

# **Layering Accompanying Turbulence Generation Due to Shear Instability and Gravity Wave Breaking**

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## **Abstract**

We describe and compare idealized, high-resolution simulations of turbulence arising due to Kelvin-Helmholtz shear instability and gravity wave breaking, believed to be the two major sources of turbulence generation near the mesopause. The two flows both share characteristics related to turbulence transition, evolution, and duration and exhibit a number of differences that have important implications for layering, layered structures, and atmospheric observations at mesopause altitudes. Common features related to layering include sharp, local gradients in turbulent kinetic energy production, dissipation, and magnitude and a clear spatial separation of the maxima of turbulent kinetic energy dissipation and thermal dissipation accompanying vigorous turbulence. Differences arise because shear instability causes turbulence and mixing confined by stratification to a narrow layer, whereas gravity wave breaking leads to a maximum of turbulence activity that moves with the phase of the wave. As a result, the effects of turbulence due to shear instability likely persist for much longer than those of turbulence due to gravity wave breaking. We also discuss the implications of these results for a number of atmospheric measurements employing radar.

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## 1. Introduction

Turbulence plays a central, but not fully quantified or understood, role in defining the evolution and structure of the atmosphere from the Earth's surface to the turbopause. At larger scales, convective heat transports largely offset radiative tendencies in accounting for the negative mean thermal gradient in the troposphere [Holton, 1979; Gill, 1982]. Similarly, turbulent transport of heat accompanying gravity wave breaking is credited with driving the mesosphere toward an adiabatic lapse rate [Garcia and Solomon, 1985], though its efficiency in heat and constituent transport has been challenged on both modeling and theoretical grounds [Strobel et al., 1985, 1987; Fritts and Dunkerton, 1985; Coy and Fritts, 1988; McIntyre, 1989]. Turbulence is known to contribute mixing and transport under more strongly stratified conditions as well, for example in the stable nocturnal boundary layer, the stratosphere, and the lower thermosphere. In all stably stratified environments, turbulence often occurs in layers of limited depth, with the turbulence extent determined initially by the scale of shear instability or wave breaking and thereafter confined vertically by stratification.

Because of the importance of turbulence in atmospheric dynamics on many scales, considerable efforts have been expended to define its roles under statically stable conditions. Applications range from constituent dispersal and surface temperature prediction (and energy consumption, etc.) near the earth's surface, to vertical mixing and transport throughout the atmosphere, to aircraft safety, laser propagation, radio communications, and astronomical observations. Field programs have employed extensive instrumentation to quantify turbulence effects throughout the lower and middle atmosphere, and these efforts have contributed greatly to our knowledge of turbulence influences statistically [Wyngaard, 1983; Hocking, 1985; Lübken, 1997; Poulos et al., 2002]. Likewise, theoretical studies have explored turbulence structure and effects under isotropic and anisotropic (stratified and/or sheared) conditions [Kolmogorov, 1941; Onsager, 1945; Bolgiano, 1959; Hill, 1978; Weinstock, 1978]. Yet, none of these studies have fully characterized turbulence influences because of the inherent limitations of, or assumptions underlying, these methodologies.

For our purposes here, the most significant indications of turbulence effects in the atmosphere have come from observations of turbulence generation, layering, and confinement by mean stratification. Early aircraft, rocket, and balloon measurements by Lilly

and Lester [1974], Rosenberg and Dewan [1975], and Cadet [1977] addressed the diffusion associated with discrete turbulent layers in the lower stratosphere. Radar observations by Sato and Woodman [1982a, b] and Woodman and Rastogi [1984] provided indications of persistent layers of strong backscatter associated with inertia-gravity wave shears in the lower stratosphere and suggested turbulence as the source of backscatter. Similar results and interpretations were offered at mesospheric altitudes by Yamamoto et al. [1988], Reid [1990], and Stitt and Kudeki [1991]. Other studies at higher spatial resolution have revealed that enhanced backscatter is associated preferentially with the edges of turbulent layers [Gossard et al., 1971; Browning, 1971; Röttger and Schmidt, 1979; Eaton et al., 1995]. In all of these cases, large  $C_N^2$  (and radar backscatter) was interpreted as evidence of turbulence. Significant insights were also provided by high-resolution balloon measurements describing both the mean thermal structure and the turbulence temperature structure parameter,  $C_T^2$ , which correlates closely with radar backscatter [Coulman et al., 1995]. These observations revealed a series of nearly adiabatic layers having sharp temperature gradients and  $C_T^2$  maxima at the edges of each. Importantly,  $C_T^2$  was usually extremely small within the turbulent layers themselves.

A complete quantification of turbulence dynamics and effects requires direct numerical simulation, or DNS, of the evolution of a turbulent process in three spatial dimensions and time because such processes are episodic and spatially localized in nature and dependent on initial and environmental conditions. It is also necessary to resolve not only the source scales, the transition to turbulence, and the inertial range, but also a significant viscous range. This is because interactions between inertial-range and viscous-range scales can impact turbulence dynamics at larger scales if the dissipation scales are not accurately represented [Jimenez, 1994]. Indeed, it has only recently become possible to achieve Reynolds numbers representative of the mesopause region in numerical simulations of geophysical processes because of the extreme resolution requirements when turbulence is intense [Werne and Fritts, 1999, 2001; Hill et al., 1999]. Initial applications of these results to calculations of radar backscatter yielded results in close agreement with observations and important insights into the interpretation of radar data [Gibson-Wilde et al., 2000]. Indeed, these results have highlighted the importance of layering accompanying turbulence in stably stratified fluids for flow evolution and measurement interpretation.

