Empirical Orthogonal Function Analysis of the Weakly Convective Atmospheric Boundary Layer. Part II: Eddy Energetics

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(Manuscript received 16 January 1995, in final form 11 August 1995)

ABSTRACT

Three-dimensional empirical orthogonal functions (EOFs), calculated from a large-eddy simulation of a weakly convective, planetary boundary layer (PBL), are used to decompose statistics for PBL turbulence into contributions from individual structures. The most energetic EOFs, corresponding largely to boundary-layer-spanning eddies, together are responsible for about one-half of the turbulent kinetic energy (TKE) throughout the boundary layer, although they carry a substantial amount of the momentum and heat fluxes only near mid-PBL. Examination of the flux profiles also reveals coupling between large roll structures and inversion-borne gravity waves. By filtering the fields through the EOFs, skewness and intermittency (kurtosis) associated with the different vertical scales are determined. Positive skewness around mid-PBL is found to be attributable to the boundary-layer spanning eddies. Intermittency, however, cannot be attributed to either large- or small-scale structures: it results from interscale interactions. Finally, equations for the flux and energy budgets of individual structures are derived. The budget analyses show clearly that the main source of TKE for large roll structures is shearing stress, while the main loss mechanism is transfer to smaller scales. The inversion-borne gravity waves gain TKE from interscale transfers and buoyant acceleration and lose TKE to shearing effects.

1. Introduction

It was shown in the companion paper (Wilson 1996, hereafter W96) how atmospheric boundary-layer turbulence can be decomposed into sums of statistically uncorrelated modes called empirical orthogonal functions (EOFs). The EOF modes often were found to have interpretations as flow structures, such as boundary-layer rolls and gravity waves. The emphasis in W96 was on the qualitative characteristics of the EOF modes. In this paper, the EOF modes for the same large-eddy simulation (LES) database are examined in a statistical, quantitative manner. Second-order statistics, such as turbulent kinetic energy (TKE), momentum, and heat fluxes, are computed for individual EOF modes. Higher-order statistics (skewness and kurtosis) are also associated with the EOFs using an indirect method. Finally, a budget equation for the second-order statistics of individual EOF modes is derived and applied. The main benefit of decomposing the statistics and budget equations in terms of EOF modes occurs when we are able to relate a mode to a particular type of coherent structure. Then we can examine, for example, the heat flux profile of a particular roll structure.

Calculation of second-order statistics, such as TKE and flux profiles, for the individual EOFs is quite simple once the modes have been computed: they are simply the product of two eigenfunctions and an eigenvalue. Furthermore, the contributions of the individual EOF modes to a second-order statistic sum to the value for the total field. In section 2 of this paper we will examine TKE and flux profiles of individual structures using this method.

The situation for statistics higher than second order, such as skewness and kurtosis, is somewhat more complicated. Since only second-order statistics are incorporated into the EOF analysis, we must determine the higher-order statistics by filtering the original fields with sets of the EOFs and then calculating the statistics of the filtered fields. For higher-order statistics it is not the case that the contributions associated with the individual structures sum to the total for the field. Higher-order statistics of the EOF modes and the overall fields are discussed in section 3.

Budget (or *tendency*) equations have been found to be a very useful tool for understanding the dynamics of atmospheric turbulence. These equations are normally derived using the Reynolds decomposition, by which the fields are decomposed into mean and fluctuating parts. In this paper we derive budget equations for second-order statistics that result when the fields are decomposed into their individual EOF modes. This makes it possible to examine the energetics and transport properties of a particular type of structure. The

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EOF budgets contain all the terms familiar from the Reynolds decomposition. For example, the TKE budget of an individual EOF mode has terms for shear and buoyancy production, pressure redistribution, turbulent transport (flux divergence), and molecular dissipation. The main distinction between the two decompositions is that the turbulent transport term in the Reynolds budget also incorporates interscale transfer effects (triad interactions) when it appears in the EOF budget. The EOF budget equations are derived and studied using LES data in section 4.

2. Flux and energy decompositions

a. Formalism

We begin by considering vertical profiles of second-order statistics (covariances) for the EOFs. As in W96, a set of state variables $\beta_i(x, y, z)$ is defined, with $\beta_1 = u/w_*$, $\beta_2 = v/w_*$, $\beta_3 = w/w_*$, and $\beta_4 = \theta/\theta_*$, where w_* and θ_* are the convective, mixed-layer scales. The height-dependent covariance is, by definition,

$$\sigma_{ij}^2(z) = R_{ij}(0, 0, z, z) = \langle \beta_i(x, y, z) \beta_j(x, y, z) \rangle. \quad (1)$$

