (e.g. Sundermeyer et al. 2014) were found to form in frontal zones with destabilizing winds.

The primary goal of this study was to examine how the interaction between surface wind-forced shear and geostrophic shear generates the coherent roll structures. We found that the coherent-structure dynamics, while similar to shear instabilities of the Ekman layer originally described in Lilly (1966), are more likely mixed instabilities that develop from the combined ageostrophic and geostrophic shear. These instabilities were found to be modulated by near-inertial currents that formed through disruption of the geostrophic balance in the mixed layer, temporarily increasing the stratification through advection of the frontal temperature gradient.

Analysis of the TKE budget shows that both geostrophic and ageostrophic shear are key components in providing energy for the growth of instabilities.

Many existing boundary layer parameterizations used in models with high resolution (e.g. 10 m) near the surface should account for frontal instabilities because they resolve geostrophic shear simulated by the large-scale circulation. However, methods that base upper-ocean mixing on surface heat and momentum fluxes alone, such as bulk layer models, may not accurately calculate the effects of fronts and geostrophic shear. More research is needed to determine if resolved geostrophic shear in typical parameterizations (e.g. Mellor and Yamada 1982) is sufficient for simulating mixing from frontal instabilities, or if coherent structures as modeled here require the inclusion of explicit dynamics, for example, through a specific non-local term in the transport equations (e.g. Smyth et al. 2002) or other frontal parameterizations (e.g. Bachman et al. 2017).
Both field measurements (e.g. D’Asaro et al. 2011; Thomas et al. 2016) and our numerical experiments indicate that mixed layer fronts can have a significant effect on the character of turbulence and the overall strength of mixing. What is not yet understood is how often frontal regions dominate the dynamics of boundary layer turbulence. Strong horizontal density gradients, similar to the examples studied here, are found in limited areas of the world ocean. Primary areas of strong gradients are located near the western boundary currents, such as the Gulf Stream and Kuroshio, and in the Southern Ocean. These regions are likely to have enhanced boundary layer mixing when winds are aligned along front such that the wind-driven shear augments the geostrophic shear.

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Table 1. Simulation parameters. Case SFC20 also has surface cooling of -20 W m\(^{-2}\).

<table>
<thead>
<tr>
<th>Case</th>
<th>(dT/dx) (°C/10 km)</th>
<th>(\tau_x) (N m(^{-2}))</th>
<th>(\tau_y) (N m(^{-2}))</th>
<th>(M (s^{-2} \times 10^{-7}))</th>
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<td>0.25</td>
<td>0.0</td>
<td>-0.1</td>
<td>0.49</td>
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<tr>
<td>SFNM</td>
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Figure Captions List

Figure 1. Initial (a) potential temperature and (b) $u$ (blue, solid) and $v$ (red, solid) velocity component profiles for the constant gradient, frontal zone cases. Also shown in (a) the potential temperature (dashed), and in (b) $u$ (blue, dashed) and $v$ (red, dashed) components at hour 16 from case SFNM. The potential temperature profile is also used to initialize the warm filament background state.

Figure 2. Surface potential temperature for a warm filament simulation initialized in geostrophic balance with (a) no surface forcing after 85 hours and with -0.1 N m$^{-2}$ wind forcing after (b) 25 hours and (c) after 52 hours.

Figure 3. Horizontal cross sections of surface $v$ component velocity (m s$^{-1}$) at hour (a) 6 and (b) 16 from case SFNM.

Figure 4. Horizontally averaged (a) $v$ component (m s$^{-1}$), (b) TKE (m$^2$ s$^{-2}$), (c) zonal departure from geostrophic balance (difference of Coriolis and pressure gradient force terms), and (d) vertical meridional momentum transport divergence, for case SFNM. Contours of horizontally averaged potential temperature (°C) are shown in (a) and (b).
Figure 5. Domain averaged TKE budget terms for case (a) SFC20, (b) NFNM, (c) WFN, (d) SFNM, and (e) SFNS: ageostrophic shear production (black), geostrophic shear production (red), buoyancy production (blue) and dissipation (black dash).