Our purposes in this paper are to describe and contrast the implications for layering and layered structures in the middle atmosphere of turbulence arising due to Kelvin-Helmholtz (KH) shear instability and gravity wave (GW) breaking. These processes are believed to be the two dominant mechanisms for turbulence generation in the free atmosphere. KH instability is most often associated with strong shears of the mean wind or accompanying low-frequency gravity waves having small vertical group velocities and slowly-evolving amplitudes and shears. Gravity wave breaking is the more common means of turbulence generation for GWs having high intrinsic frequencies and large vertical group velocities because of their more rapid amplitude growth with time. Essentially, GWs having high intrinsic frequencies rush past the necessary (but not sufficient) condition for dynamical instability of a plane parallel shear flow (a Richardson number  $Ri < 1/4$ , see below) and quickly become convectively unstable ( $Ri < 0$ ), though this is not strictly the condition for GW instability of a “convective” type (see Fritts and Alexander, 2002]). KH shear instability appears to be more common at lower altitudes, the troposphere and lower stratosphere, where vertical wavelengths and vertical group velocities tend to be small. GW breaking becomes increasingly important at higher altitudes where wave scales and group velocities are larger and is likely the dominant source of turbulence in the mesosphere and lower thermosphere.

We begin in Section 2 by describing briefly the numerical methods employed for these studies. An idealized KH instability evolution and turbulence transition, and its implications for layering, are described in Section 3. The evolution of a breaking GW, its turbulence morphology, and implications for layering are discussed in Section 4. Section 5 compares and contrasts the influences of turbulence arising due to these two very different sources. Our conclusions are presented in Section 6.

## 2. Numerical Formulation

Our numerical simulations of KH instability and GW breaking were performed with an incompressible spectral code optimized for performance on various supercomputer architectures, primarily the Cray T3E and the SGI Origin series. These simulations were performed with resources provided as part of a Department of Defense High Performance Computing “Challenge” resource allocation and consumed in excess of 100,000 hours each. Each application employed a triply-periodic version of the code using Fourier basis functions in three directions. The specific formulation of the spectral code was described

in detail by Werne and Fritts [1999, 2001] and will not be repeated here. Details specific to each class of simulation are provided below.

## 2.1 KH Instability

Because the code formulation is nondimensional, results are scalable to any problem for which the choices of the nondimensional parameters  $Ri_0$ ,  $Re_0$ , and  $Pr$  are appropriate. For our KH instability simulations, these choices imply spatial scales and a kinematic viscosity,  $\nu$ , in close agreement with values expected near the mesopause. Because the computational code solves the incompressible Navier-Stokes equations, temperature and potential temperature are equivalent and we will refer only to temperature in discussing the model results hereafter.

Simulations of KH instability were performed with a domain aligned horizontally, an initial horizontal shear flow given by

$$U(z) = U_0 \tanh(z/h), \tag{1}$$

and an initially uniform stratification with temperature gradient  $\beta$  and buoyancy frequency  $N$ . Dimensions of the computational domain were specified in terms of the shear scale as  $(X_0, Y_0, Z_0) = (4\pi, 4\pi/3, 8\pi)h$ , with  $X_0$  the streamwise (along shear) direction. The ratio  $X_0/h = 4\pi$  was chosen to be consistent with the wavelength of the most rapidly growing mode in the linear viscous stability theory for these initial profiles.  $Z_0/h = 8\pi$  was chosen to ensure a minimal influence of the upper and lower domain boundaries on the KH evolution [Werne and Fritts, 1999].

Our choices of

$$Ri_0 = N^2/U_z^2 = N^2 h^2/U_0^2 = 0.05, \tag{2}$$

$$Re_0 = U_0 h/\nu = 2500, \tag{3}$$

and

$$Pr = \nu/\kappa = 1 \tag{4}$$

are then consistent with mesopause values of a shear depth  $h \sim 240$  m, a KH wavelength  $X_0 \sim 3$  km, a velocity scale  $U_0 \sim 10$  ms<sup>-1</sup>, a stratification  $N^2 \sim 10^{-4}$  s<sup>-2</sup>, and a kinematic

viscosity  $\nu \sim 1 \text{ m}^2\text{s}^{-1}$ . With these choices for scales, a buoyancy period corresponds to 28 time units.

## 2.2 GW Breaking

Instability and turbulence accompanying gravity wave breaking was first studied numerically at relatively coarse spatial resolution by Andreassen et al. [1994], Fritts et al. [1994, 1996], and Isler et al. [1994] in an atmospheric context and by Winters and D’Asaro [1994] in an oceanic context. Subsequent studies by Andreassen et al. [1998] and Fritts et al. [1998] addressed turbulence dynamics with only slightly enhanced resolution. All of the atmospheric studies were constrained by the need to confine turbulence to the interior of the model domains, and this was accomplished by imposing a mean shear flow. The joint desires to increase model resolution and perform studies in the absence of a mean shear flow were the motivations for the simulations described here.

Our current simulations of GW breaking were performed in a computational domain aligned along the phase of the gravity wave. Hence the wavelengths in the domain do not correspond to horizontal and vertical wavelengths in the atmosphere. Instead, the “vertical” direction is normal to the phase surfaces and inclined from true vertical at the angle of the GW phase lines from the horizontal,  $\theta = \sin^{-1}(\omega/N)$ , where  $\omega$  is the intrinsic frequency of the GW, here assumed to be  $\omega = N/3$ . Gravity is likewise inclined at this same angle from “vertical” in this coordinate system. The advantage to this approach is the ability to easily average wave and turbulence quantities along the GW phase in the analysis of these results. A schematic of this geometry is shown in Figure 1. We note here that it is the ratio of  $\omega/N$  (together with other parameters) rather than  $N$  itself that dictates GW instability properties. Hence our results are relevant to both weakly and strongly stratified environments.

With a streamwise direction along the phase of the GW, the streamwise wavelength in this coordinate system is infinite. The wavenumber in the normal direction is the total wavenumber of the GW,  $k_{tot}^2 = k^2 + m^2$ , where  $k$  and  $m$  are the horizontal and vertical wavenumbers in the atmosphere and  $k_{tot} = 3k$  with our choice of  $\omega$ .