The angle brackets indicate ensemble average. Cases of special interest include the turbulent kinetic energy (TKE, sum over $i = j = 1, 2, 3$), the longitudinal momentum flux ($i = 1, j = 3$), and the temperature flux ($i = 3, j = 4$). As shown in W96, the covariances can be written as a sum over EOF modes:

$$\sigma_{ij}^2(z) = \sum_n [\sigma_{ij}^{(n)}(z)]^2, \quad (2)$$

where

$$[\sigma_{ij}^{(n)}(z)]^2 = \iint \Phi_{ij}^{(n)}(k_x, k_y, z, z) dk_x dk_y, \quad (3)$$

and

$$\Phi_{ij}^{(n)}(k_x, k_y, z, z) = \lambda^{(n)}(k_x, k_y) \hat{\phi}_i^{(n)}(k_x, k_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z). \quad (4)$$

The carat indicates the horizontal Fourier transform, with k_x and k_y being the horizontal wavenumbers and the superscript (n) the EOF index. The eigenvalues are the $\lambda^{(n)}$, and the eigenfunctions (EOFs) are the $\phi_i^{(n)}$'s.

It is often valid to associate increasing EOF index with decreasing vertical spatial scale. For example, we might attribute $\sigma_{ij}^{(1)}$ to large, boundary-layer-spanning eddies or to inversion-spanning wave motions. This is because energy decreases with increasing EOF index (by definition) and energy *usually* decreases with spatial scale. This connection is demonstrated in Fig. 1, which shows the real part of the temperature profiles for EOFs at wavenumber B, $(\kappa_x, \kappa_y) = (5/4, 1)$. (Refer to W96 for the wavenumber labelling scheme.) EOF 1 is observed to have no significant zero crossings, while EOF 2 has one. Although the structure becomes more

FIG. 1. Real part of the EOFs for temperature at $(\kappa_x, \kappa_y) = (5/4, 1)$. The solid line is for EOF 1, dotted 2, dashed 3, dash-dotted 4.

noisy for EOFs 3 and 4, they clearly have multiple zero crossings. We should point out that the EOFs at B, since they primarily represent temperature fluctuations at and around the inversion level, provide a particularly strong example of the connection between EOF index and vertical scale. At other locations in the horizontal wavenumber domain this connection is not always so clear. Hence, although the association of increasing EOF index with decreasing vertical spatial scale will often be made in this paper for the purpose of simplicity, the reader should keep in mind the limitations of this approach. Moser (1994) has dealt with the characterization of spatial scales corresponding to EOF modes in a more precise manner; perhaps his results can be applied to future EOF studies of BL turbulence.

b. Integrated profiles

As in W96, we use data from a large-eddy simulation (LES) for the EOF case study. The simulation was very weakly convective, with geostrophic wind 22.5 m s^{-1} , and surface temperature flux 0.03 K m s^{-1} . The mixed-layer scales were $w_* = 0.79 \text{ m s}^{-1}$ and $\theta_* = -0.038 \text{ K}$, the friction velocity was $u_* = 0.69 \text{ m s}^{-1}$, and $-z_i/L$ was 0.59. More details on the run can be found in W96.

Figure 2a shows the fraction of the resolved TKE due to the EOF 1, $\sum_{\alpha=1}^3 [\sigma_{\alpha\alpha}^{(1)}(z)]^2$, and to the sum of the first three EOFs, $\sum_{n=1}^3 \sum_{\alpha=1}^3 [\sigma_{\alpha\alpha}^{(n)}(z)]^2$. In both

FIG. 2. (a) Fractions of the resolved TKE that are due to the first EOF (solid line) and the sum of the first three EOFs (dotted line). (b) Fractions of the total TKE. Also shown is the resolved TKE (dashed line).

cases, the EOFs contributions to TKE change little with height: the first EOF accounts for about 50% of the resolved TKE throughout the BL, whereas the sum of the first three EOFs accounts for about 80% of the resolved TKE. Figure 2b is similar to Fig. 2a, except that the fraction of the total (resolved plus subgrid) TKE is shown. We observe that, at a height of $0.1z_i$, the BL-scale structures (as accounted for by the first EOF) contain about 31% of the total TKE. At $0.6z_i$, the BL-scale structures contain about 49% of the total TKE. Note that the resolved TKE accounts for 85%–90% of the total TKE over most of the BL, except very near the ground, where only 50% of the TKE is resolved. The conclusion to be drawn from these results is that largest, BL-scale structures, represented by the first EOF, are responsible for about one-half of the TKE in the boundary layer. The majority of the remaining TKE exists in other large-scale structures represented by EOFs 2 and 3.

Figures 3a,b show a similar analysis for the momentum flux, and Figs. 4a,b for the heat flux. At a height of $0.1z_i$, the first EOF is found to carry only 14% of the total momentum flux and 7% of the total heat flux. Near mid-BL, at $0.6z_i$, the first EOF is responsible for a much larger fraction of the fluxes: 55% of the total momentum flux and 25% of the total heat flux. Overall, the first EOF contributes about 50%–65% of the resolved momentum flux and 40%–55% of the resolved heat flux. The sum of the first three EOFs contributes 75%–95% of the resolved momentum flux (although somewhat less near the inversion) and 70%–90% of the resolved heat flux. (The discontinuity at $0.5z_i$ in the curves in Figs. 4a,b results from the vanishing heat flux at that level.)