Figure 6. Horizontally averaged TKE budget terms vs depth for case SFNM at (a,c) 6 hr and (b,d) 17 hr. Terms in (a) and (b) are ageostrophic shear production (black), geostrophic shear production (red), buoyancy production (blue), vertical transport (magenta), and dissipation (dashed). Terms in (c) and (d) are total (black) and geostrophic (dashed) meridional, and zonal (red), shear production.

Figure 7. Growth rates vs. wavenumber vector angle $\phi$ and wavelength $\lambda$ from the frozen-field linear instability calculation for the SFNM hour-16 mean profile and lateral temperature gradient (color-filled contours). The centers of instability for the neutral Ekman-spiral profile and for the symmetric and baroclinic modes of the pure-geostrophic profile are indicated (white contours and labels). The modes at $\phi = -24^\circ$ and $\phi = -16^\circ$ with 300-m wavelength, for which the modes structures are shown in Fig. 8a and Fig. 8b, respectively, are indicated (magenta and purple dots).

Figure 8. Horizontal and vertical velocity vectors (reference vector at lower right) in the vertical plane parallel to the wavenumber angle $\phi$, and horizontal velocity normal to $\phi$ (contours) for the SFNM hour-16 linear instability modes with wavelength 300 m, from the calculation shown in Figure 8. (a) mode with $\phi = -24^\circ$, and (b) mode with $\phi = -16^\circ$. The absolute value of the velocity amplitude is arbitrary in each case.
Figure 9. Cross-front section for Case SFNM of the (a) v component velocity (shaded) and potential temperature (contour interval 0.025 °C) at hour 17 from y = 1200 m, and the meridional average absolute momentum (blue dashed, contour interval 0.05 m s\(^{-1}\)) and potential temperature (black, contour interval 0.025 °C) at hour (b) 17 and (c) 24.

Figure 10. Horizontally averaged potential vorticity \( q \) (s\(^{-3}\)) for Case SFNM (shading; \( q = 0 \) contour in red), along with contours of \( Ri = 0.25 \) (green) and \( Ri = 1.0 \) (black).

Figure 11. Horizontally averaged vertical buoyancy flux (shaded) for Case SFNM, along with diagnosed convective depth \( h \) from (7) using computed \( B_{wind} \) (solid line) and \( EBF \) (dashed line).

Figure 12. Same as Figure 3 but for case NFNM.

Figure 13. Same as figure 4ab for (a) case NFNM and (b) case SFNS.

Figure 14. Same as Fig. 4ab, but for case SFSM with warm-to-cold Ekman transport.

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Figure 16. Meridional velocity at hour 22 from a depth of 50 m for case SFSM with winds from the south.
Figure 17. Horizontally average (a) $v$ velocity component (m s$^{-1}$) and temperature ($^\circ$C contoured), (b) TKE and temperature, and (c) potential vorticity for case SFC20. Overlaid on (c) are contours of $Ri = 0.25$ (green), $Ri = 1.0$ (black), and potential vorticity $q = 0.0$ (red).

Figure 18. Surface meridional velocity (m s$^{-1}$) at hour 19 for case SFC20.

Figure 19. Same as figure 10b-c, but for case SFC20 at hour (a) 19 and (b) 22.

Figure 20. Horizontally averaged TKE budget terms from hour 22 for (a) case SFSM with stabilizing Ekman flux winds, and (b) case SFC20 with surface cooling, but no wind forcing. Terms are defined as in Fig. 6a-b.

Figure 21. TKE averaged in the horizontal and over the simulation period for cases with (a) different temperature gradient values for cases SFNM (“1.0”), SFSM (“1.0 up”), MFNM (“0.5”), WFNM (“0.2”), and NFNM (“NF”), and (b) wind directions for cases SFNM, SFEM, SFWM, SFSM. Wind stress magnitude in all cases is 0.1 N m$^{-2}$.

Figure 22. Plots of the dissipation rate, $\varepsilon$, from the LES model averaged horizontally and between the hours of 15 and 36 for (a) moderate and (b) weak winds, and as predicted by Eq. (13) for (c) moderate and (d) weak winds.
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