In this coordinate system, we choose length and time scales  $l = 2\pi/k_{tot}$  and  $t = T_{BV} = 2\pi/N$  (the buoyancy period), and the relevant nondimensional quantities are

$$a = u'_{tot}/U_0 = u'/c, \tag{5}$$

$$Re_0 = U_0 l/\nu = l^2/t\nu = 2\pi N/k_{tot}^2\nu, \tag{6}$$

and again

$$Pr = \nu/\kappa = 1, \tag{7}$$

where  $a$  is wave amplitude relative to that for marginal convective instability,  $u'_{tot}{}^2 = u'^2 + w'^2$ ,  $U_0 = l/t$ , and  $u'$ ,  $w'$ , and  $c$  are the corresponding horizontal and vertical velocities and the horizontal phase speed of the gravity wave in the atmosphere. The nondimensional GW period is  $T_{GW}/T_{BV} = N/\omega = 3$ . As in our KH simulations,  $Re_0$  is a measure of dissipation and thus turbulence intensity and spectral extent, but we chose to not have dissipation act on the primary wave in order to assess instability growth rates as a function of wave amplitude, compare with linear theory, and evaluate the effects of turbulence on wave amplitude apart from dissipation. For the simulation discussed here, we chose  $a = 1.1$  and  $Re_0 = 1000$ , corresponding to a weakly overturning wave and relatively weak dissipation of turbulence and other motions excited by wave breaking. The computational domain was chosen to have dimensions of  $(X_0, Y_0, Z_0) = (3.4, 2.2, 1)l$  (streamwise, spanwise, and “vertical”). A maximum resolution of  $(N_x, N_y, N_z) = (1440, 720, 400)$  was required to describe wave instability and turbulence generation for our chosen  $Re_0$ .

One interesting implication of our choice of computational domain is that the nonlinearities in this simulation are necessarily different from those that would have occurred in a domain aligned horizontally. With a sufficiently large domain (and multiple wavelengths in each direction), there would be no practical difference in the description of the dynamics. But imposed periodicities because of periodic boundary conditions do constrain the possible solutions with either choice of domain orientation when the domain is only a single wavelength. A horizontal domain, for example, would have imposed instability structures and higher wavenumber GWs having harmonics of the atmospheric wavenumbers  $(k, l, m)$ , with  $l$  here the wavenumber of the gravest spanwise mode. A slanted domain, on the other hand, admits only harmonics of that domain in each direction, which may have no relation to the horizontal atmospheric wavenumbers. Practically, as long as our focus is on instability dynamics and the computational domain provides sufficient spectral resolution of the dominant instability and turbulence scales, the results will not depend strongly on these choices.

### 3. Turbulence Generation and Layering Accompanying KH Instability

The evolution of KH instability, the transition to turbulence, and the dynamics of the turbulence cascade have been described in our earlier studies [Palmer et al., 1996; Fritts et al., 1996; Werne and Fritts, 1999, 2001; Fritts and Werne, 2000]. Other studies have applied these results in the interpretation of electron spectra and radar backscatter at mesopause altitudes [Hill et al., 1999; Gibson-Wilde et al., 2000]. Here we will only summarize these aspects of the evolution and focus instead on the implications of KH instability for atmospheric layering.

#### 3.1 Instability and Turbulence Evolution

KH instability arises initially as a two-dimensional (2D) instability of a shear flow exhibiting an inflexion point and  $Ri_0 < 1/4$ . The vorticity associated with the KH instability is spanwise, or aligned with that of the mean shear flow. Thus the instability can be thought of as organizing the initial mean vorticity into streamwise localized maxima which cause closed streamlines or billows. These billows entrain heavier fluid from below and lighter fluid from above, resulting in alternating bands of positive and negative static stability. Opposite horizontal density gradients on either side of the entrainment regions also lead to baroclinic generation of positive and negative spanwise vorticity, both enhancing the initial spanwise vorticity and creating spanwise vorticity of the opposite sign to that of the initial shear flow [Palmer et al., 1996].

The details and the energetics of KH billow development depend very sensitively on  $Ri_0$  and to a lesser extent on  $Re_0$  (there is also a dependence on  $Pr$ , but this is not relevant in the atmosphere). Values of  $Ri_0 \sim 0.2$  lead to billows that are relatively shallow and weak, whereas  $Ri_0 \sim 0.05$  or less lead to billows that are energetic and have a ratio of billow height to wavelength exceeding  $1/2$  [Thorpe, 1973]. Values of  $Re_0 < 300$  strongly suppress 3D secondary instabilities [Fritts et al., 1996], whereas values of  $Re_0 > 1000$  are required to achieve vigorous turbulence [Werne and Fritts, 1999, 2001]. Such values of  $Re_0$  are realistic near the mesopause because of the exponential increase of kinematic viscosity with altitude and characteristic billow scales at these altitudes. But values of  $Re_0$  representative of KH instability at lower altitudes may be  $10^3$  to  $10^4$  larger. Fortunately, the values of  $Re_0$  that can be addressed with current supercomputers,  $Re_0$  up to 2500 for  $Ri_0 = 0.05$ , are likely representative of KH instability and turbulence transitions at much higher  $Re_0$  for reasons that will be discussed below. Our choice

of  $Ri_0$  appears representative of KH instability in the atmosphere based on KH billows observed in clouds and with various atmospheric radars.