FIG. 3. (a) Fractions of the resolved momentum flux that are due to the first EOF (solid line) and the sum of the first three EOFs (dotted line). (b) Fractions of the total momentum flux. Also shown is the resolved momentum flux (dashed line).

In comparison to the TKE, the fractions of the momentum and heat fluxes resolved by the first few EOFs are much less near the surface and near the inversion. In particular, the first few EOFs contain a vanishing amount of the total fluxes near the surface. This leads us to the important conclusion that while the large, BL-spanning structures contribute substantially to the TKE near the surface, they are not directly responsible for the transport of momentum and heat. The large, coherent structures can still play an important indirect role, though, by triggering the generation of smaller eddies, which in turn carry most of the flux. Evidence for this view will be presented in section 3.

FIG. 4. (a) Fractions of the resolved heat flux that are due to the first EOF (solid line) and the sum of the first three EOFs (dotted line). (b) Fractions of the total heat flux. Also shown is the resolved heat flux (dashed line).

c. Individual structures

The quantity $\Phi_{ij}^{(n)}(k_x, k_y, z, z)$ is the contribution of an EOF mode (k_x, k_y, n) to the covariance σ_{ij}^2 . These modal covariances can be computed directly from the eigenfunctions and eigenvalues using Eq. (4).

The modal EOF energy, TKE, momentum flux, and heat flux profiles for wavenumber B, $(\kappa_x, \kappa_y) = (5/4, 1)$, are shown in Fig. 5. (The lettering scheme for the EOFs was discussed in W96.) EOF B1 contains many times more EOF energy than B2 or the other modes at this wavenumber. The reason is that B1 has much stronger temperature fluctuations than B2. The difference in TKE between B1 and B2 is not nearly so great. In fact, the TKE in B2 peaks at $z/z_i = 0.9$ and is about twice as great as B1 there. The TKE in B1 peaks just above the inversion at around $z/z_i = 1.1$.

Both the momentum and heat flux profiles for B2 have the appropriate sign for down gradient transport, but transport is counter gradient for B1. The heat flux for B1 is strongly positive in the region from about $z/z_i = 1$ to 1.2 . If one examines the flow realization for B1 in W96, it is clear that temperature and vertical velocity are nearly in phase quadrature. Perfect phase quadrature would yield zero heat flux; there is a small but dynamically significant difference from phase quadrature in mode B1.

Energy and flux profiles for wavenumber D, $(\kappa_x, \kappa_y) = (-1/5, 1/5)$, are shown in Fig. 6. Structure D1 has positive heat flux and negative momentum flux up to $z/z_i = 0.8$. Interestingly, D1 has a countergradient heat flux region from about $z/z_i = 1$ to 1.2 , which is very similar to B1. This could indicate coupling to a gravity wave. The TKE in D1 peaks near the surface, at $z/z_i = 0.2$. The TKE in D2 peaks much higher in the BL at about $z/z_i = 0.7$. The heat and momentum fluxes in D2 are negligible up to a height $z/z_i = 0.3$, but the heat

flux has a pronounced minimum at $z/z_i = 0.7$. Apparently D2 is involved in the entrainment of warm air at the inversion level.

Energy and flux profiles for wavenumber E, $(\kappa_x, \kappa_y) = (-1/3, 1)$, are shown in Fig. 7. Structure E1 clearly contains more EOF energy than E2. But within the lower BL, the EOF energy, TKE, momentum, and heat fluxes of E2 exceed those of E1. The heat flux for E1 changes sign at mid-BL, whereas E2 remains positive throughout most of the BL. (This behavior can also be deduced from the flow realizations for these structures shown in W96.) It is interesting that beginning at a height $z/z_i \approx 0.9$, the heat flux profile and other profiles for E1 bear a strong resemblance to that of B1. In W96, E1 and E2 were called inflection-point and thermal roll modes, respectively, in order to distinguish between their distinct heat transport properties. Since B1 was established as a gravity wave mode in W96, E1 is apparently a BL roll coupled to an inversion-borne gravity wave. Such coupling between BL motions and gravity waves has been discussed by Stull (1976), Mason and Sykes (1982), Clark et al. (1986), and Kuettner et al. (1987), among others.

Lastly, we consider the energy and flux profiles for wavenumber F, $(\kappa_x, \kappa_y) = (-1/3, 2)$, in Fig. 8. The TKE for F1 peaks around mid BL, at $z/z_i = 0.4$, while F2 peaks at $z/z_i = 0.7$, and F3 at $z/z_i = 0.2$. Because each EOF seems to be concentrated in its own distinct region of space, we should not be too hasty to interpret these EOFs as physically meaningful structures. They could be strongly influenced by the vertical finite-differencing scheme in the LES. Still, it is worth noting the strong similarities between the momentum and heat flux profiles of E1 and F2, and to a lesser extent between B2, D2, and F1. The flux profiles of D1, F2, and F3 are also quite similar, at least up to $z/z_i = 0.8$.