The turbulence transition accompanying KH instability within a stratified fluid comprises streamwise-aligned rolls that derive their eddy kinetic energy from both shear and buoyancy within regions of the KH billows that exhibit convective instability and counter-sign spanwise vorticity [Thorpe, 1985, 1987; Fritts et al., 1996; Smyth, 1999]. The spanwise scale of these rolls is dictated by the depth of the layer triggering instability [Klaassen and Peltier, 1985; Fritts et al., 1996], which is dependent in turn on  $Re_0$ . Large dissipation (or small  $Re_0$ ) leads to larger scales and slower growth of secondary instability. For  $Re_0 > 1000$  or so, however, the spanwise scale of secondary instability asymptotes to a value dependent on the initial shear depth and does not decrease further as  $Re_0$  increases. This is why we stated above that simulations with  $Re_0 \sim 1000$  to 2500 likely provide a reasonable initial description of KH dynamics and effects even when the environmental  $Re_0$  is much larger. The initial occurrence and streamwise alignment of these rolls is shown in the upper left panel of Figure 2. The 2D billow motion in these images is counterclockwise and the subdomain displayed is the central 1/3 of the full domain depth.

The streamwise-aligned rolls comprising secondary instability within the 2D KH billows initiate a transition to full turbulence via mutual and self vortex interactions. These interactions were initially described in numerical simulations of gravity wave breaking by Arendt et al. [1998] and Fritts et al. [1998] and in our initial KH simulations by Fritts and Werne [2000]. Essentially, the interactions among neighboring vortices spawn a series of perturbations to the vortices that can be viewed most simply as twist waves [Kelvin, 1880; Arendt et al., 1997]. Their finite-amplitude effects, however, include vortex breakup and fragmentation that appear to underlie the turbulence cascade to smaller scales of motion [Fritts et al., 1998]. The top center panel in Figure 2 displays the 3D vortex field within a KH billow at an intermediate stage in this transition to turbulence. One can see a predominance of vortices originating with the secondary, streamwise-aligned instability structures. But these structures exhibit a multitude of perturbations, are less coherent along their axes, and display an increasing isotropy relative to earlier stages of the evolution.

The most vigorous turbulence accompanies breakdown of the coherent, quasi-2D bil-

low structure and evolution towards a quasi-homogeneous turbulence layer in the horizontal. Spectra spanning this stage of the evolution exhibit a fairly broad inertial range (extending over more than a decade of scales) and apparently increasing turbulence isotropy with time [Werne and Fritts, 1999, 2001]. The panel at the upper right in Figure 2 displays the vortex structures as the turbulence layer approaches horizontal homogeneity, though the turbulence intensity still suggests a residual KH billow structure to the right of center of the domain. Importantly for our discussion below, we see that although the turbulence layer at later times has expanded to approximately the depth of the initial KH billow, it appears to be fairly strongly constrained in the vertical due to other factors.

### 3.2 Layering Accompanying KH Instability

Images in the lower panels of Figure 2 display the mechanical (yellow/red) and thermal (blue) energy dissipation fields corresponding to the vortex images displayed above. The most important features of the evolutions of these fields include 1) an initial alignment of both mechanical and thermal energy dissipation with the streamwise-aligned secondary instability structures (lower left panel), 2) a rapid spatial separation of the two dissipation fields accompanying vigorous turbulent mixing of the billow cores (and destruction of the thermal gradients and reduction of thermal dissipation in the interior of the mixing layer), and 3) attainment of a state of decaying turbulence intensities having the largest mechanical energy dissipation in the center of the turbulent layer and the largest thermal energy dissipation in strongly stratified edge regions. It is this behavior that motivated efforts to apply these data in the interpretation of electron density and radar backscatter measurements accompanying shear instability by Hill et al. [1999] and Gibson-Wilde et al. [2000].

The stages of KH instability and turbulence transition, as well as the implications of localized turbulence for mean atmospheric structure, are displayed in another format in Figure 3. Spanwise-averaged temperature and streamwise velocity are shown at eight times throughout the KH evolution in the upper two panels. In each case, solid lines are the profiles through the center of the billow and dashed lines are through the braid between adjacent billows. Profiles through the billow centers at early times quantify the discussion above concerning entrainment dynamics, with alternating gradients of temperature and streamwise velocity (or alternating spanwise vorticity) seen during the first two times. Clearly, entrainment and overturning within the KH billow establish

an approximately adiabatic mean thermal structure before secondary instabilities and turbulence arise. These profiles also illustrate the rate at which both secondary instability and turbulence annihilate the thermal gradients within the billow core. The fourth profile of temperature (at  $t = 90$ ) shows an essentially adiabatic gradient with only very weak fluctuations within the billow core. The corresponding velocity profile exhibits more variability due to the persistent billow structure and the presence of large- and small-scale turbulent motions within the quasi-2D flow. Only after this homogenization of the billow core does billow turbulence begin to shear and extend horizontally, leading to the merging of the solid and dashed profiles at later times.

Profiles of Richardson number and mechanical energy and thermal dissipation rates based on spanwise and streamwise averages of the relevant fields are shown in the center and lower panels of Figure 3 at the same eight times throughout the KH evolution. Clearly, these quantities are dominated by structure within the KH billow, since flow outside the billow is stably stratified and exhibits negligible mechanical or thermal energy dissipation. While a horizontal average of the full domain does not fully describe the mean environment in the presence of a large-amplitude billow, it is nevertheless clear that the annihilation of the thermal gradients by billow turbulence drives the mean  $Ri$  to values near zero within the region of active turbulence until late stages of the evolution. As billow turbulence shears and expands horizontally, it entrains the stratified fluid between adjacent billows and evolves towards a horizontally homogeneous layer having a mean  $Ri$  near or marginally above  $1/4$ . The edge regions of the turbulent layer retain sharp gradients in both temperature and streamwise velocity as the layer restratifies.