FIG. 5. Vertical profiles of second-order statistics for individual EOF modes at wavenumber B. (a) EOF energy. (b) TKE. (c) Momentum flux. (d) Temperature flux. Solid line: B1. Dotted line: B2. Dashed line: B3. Dash-dotted line: B4. Total at B: circles.

FIG. 6. Vertical profiles of second-order statistics for individual EOF modes at wavenumber D. (a) EOF energy. (b) TKE. (c) Momentum flux. (d) Temperature flux. Solid line: D1. Dotted line: D2. Dashed line: D3. Dash-dotted line: D4. Total at D: circles.

3. Higher-order statistics of the structures

As discussed in W96, the EOF analysis does not retain information on statistics higher than second order, such as skewness and kurtosis. This is because the third- and higher-order statistics depend on mutual phasing (i.e., interactions) between Fourier modes, and the spectral density tensor used to compute the EOFs has no such phase information. Unfortunately, the higher-order statistics do contain important information on turbulence structure that is frequently of much interest. For example, positive skewness means that the updrafts are stronger than the downdrafts. Values of the kurtosis above 3 mean that the turbulence is more intermittent than a Gaussian process. And so the question arises as to how we can derive higher-order statistics for structures found using the EOF decomposition. The simplest way to restore the required phase information is to calculate the projection of the EOFs onto the original field; that is, filter the fields through the EOFs. The phase information is preserved in the filtered fields.

In filtering the fields, it is important to remember that the filtering must be done using a *set* of EOFs, not just a single mode. Filtering with a single mode would result in a loss of all information on interactions, hence yielding zero skewness and Gaussian kurtosis. In the following analysis each set of EOFs used in the filtering operation includes all horizontal wavenumbers at a single, fixed EOF index. The intention of filtering with sets of modes defined in this manner is to isolate the skewness and kurtosis attributable to various vertical spatial scales.

The projection coefficients of the EOFs are (W96)

$$\hat{a}_n(k_x, k_y) = \int \hat{\beta}_i(k_x, k_y, z) \hat{\phi}_i^{(n)*}(k_x, k_y, z) dz. \quad (5)$$

Hence the part of the field accounted for by EOF n is

$$\hat{\beta}_\alpha^{(n)}(k_x, k_y, z) = \hat{a}_n(k_x, k_y) \hat{\phi}_\alpha^{(n)*}(k_x, k_y, z). \quad (6)$$

The skewness and kurtosis associated with EOF n are then

$$S_\alpha^{(n)}(z) = \frac{\langle [\hat{\beta}_\alpha^{(n)'}(x, y, z)]^3 \rangle}{[\sigma_\alpha^{(n)}(z)]^3} \quad (7)$$

and

$$K_\alpha^{(n)}(z) = \frac{\langle [\hat{\beta}_\alpha^{(n)'}(x, y, z)]^4 \rangle}{[\sigma_\alpha^{(n)}(z)]^4}. \quad (8)$$

We computed skewness and kurtosis by approximating the ensemble averages as horizontal averages over a single snapshot of the field. Smoother curves probably could have been obtained by averaging over more snapshots; however, the amount of data generated would have been prohibitive.

Figure 9 shows the vertical velocity skewnesses of the unfiltered field and the EOFs $n = 1, 2$, and 5. The skewness of the unfiltered velocity field is negative near the surface, increases with height, becomes positive around mid-BL, and decreases as the inversion is approached. This behavior is not unlike the Rayleigh-Bénard and cloud-topped cases considered by Moeng and Rotunno (1990). In contrast, experimental data for convective boundary layers do not exhibit a ground-based region of negative skewness (Wyngaard 1988). However, it should be pointed out that our simulation is only very weakly convective. Presumably the negatively skewed region would shrink if the surface heat flux were increased.

The dotted line in Fig. 9 is the skewness associated with EOF 1, $S_3^{(1)}(z)$. It is positive over most of the BL, implying that BL-scale structures are positively skewed; that is, their updrafts are stronger than their

FIG. 7. Vertical profiles of second-order statistics for individual EOF modes at wavenumber E. (a) EOF energy. (b) TKE. (c) Momentum flux. (d) Temperature flux. Solid line: E1. Dotted line: E2. Dashed line: E3. Dash-dotted line: E4. Total at E: circles.

downrafts. Smaller-scale structures (EOFs 2 and 5, dashed and dash-dotted lines, respectively) are not so strongly skewed. In fact, EOF 5 has negative skewness near the surface. Apparently it is the small-scale structures that cause the unfiltered fields to have negative skewness at the surface. It is interesting that Hunt et al. (1988) found the opposite trend in actual data for convective boundary layers, namely that the small eddies contribute positively to the skewness near the surface. The disagreement could be due either to the small surface heat flux in our simulation, to the finite resolution of LES, or to the fact that we have used vertical filtering, whereas Hunt et al. used horizontal filtering.

The vertical velocity kurtosis is plotted in Fig. 10. The kurtosis of the unfiltered field peaks at the surface

and at $z \approx 0.8z_i$. The peak values, about 4.5, are well above the value for a Gaussian process, 3. This tells us that the vertical velocity is very intermittent at the surface and below the inversion. In contrast, the individual EOFs all have kurtosis near the Gaussian value. Lumley and Takeuchi (1976) have previously noted that statistics of bandpass filtered turbulence become more Gaussian as the pass band is narrowed. This is apparently the reason why the kurtoses of the individual EOFs are more nearly Gaussian than the unfiltered field. Therefore intermittency must result from coherent interactions among eddies of differing scales.

Intermittency of covariances, such as fluxes, can be studied using the method of Siegel (1995). Siegel used wavelet transforms to decompose the fluxes into con-

FIG. 8. Vertical profiles of second-order statistics for individual EOF modes at wavenumber F. (a) EOF energy. (b) TKE. (c) Momentum flux. (d) Temperature flux. Solid line: F1. Dotted line: F2. Dashed line: F3. Dash-dotted line: F4. Total at F: circles.

FIG. 9. Vertical velocity skewness associated with the EOFs. The solid line is the unfiltered field. EOF 1: dotted line. EOF 2: dashed line. EOF 5: dash-dotted line.

FIG. 10. Vertical velocity kurtosis associated with the EOFs. The solid line is the unfiltered field. EOF 1: dotted line. EOF 2: dashed line. EOF 3: dash-dotted line.

tributions by scale. In this paper, the scale decomposition is accomplished with EOFs rather than wavelets. The kurtosis of a flux is a joint eighth moment:

$$K_{ij}^{(n)}(z) = \frac{\langle [\beta_i^{(n)'}(x, y, z) \beta_j^{(n)'}(x, y, z)]^4 \rangle}{[\sigma_i^{(n)}(z) \sigma_j^{(n)}(z)]^4}. \quad (9)$$

As shown by Siegel (1995), the joint kurtosis of a Gaussian process is

$$K_{ij,G}^{(n)}(z) = 24[\rho_{ij}^{(n)}(z)]^4 + 72[\rho_{ij}^{(n)}(z)]^2 + 9, \quad (10)$$

where

$$\rho_{ij}^{(n)}(z) = \frac{\langle \beta_i^{(n)'}(x, y, z) \beta_j^{(n)'}(x, y, z) \rangle}{\sigma_i^{(n)}(z) \sigma_j^{(n)}(z)} \quad (11)$$

is the correlation coefficient for $\beta_i^{(n)'}$ and $\beta_j^{(n)'}$.

In Fig. 11, we plot the normalized difference between the actual joint kurtosis and the Gaussian prediction; that is, $[K_{ij}^{(n)} - K_{ij,G}^{(n)}]/K_{ij,G}^{(n)}$. The kurtosis of the unfiltered fields has a strong peak, well above the Gaussian value, just below the inversion level. A lesser maximum occurs near the ground. On the other hand, EOFs 1 and 2, as well as the unfiltered field between $0.1z_i$ and $0.5z_i$, actually have kurtosis slightly below that of a Gaussian process. As the EOF index increases, the kurtosis approaches that of a Gaussian process. This means that the momentum flux carried by the individual structures, as well as the total resolved momentum flux in much of the lower BL, cannot be characterized as intermittent. We must remember, though, that much of the momentum flux is unresolved by the LES near the ground. The momentum flux from small-scale structures, unresolved by the LES, could still be highly intermittent.

The behavior of the temperature flux kurtosis, Fig. 12, is quite similar to the momentum flux. The main difference is that the maximum occurs lower in the BL around $0.6z_i$.

4. EOF budget equations

The topic of this section is budget equations for covariances of individual EOF modes. By budget equation, we mean an equation that breaks down the time rate of change of the statistical quantity into contributions from the relevant physical forcings.

This study is actually far from the first to consider decomposition of the TKE and other budgets into contributions from individual modes. The EOF decomposition is in fact closely related to the Fourier spectral decomposition. In the spectral decomposition, the wavenumber is inversely proportional to the scale, whereas in the EOF de-

FIG. 11. Momentum flux kurtosis associated with the EOFs. The normalized difference between the kurtosis and the prediction for a joint Gaussian process is plotted. The solid line is the unfiltered field. EOF 1: dotted line. EOF 2: dashed line. EOF 3: dash-dotted line.