Profiles of mechanical energy and thermal dissipation,  $\epsilon$  and  $\chi$ , exhibit very different evolutions. This is because  $\epsilon$  provides a measure of turbulence intensity and mixing efficiency while  $\chi$  is a maximum where mixing or advection have resulted in sharp thermal gradients. As noted above, initial maxima of both  $\epsilon$  and  $\chi$  occur in the billow edge regions where secondary instabilities first lead to strong small-scale gradients. Vigorous turbulence and mixing within the billow core rapidly annihilates initial thermal gradients, however, and drives these gradients and maxima of  $\chi$  to the billow edges where sharp gradients in  $\epsilon$  persist, even in the mean profiles displayed in Figure 3. These differences persist throughout the further transition from turbulence confined to the billow interior to a turbulence layer that has achieved approximate horizontal homogeneity. While

detailed energy budget studies remain to be performed, it appears from these profiles that the largest mechanical energy dissipation rates accompany the horizontal expansion of billow turbulence, the entrainment of stratified fluid from outside the billow, and the gradual increase of the mean Richardson number to values near or marginally above  $1/4$ . Indeed, it is the entrainment of stratified fluid that suppresses vertical motions, drives the turbulence decay, and ultimately results in the attainment of a new dynamically stable mean state.

For the purposes of this paper, both the evolution of the turbulence layer and the structure of the altered mean state have important implications. We noted in a previous publication [Gibson-Wilde et al., 2000] that KH instability, turbulence, and mixing cause radar measurements of such events to differ significantly from previous assumptions. Radar measurements of spectral width have often been interpreted as a measure of turbulence intensity, with the hope that such measurements would permit a quantification of turbulence and mixing as functions of altitude. However, the simulations of radar backscatter by Gibson-Wilde et al. [2000] demonstrated that the most intense turbulence contributes little or no backscatter because of its rapid annihilation of thermal (and refractive index) gradients. Instead, the largest backscatter occurs in the edge regions of these turbulent layers where  $\epsilon$  values and turbulence spectral widths are smaller. Likewise, a direct computation of turbulence velocities and  $\epsilon$  revealed that the theory by Weinstock [1978] relating these quantities under the assumption of uniform stratification is flawed. A comparison of the theoretical and computed profiles was performed by Gibson-Wilde et al. [2000] and revealed that the theory and the DNS results differed whether a mean or local stratification profile was employed. Such simulations are thus allowing us to evaluate previous assumptions and theories quantitatively for the first time, and the results are reshaping our understanding of these turbulence effects.

The layering of the mean flow driven by KH instability and turbulence is apparently pervasive throughout the atmosphere and may have a number of previously unappreciated effects. Examples of layering observed in high-resolution balloon measurements of potential temperature by Coulman et al. [1995] are displayed in Figure 4. These profiles indicate that the troposphere and lower stratosphere are often composed of multiple layers that are alternately weakly stratified (or nearly adiabatic) and strongly stratified, causing these authors to suggest that such layering is a result of multiple events of shear

instability. Typical depths of these layers range from less than 100 m to  $\sim 1$  km and likely increase with altitude. Indeed, such a suggestion is entirely consistent with the radar observations by Sato and Woodman [1982a, b] of enhanced radar backscatter and apparent turbulence at similar altitudes noted in the introduction. The additional clarification that comes with the balloon measurements is characterization of temperature fine structure, via the temperature structure function parameter,  $C_T^2$ . An expanded view of this quantity, its relation to the potential temperature profiles, and the measured Richardson number for two profiles are shown in the upper two panels of Figure 5. The same fields derived from our KH simulation at  $t = 160$  are shown for comparison in the lower panel of Figure 5. In both the observations and the numerical results, strong maxima of  $C_T^2$  are associated with the edges of layers apparently arising from localized turbulent mixing due to KH instability. The temperature profiles themselves may contribute to sharp gradients in quantities, such as noctilucent cloud (NLC) particle size or growth rate, that are strongly temperature sensitive, given the rapid transition from near adiabatic to strongly stratified thermal structure at the upper edges of such mixed layers and the persistence of such edge regions on the time scales relevant to NLC particle growth and decay.

Characterization of temperature fine structure is less advanced near the mesopause, but there are nevertheless a number of indications of similar structure at these altitudes. VHF radar measurements at MU, SOUSY, and Jicamarca reveal persistent layers of enhanced backscatter reminiscent of the layers in the lower stratosphere [Yamamoto et al., 1988; Reid, 1990; Stitt and Kudeki, 1991], while VHF measurements at Poker Flat and UHF measurements at EISCAT have inferred extremely narrow spectral widths suggestive of enhanced  $C_T^2$  or electron density gradients in the absence of strong turbulence [Ulwick et al., 1988; Hoppe and Fritts, 1995]. Likewise, high-resolution rocket measurements have revealed layers of plasma or electron density fluctuations with and without associated neutral turbulence, often in very close proximity [Ulwick et al., 1988; Lübken et al., 1993, 2002]. Finally, direct applications of our KH turbulence simulations to rocket measurements of electron densities and spectra have suggested that there are times when the edges of turbulent layers can yield electron spectra in reasonable agreement with observations [Hill et al., 1999]. Clearly much remains to be accomplished in understanding the physical processes underlying such occurrences of layering. But it is not possible at

this stage to exclude the role of atmospheric turbulence and its confinement by stratification in at least some cases.

#### 4. Turbulence Generation and Layering Accompanying GW Breaking

All of our high-resolution GW breaking simulations to date examined waves having  $\omega = N/3$ ,  $Re_0 = 500$ , 1000, or 2000, and  $a = 0.9$ , 1.1, or 1.3. Here we will discuss only the  $a = 1.1$  case (with  $Re_0 = 1000$ ), as that is arguably most relevant to the mesopause region.

The instability dynamics and turbulence generation arising from GW breaking in the absence of mean shear (at least for the wave parameters considered to date) exhibit significant similarities to our previous simulations at lower resolution and in the presence of a mean shear. Initial instabilities comprise streamwise-aligned counter-rotating vortices that are largely confined to the region of convective instability within the wave. The streamwise vortices link via “hairpin” or loop vortices at one end, where they exhibit primarily spanwise vorticity. And these loop vortices act as sites of especially strong vortex interactions that drive the evolution towards increasing complexity and smaller scales of motion. Important differences in instability structure between the current unsheared and previous sheared mean state results include 1) a horizontal instability alignment within the unstable phase of the GW without mean shear (consistent with the stability analysis by Lombard and Riley [1996], but differing from the orientation in our sheared simulations [Fritts et al., 1994; Andreassen et al., 1998]) and 2) development of the vortex loops at the leading (upstream) edge of the unstable layer, as opposed to wave breaking in a mean shear, where vortex loops occurred at the lower, trailing edge of the instability.