FIG. 12. Temperature flux kurtosis associated with the EOFs. The normalized difference between the kurtosis and the prediction for a joint Gaussian process is plotted. The solid line is the unfiltered field. EOF 1: dotted line. EOF 2: dashed line. EOF 3: dash-dotted line.

composition the relationship between scale and EOF index is not always so clear. A special case is that of three-dimensional spatial homogeneity, for which the EOF and spectral analyses yield equivalent results. (As discussed in W96, the EOFs are simply harmonic functions in homogeneous spatial directions. In an inhomogeneous direction, the vertical in our case, the EOFs must be determined from an eigenanalysis of the correlation function.) Brasseur and Wei (1994) studied the TKE spectral budget and interscale transfers in a low Reynolds number flow simulation and include many references to earlier work. Lumley and Panofsky (1964) and Borkowski (1969) developed spectral budget models for atmospheric turbulence that included anisotropy. Lumley and Panofsky also considered inhomogeneous turbulence in which the integral length scale varied in proportion to height. McBean and Elliot (1975) considered the balance between shear production, buoyancy production, interscale transfer, and viscous dissipation in 1D longitudinal spectra. Our budget analysis deals with a more complicated situation than was considered by these earlier authors since it incorporates inhomogeneity in the vertical direction.

Previous researchers, such as Lenschow and Stephens (1980), Young (1988), and Schumann and Moeng (1991), have also developed budget equations for individual structures. Specifically, they dealt with thermal plumes in convective boundary layers. All used conditional sampling techniques to distinguish between the plumes and their background environment. The plume budget analyses developed by these authors are designed for spatially compact structures: the nonlinear terms in the budget represent gain-loss between the plume and its environment. Mathematically, the nonlinear terms are the flux divergence of the budgeted quantity at the plume boundary.

The EOF budgets are not directly comparable with the conditionally sampled plume budgets. This is because the EOF structures have no boundaries; they are in fact harmonic in the horizontal directions, containing alternating updrafts and downdrafts of equal strength. The nonlinear terms in the EOF budget represent interactions between structures having different spatial scales, rather than flux-divergence across spatial boundaries.

a. Decomposition

Derivation of the EOF covariance budget begins by relating the time derivative of the EOF covariance to the time derivative of the field variables. Differentiating (2), we have

$$\frac{\partial \sigma_{ij}^2(z)}{\partial t} = \sum_n \iint \frac{\partial \Phi_{ij}^{(n)}(k_x, k_y, z)}{\partial t} dk_x dk_y. \quad (12)$$

By Parseval's theorem, the covariance can also be written as an integration over the wavenumber domain:

$$\sigma_{ij}^2(z) = \iint \langle \hat{\beta}_i(k_x, k_y, z) \hat{\beta}_j^*(k_x, k_y, z) \rangle dk_x dk_y. \quad (13)$$

Taking the time derivative of this expression, we have

$$\frac{\partial \sigma_{ij}^2(z)}{\partial t} = \sum_n \iint \left(\left\langle \frac{\partial \hat{\beta}_i}{\partial t} \hat{\beta}_j^* \right\rangle + \left\langle \hat{\beta}_i \frac{\partial \hat{\beta}_j^*}{\partial t} \right\rangle \right) dk_x dk_y. \quad (14)$$

Equating (12) and (14) and expanding the undifferentiated $\hat{\beta}$ s in terms of the EOFs, we find

$$\frac{\partial \Phi_{ij}^{(n)}(k_x, k_y, z)}{\partial t} = \left\langle \frac{\partial \hat{\beta}_i}{\partial t} \hat{a}_n^* \right\rangle \hat{\phi}_j^{(n)*} + \left\langle \hat{a}_n \frac{\partial \hat{\beta}_j^*}{\partial t} \right\rangle \hat{\phi}_i^{(n)}. \quad (15)$$

The quantity $\partial \Phi_{ij}^{(n)}(k_x, k_y, z)/\partial t$ can be identified as the contribution to the covariance budget from an individual EOF mode (k_x, k_y, n) .

In order to calculate the EOF covariance budget explicitly, an expression for $\partial \hat{\beta}_i/\partial t$ is still needed. We call this the state equation, and it is derived in nondimensional form in the appendix. Taking the Fourier transform of the state equation (A8) (see appendix) and defining $k_x'' = k_x - k_x'$, $k_y'' = k_y - k_y'$, we find

$$\begin{aligned} \frac{\partial \hat{\beta}_i(k_x, k_y, z)}{\partial t} = & - \iint \hat{\beta}_j(k_x', k_y', z) \hat{D}_j(k_x'', k_y'') \\ & \times \hat{\beta}_i(k_x'', k_y'', z) [1 - \delta(k_x', k_y') - \delta(k_x'', k_y'')] \\ & \times dk_x' dk_y' - \hat{\beta}_j(0, 0, z) \hat{D}_j(k_x, k_y) \hat{\beta}_i(k_x, k_y, z) \\ & - \hat{\beta}_j(k_x, k_y, z) \hat{D}_j(0, 0) \hat{\beta}_i(0, 0, z) \\ & - \hat{D}_i(k_x, k_y) \hat{p}(k_x, k_y, z) - \hat{\beta}_4(k_x, k_y, z) \\ & \times [1 - \delta(k_x, k_y)] \delta_{i3} - \frac{1}{\text{Ro}} \epsilon_{ijk} \Omega_j \hat{\beta}_k(k_x, k_y, z) \\ & + \frac{1}{\text{Re}} \nu_{ik} \hat{D}_j(k_x, k_y) \hat{D}_j(k_x, k_y) \hat{\beta}_k(k_x, k_y, z), \quad (16) \end{aligned}$$