##### 4.1 Instability and Turbulence Evolution

Volumetric views of the vorticity structures within the inclined computational domain at times of  $t = 5.26$ , 11.25, and 12.66 (in buoyancy periods) are displayed in the upper panels of Figure 6. For reference, the group velocity is inclined along the slanted domain and is upward and to the right, while the phase velocity of the wave is downward and to the right and normal to the lower domain boundary (see insert in the upper left panel). The lower panels in Figure 6 display the same volumes seen from above.

Initial instability of the breaking GW appears to be a merging of the horizontal, streamwise-aligned counter-rotating vortices anticipated by Lombard and Riley [1996] and a simultaneous formation of vortex loops linking adjacent streamwise vortices. There

is no tendency here, as in our earlier wave breaking simulations in mean shear, for streamwise rolls to precede formation of vortex loops via secondary KH instability of intensified vortex sheets [Fritts et al., 1994; Andreassen et al., 1998]. The loops, as well as the localization of the streamwise vortices within the unstable phase of the GW, were not anticipated by Lombard and Riley [1996]. But it is nevertheless impressive that the linear stability analysis was able to capture as many characteristics of the initial instability structure as it has. What is perhaps most surprising in this initial evolution of the instability structure is the occurrence of the loops at the upstream (leading or lower) edge of the phase of the GW that is convectively unstable, given that it was the opposite edge of the unstable phase that led to loop formation in the presence of mean shear). However, this can be understood qualitatively by recognizing that wave breaking in 2D (either where dynamically favored or numerically constrained) occurs via 2D rolling motions at a comparable site in the wave field where the horizontal wave velocity exceeds the horizontal phase speed,  $u' > c$ . Where this 2D behavior has been observed, it has led to rolling structures within the wave field having the same spanwise vorticity as the vortex loops in Figure 6 [Koop and McGee, 1986; Walterscheid and Schubert, 1990; Andreassen et al., 1994]. The simultaneous occurrence of the streamwise vortices and the loops having spanwise vorticity is apparently associated with the horizontal orientation of the instability, causing an immediate co-location of the two structures. Loop formation in our previous simulations with mean shear was delayed until spanwise vortex sheet intensification because initial streamwise vortices were aligned along the phase of the GW. Note that the vortex structures seen in the left panels of Figure 6 have extremely small amplitudes and virtually no impact on GW structure at that time.

The subsequent evolution of vortex structures in the GW breaking simulation exhibits a rapid increase in complexity and a cascade of energy and enstrophy to smaller scales of motion. Specifically, the vortex loops seen near the center of the domain in the left panels of Figure 6 represent the sites of the most vigorous vortex dynamics and cascade processes as the evolution proceeds. These sites comprise the knots of complex small-scale activity seen in the center panels and to a lesser extent in the right panels. For reference, these sites are those with the least streamwise structure at three approximately uniformly spaced locations in the center panels. The knots of vortex structure also trace the downward progression of the unstable phase of the GW with time.

We quantify the effects of GW breaking further by displaying the domain-averaged wave amplitude,  $a$ , and vertical heat flux,  $\overline{w'T'}$ , as functions of time in Figure 7. Corresponding profiles of wave velocities and temperature are shown in Figure 8 at the stages of the evolution denoted by arrows in Figure 7 (top). Initial wave breaking is accompanied by a large positive vertical heat flux because of the role of instability in removing the superadiabatic lapse rate resulting from GW overturning. This pulse of large heat flux persists for less than a wave period ( $T_{GW} = 3$ ) and  $\overline{w'T'}$  oscillates about zero thereafter. The GW amplitude decreases during the instability growth and vertical mixing from the initial value of  $a_i = 1.1$  to a final value of  $a_f \sim 0.33$ . In fact, this severe amplitude reduction is one of the most surprising results of the GW breaking simulation, as theoreticians and modelers have assumed for many years that instability will drive GW amplitudes towards a state of marginal stability with  $a \sim 1$ .

Vertical profiles of GW velocities and temperature displayed in Figure 8 are plotted subtracting the linear GW phase speed to permit an assessment of the impact of wave breaking on the relative phases of the perturbation quantities. As displayed here, positive velocities are to the left and coincide with the unstable phase of the GW (where  $dT/dz$  is negative). Velocities are redundant because they must remain in the ratio  $u'/w' = 2\sqrt{2}$  with our choice of domain orientation. The first six profiles span the wave breaking and mixing phase of the evolution. These reveal both the amplitude reduction noted above and departures from sinusoidal structure in the vertical because of instability and mixing primarily in the unstable phase of the GW. The effects of localized instability and mixing include 1) an initial reduction of the wave amplitude in the direction of wave propagation (to the left here), 2) an initial expansion of the vertical extent of the upward phase of the wave motion (and of the associated negative temperature gradient), 3) a corresponding increase of the wave shear below the unstable phase of the GW (the middle of the profiles), and 4) a downward advance of the phase of the GW in both velocity and temperature profiles. The latter profiles reveal that the GW structure returns to nearly sinusoidal profiles in approximate quadrature in the  $\sim 16$  buoyancy periods following wave breaking. The late-time implications of wave breaking are thus an amplitude reduction far larger than anticipated theoretically and a phase advance of the resultant GW.