where

$$\hat{D}_j(k_x, k_y) = \begin{cases} ik_x & j = 1 \\ ik_y & j = 2 \\ \partial/\partial z & j = 3 \\ 0 & j = 4 \end{cases}, \quad (17)$$

and ϵ_{ijk} , ν_{ik} , Ro , and Re are defined in the appendix. In writing the nonlinear term, the parts of the integral representing mean-turbulent interactions have been separated out from the turbulent-turbulent interactions. We associate the terms on the right-hand side with non-

linear interactions, mean advection, gradient production, pressure transport, buoyancy, Coriolis effect, and molecular effects, respectively.

b. Covariance budget

The next step in finding the EOF covariance budget is to multiply (16) by $\hat{a}_n^* \hat{\phi}_j^{(n)*}$ and take the expected value. At this point we also expand the $\hat{\beta}_i$ on the right side of the equation in terms of the EOFs and make use of statistical orthogonality of the EOF coefficients. The result is

$$\begin{aligned} \left\langle \frac{\partial \hat{\beta}_i(k_x, k_y, z)}{\partial t} \hat{a}_n^*(k_x, k_y) \right\rangle \hat{\phi}_j^{(n)*}(k_x, k_y, z) = & - \sum_p \sum_q \iint \langle \hat{a}_p(k'_x, k'_y) \hat{a}_q(k''_x, k''_y) \hat{a}_n^*(k_x, k_y) \rangle \\ & \times [1 - \delta(k'_x, k'_y) - \delta(k''_x, k''_y)] \times \hat{\phi}_l^{(p)}(k'_x, k'_y, z) \hat{D}_l(k''_x, k''_y) \hat{\phi}_i^{(q)}(k''_x, k''_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z) dk'_x dk'_y \\ & - \lambda_n(k_x, k_y) [ik_x \hat{\beta}_i(0, 0, z) + ik_y \hat{\beta}_j(0, 0, z)] \hat{\phi}_i^{(n)}(k_x, k_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z) \\ & - \lambda_n(k_x, k_y) \frac{\partial \hat{\beta}_i(0, 0, z)}{\partial z} \hat{\phi}_3^{(n)}(k_x, k_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z) - \langle \hat{a}_n^*(k_x, k_y) \hat{D}_i(k_x, k_y) \\ & \times \hat{p}(k_x, k_y, z) \rangle \hat{\phi}_j^{(n)*}(k_x, k_y, z) - \lambda_n(k_x, k_y) \hat{\phi}_4^{(n)}(k_x, k_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z) \delta_{i3} - \frac{1}{\text{Ro}} \epsilon_{ilk} \Omega_l \lambda_n(k_x, k_y) \\ & \times \hat{\phi}_k^{(n)}(k_x, k_y, z) \hat{\phi}_j^{(n)*}(k_x, k_y, z) + \frac{1}{\text{Re}} \nu_{ik} \lambda_n(k_x, k_y) \hat{\phi}_j^{(n)*}(k_x, k_y, z) \hat{D}_l(k_x, k_y) \hat{D}_l(k_x, k_y) \hat{\phi}_k^{(n)}(k_x, k_y, z). \quad (18) \end{aligned}$$

The mean advection terms were simplified by assuming zero mean vertical velocity; the gradient production terms were simplified using horizontal homogeneity.

Now, to complete the EOF covariance budget (15), we need to switch the indices i and j in (18), take the complex conjugate, and add the result to the unaltered version of (18). The advection terms are found to cancel out during the process. The result is

$$\begin{aligned} \frac{\partial \Phi_{ij}^{(n)}(k_x, k_y, z)}{\partial t} = & \Gamma_{ij}^{(n)}(k_x, k_y, z) \\ & + \Gamma_{ji}^{(n)*}(k_x, k_y, z) - \Phi_{3j}^{(n)}(k_x, k_y, z) \frac{\partial \langle \beta_i(z) \rangle}{\partial z} \\ & - \Phi_{i3}^{(n)}(k_x, k_y, z) \frac{\partial \langle \beta_j(z) \rangle}{\partial z} - \Pi_{ij}^{(n)}(k_x, k_y, z) \\ & - \Pi_{ij}^{(n)*}(k_x, k_y, z) - \Phi_{4j}^{(n)}(k_x, k_y, z) \delta_{i3} \\ & - \Phi_{i4}^{(n)}(k_x, k_y, z) \delta_{j3} - \frac{\Omega_l}{\text{Ro}} [\epsilon_{ilk} \Phi_{kj}^{(n)}(k_x, k_y, z) \\ & + \epsilon_{jlk} \Phi_{ik}^{(n)}(k_x, k_y, z)] + \frac{1}{\text{Re}} [\nu_{ik} \epsilon_{jk}^{(n)}(k_x, k_y, z) \\ & + \nu_{jk} \epsilon_{ik}^{(n)*}(k_x, k_y, z)], \quad (19) \end{aligned}$$

where $\Gamma_{ij}^{(n)}(k_x, k_y, z)$ is the nonlinear term [the double-summation on the right-hand side of (18)],

$$\Pi_{ij}^{(n)}(k_x, k_y, z) = \langle \hat{a}_n^* \hat{D}_i \hat{p} \rangle \hat{\phi}_j^{(n)*}, \quad (20)$$

and

$$\epsilon_{jk}^{(n)}(k_x, k_y, z) = \lambda_n(k_x, k_y) \hat{\phi}_j^{(n)*} \hat{D}_l \hat{D}_l \hat{\phi}_k^{(n)}. \quad (21)$$