Profiles of eddy (or turbulent) kinetic energy (3D), kinetic energy production and dissipation, thermal dissipation, and an estimate of  $C_T^2$  are displayed in Figure 9 at

the times denoted by arrows in Figure 7. As in Figure 8, these profiles are displayed relative to the GW phase, with the phase of maximum initial instability at  $z/\lambda_z = 0.75$  in each panel. The turbulent kinetic energy is seen to achieve a broad initial distribution spanning the unstable phase and extending into the adjacent stable phases of the GW (see profile 2). Accompanying initial mixing and phase advance, however, turbulent kinetic energy remains a maximum at the lower edge of the formerly unstable layer, as noted in the discussion of the vortex structures in Figure 6. Thus the most energetic turbulent motions advance with the phase of the GW, but disappear quickly after cessation of convective instability. All of these quantities become negligible by  $t \sim 20$ , or  $\sim 3$  GW periods beyond initial instability.

The reason that turbulent kinetic energy remains a maximum at the lower edge of the initially unstable layer becomes apparent when we examine the sources and sinks of turbulent kinetic energy. Turbulent kinetic energy production (solid lines, second panel) and dissipation (short dashed lines second panel, and solid lines fourth panel) of Figure 9 reveal an active source of turbulence extending beyond the most vigorous stages of wave breaking. The persistent structure seen in profiles 3 to 7 suggest a primarily shear-driven source of turbulent kinetic energy in the high-shear portion of the GW (see Figure 8, top), with a compensating return of turbulent energy to the GW (a sink of turbulent kinetic energy) near the velocity maximum above. Without further analysis, we cannot say whether this restores kinetic or potential energy to the GW, but one or the other must occur. Turbulent kinetic energy dissipation achieves a maximum where the production is a maximum and remains large across the turbulent wake extending upward within the GW phase structure. Thus the turbulent kinetic energy profile represents a balance between production, advection, and dissipation, with the continued alignment of turbulent kinetic energy with the descending phase of the GW occurring largely because dissipation acts strongly on the turbulence being left in the wake of the descending GW phase. Note, for example, that turbulent energy dissipation decreases by  $\sim 10$  times across a vertical wavelength of the GW, suggesting that very little turbulence survives being advected into the adjacent (upper) stable phase of the GW.

## 4.2 Layering Accompanying GW Breaking

Layering due to GW breaking is necessarily more transient than that due to KH instability because of the continuous vertical progression of the GW phase and because

strong GW breaking and turbulence are typically confined to  $\sim 1$  GW period for higher-frequency motions. This argues against permanent effects of localized mixing, except possibly in cases where GW localization and/or superposition initiate a localized patch of turbulence that does not progress through the atmosphere with the phase of the GW. However, this is speculative at present as such simulations have not yet been performed.

The transient layering that accompanies GW breaking includes responses to both 1) localized turbulence at early stages of the evolution and 2) the structure of the more nearly homogeneous turbulence (along the GW phase) during the decay stage. At early stages in the evolution, localized regions of strong turbulence induce similarly localized patches of strong mixing, each with thermal gradients at the edges that are enhanced relative to other regions of the flow. These regions are similar locally to the turbulent layer due to KH instability, where strong gradients arise at the edges due to efficient mixing within the turbulent layer. In particular, the most intense vortex knots in the upper panels correspond to regions of separated  $\epsilon$  and  $\chi$  (not shown).

At larger scales (and later times), layering is more uniform along the GW phase because sources and sinks of turbulent kinetic energy are localized within the GW phase and turbulence is decaying. The lower edge of the turbulent kinetic energy maximum lies adjacent to the more strongly stratified phase of the GW below. As in the KH simulations, significant turbulent kinetic energy (and dissipation) adjacent to stable stratification implies large thermal gradients and small-scale thermal structure. This implies, in turn, large thermal dissipation and  $C_T^2$  (see the third and fifth panels of Figure 9) during the decay phase of turbulence. Importantly, the maxima of thermal dissipation and  $C_T^2$  and the maximum in  $\epsilon$  occur in different phases of the GW. Note, however, that this stage persists for only  $\sim 1$  GW period, and that apparent layering and variations of turbulence and its effects across the GW field decay quickly thereafter.

## 5. Comparison and Discussion of Turbulence Layering and Anisotropy

Our discussion above addressed two very different processes that result in turbulence generation and layering in the atmosphere. KH instability arises at a dynamically unstable shear layer (with  $Ri < 1/4$ ) due to mean or low-frequency GW shear, evolves on a time scale of several buoyancy periods, and results in turbulence and mixing that are confined by stratification to a thin layer about the initial shear layer. For the parameters studies here, the turbulence layer depth is  $\sim 3$  times that of the initial shear layer. GW

breaking involves overturning of the stable thermal structure of the atmosphere, evolves on a time scale of a GW period or less, and results in turbulence and mixing that are closely tied to, and move with, the unstable phase of the GW.

Similarities between the turbulence and layering in the two flows include 1) related transitions to turbulence via streamwise-aligned vortex structures deriving kinetic energy from both buoyancy and shear sources, 2) transitions to full turbulence via vortex interactions and twist-wave dynamics common to both flows, 3) expansion, mixing, and influences of turbulence beyond the initial region of instability, 4) a turbulence duration, at least for the flows examined here, of several buoyancy periods or less, 5) sharp gradients in turbulence quantities in edge regions, and 6) spatial separation of the peak turbulent kinetic energy and thermal dissipation. Indeed, the latter similarity implies that radar measurements of both flows will be biased towards the maximum of  $C_T^2$  and relatively less sensitive to the maximum in  $\epsilon$ , causing radar estimates of  $\epsilon$  to be inaccurate in both cases [Gossard et al., 1971; Browning, 1971; Röttger and Schmidt, 1979; Eaton et al., 1995; Gibson-Wilde et al., 2000].

Despite these similarities, there are also significant differences between the turbulence and layering occurring due to KH instability and GW breaking. The major differences arise because turbulence due to KH instability is localized and confined by mean stratification, whereas turbulence accompanying GW breaking sweeps through the fluid following the phase of the GW in which the most vigorous turbulence sources are operative. This enables sharper and more persistent edge regions accompanying KH instability, which can persist far beyond the duration of the turbulence event. Sharp temperature gradients, especially at the upper edge, may play a role in layering of quantities, such as NLC particles or aerosols, that are strongly temperature dependent.

Though we have yet to perform GW breaking simulations for significantly smaller  $\omega$ , we speculate that a slower vertical phase velocity would enable more confined turbulence generation within the GW, thinner layers of turbulence, and a sharper spatial separation between maxima of  $C_T^2$  and  $\epsilon$ . For both high and low intrinsic frequencies, the occurrence of turbulence primarily within the most unstable phase of the GW seems to support the arguments for weak mixing and a large turbulent Prandtl number due to GW breaking advanced by Fritts and Dunkerton [1985], Coy and Fritts [1988], and McIntyre [1989]. Mixing in the case of KH instability is relatively efficient within a turbulent layer if

constituents behave like temperature. The uncertainty is how effectively successive turbulent layers diffuse the sharp gradients created by earlier turbulence events [Rosenberg and Dewan, 1975; Cadet, 1977]. Finally, while biases in radar estimates of  $\epsilon$  appear likely in both flows, biases in estimates of mean vertical motions appear likely only due to GW breaking, where  $C_T^2$  maxima occur largely in the descending phase of the GW and support the arguments of Nastrom and VanZandt [1994] and Hoppe and Fritts [1995].

## 6. Conclusions

We have described and compared simulations of turbulence arising due to KH instability and GW breaking as well as the implications of these turbulence events for layering and layered structures in the atmosphere. The two flows share many characteristics related to turbulence transition, evolution, and duration, and these characteristics impose some similarities on turbulence layering common to both flows. Perhaps the most relevant is the separation of maxima of  $C_T^2$  and  $\epsilon$ , given the implications of such separations for atmospheric measurements employing radars. But the two turbulent flows also exhibit a number of differences that have important implications for layering and layered structures. The differences arise because of the different vertical motion (or lack of) of the turbulence source, with the effects of turbulence due to KH instability potentially more significant and longer lasting than those due to GW breaking. Whereas layering, enhanced radar backscatter, and vertical wind measurement biases are likely significant accompanying GW breaking only for a few buoyancy periods, the layering, thermal gradients, enhanced backscatter, and effects of local mixing due to KH instability remain features of the flow long after turbulence has subsided.

While turbulence does not account for, or even play a role in, all layering processes at mesopause altitudes, its role in defining the large- and small-scale structure of the atmosphere, and in influencing many atmospheric processes and measurements, is unequivocal. Given this, the role of numerical studies of turbulence will play a key role in further quantifying these influences in the future.

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## Figure Captions

**Figure 1.** Geometry employed for the GW breaking simulation. The domain is inclined along the GW phase such that the group velocity is along the streamwise ( $x$ ) direction. In this geometry, the streamwise wavelength is infinite and gravity and stratification both have streamwise and “vertical” components.

**Figure 2.** Volumetric views of vorticity and dissipation fields arising due to KH instability at  $t = 50, 70,$  and  $120$  (left to right, with  $T_{BV} = 28$ ). The vorticity fields (top panels) and turbulent kinetic energy dissipation ( $\epsilon$ ) and thermal dissipation ( $\chi$ ) fields (bottom panels) are viewed from the side and ahead (from  $x, y > 0$ ). Dissipation fields are shown in yellow/red and blue, with larger values opaque and smaller values transparent. Motions are to the left in the upper portion of the domain and to the right in the lower portion of the domain.

**Figure 3.** Profiles of  $T, U(z), Ri, \epsilon,$  and  $\chi$  averaged spanwise (and streamwise in the lower three panels) at  $t = 50, 60, 70, 90, 105, 120, 160,$  and  $300$  for the KH simulation. Solid (dashed) lines in the upper two panels are through (between) billows. Horizontal scales display the magnitudes for each quantity and successive profiles are offset uniformly in each case. Thus  $Ri$ , for example, exhibits variations between 0 and 1 except at the earliest times, with the value  $Ri = 1/4$  shown with a dashed line for the final profile. All units are nondimensional.

**Figure 4.** Profiles of  $C_T^2, \theta,$  and  $Ri$  obtained by Coulman et al. [1995] and displaying a series of active or past KH turbulence events (reprinted with permission of Applied Optics).

**Figure 5.** As in Figure 4, but close-ups of two KH turbulence events (upper two panels, after Coulman et al. [1995], reprinted with permission of Applied Optics) and from our KH simulation (lower panel) at  $t = 160$ .

**Figure 6.** As in Figure 2, but for vorticity fields arising due to GW breaking at  $t = 5.26, 11.25,$  and  $12.66$  (left to right, with  $T_{BV} = 1$  and  $T_{GW} = 3$ ). The vorticity fields are viewed from the side and above (top and bottom panels). Motions are initially up and to the right in the upper portion of the domain and down and to the left in the lower portion of the domain, and the GW phase progresses downward with time.

**Figure 7.** GW amplitudes,  $u'_{tot}$  and  $T'$  (bottom), and heat flux,  $\overline{w'T'}$  (top), averaged streamwise and spanwise, as functions of time. The initial GW amplitude corresponds to  $a_i = 1.1$ , the final amplitude is  $a_f \sim 0.33$ , and time is in buoyancy periods.

**Figure 8.** Profiles of GW velocities,  $u'$  and  $w'$  (top), and temperature,  $T'$  (bottom), at  $t =$

5.26, 11.25, 12.66, 12.83, 12.97, 13.58, 13.90, 19.76, and 30. Scales show nondimensional amplitudes and successive profiles are displaced uniformly.

**Figure 9.** As in Figure 8 for turbulent kinetic energy (top), turbulent kinetic energy production and dissipation rates (second panel, solid and short dashed lines), thermal dissipation (third panel), viscous dissipation (fourth panel), and an estimate of  $C_T^2$  (bottom).