Equation (19) is our final result for the EOF covariance budget. It has a term by term correspondence to the traditional Reynolds decomposition (e.g., Stull 1988). One simply sums each term in the EOF budget over all modes (k_x, k_y, n) to obtain the corresponding term in the Reynolds budget. The only subtlety lies in the nonlinear term Γ_{ij} . As it stands in (19), the nonlinear term includes both turbulent transport (flux divergence) and interscale transfer (triad interactions) effects. It becomes a pure flux divergence only after the summation over EOF modes.

There is also a term by term correspondence of the EOF budget to spectral decompositions (e.g., Borowski 1969), provided that the flow is homogeneous. One simply integrates the EOF budget over the flow volume. The nonlinear term in the EOF budget reduces to a pure interscale interaction term after the integration.

c. TKE budget

An important special case of the EOF covariance budget is the TKE. The TKE of an EOF mode (k_x, k_y, n) is defined as

$$T^{(n)}(k_x, k_y, z) = \frac{1}{2} [\Phi_{11}^{(n)}(k_x, k_y, z) + \Phi_{22}^{(n)}(k_x, k_y, z) + \Phi_{33}^{(n)}(k_x, k_y, z)]. \quad (22)$$

The TKE budget equation follows directly from (19):

$$\begin{aligned} \frac{\partial T^{(n)}(k_x, k_y)}{\partial t} = & -\Re[\Gamma_{11}^{(n)}(k_x, k_y, z) + \Gamma_{22}^{(n)}(k_x, k_y, z) \\ & + \Gamma_{33}^{(n)}(k_x, k_y, z)] - \Re \left[\Phi_{31}^{(n)}(k_x, k_y, z) \frac{\partial \langle \beta_1(z) \rangle}{\partial z} \right. \\ & \left. + \Phi_{32}^{(n)}(k_x, k_y, z) \frac{\partial \langle \beta_2(z) \rangle}{\partial z} \right] - \Re[\Pi_{ii}^{(n)}(k_x, k_y, z)] \\ & - \Re[\Phi_{34}^{(n)}(k_x, k_y, z)] + \frac{1}{\text{Re}} [\epsilon_{11}^{(n)}(k_x, k_y, z) \\ & + \epsilon_{22}^{(n)}(k_x, k_y, z) + \epsilon_{33}^{(n)}(k_x, k_y, z)], \quad (23) \end{aligned}$$

where $\Re(\cdot)$ signifies the real part. Note that the Coriolis term vanishes from the energy equation. (The reader may initially think there is a sign error on the heat flux term since a positive heat flux produces TKE. It must be remembered, however, that the temperature fluctuation is normalized by θ_* , which is negative.)

The pressure term can be simplified using the continuity equation. This facilitates comparison with previous results given in the literature. Fourier transforming the continuity equation, and expanding the velocities in terms of the EOFs, one obtains

$$\sum_n [\hat{a}_n \hat{D}_i(k_x, k_y) \hat{\phi}_i^{(n)}] = 0. \quad (24)$$

Multiplying both sides by $\hat{a}_m^*$, taking the expected value and using statistical orthogonality of the coefficients, we find

$$\hat{D}_i(k_x, k_y) \hat{\phi}_i^{(n)} = 0 \quad (25)$$

for all n . That is, the EOFs must individually satisfy continuity.

The pressure term in the TKE equation is the real part of

$$\begin{aligned} \Pi_{ii}^{(n)}(k_x, k_y, z) = & (ik_x \hat{\phi}_1^{(n)*} + ik_y \hat{\phi}_2^{(n)*}) \langle \hat{a}_n^* \hat{p} \rangle \\ & + \frac{\partial}{\partial z} \langle \hat{\phi}_3^{(n)*} \hat{p} \hat{a}_n^* \rangle - \frac{\partial \hat{\phi}_3^{(n)*}}{\partial z} \langle \hat{a}_n^* \hat{p} \rangle. \quad (26) \end{aligned}$$

The first, second, and fourth terms of (26) cancel as a result of continuity, and we are left with

$$\Pi_{ii}^{(n)}(k_x, k_y, z) = \frac{\partial}{\partial z} \langle \hat{\phi}_3^{(n)*} \hat{p} \hat{a}_n^* \rangle. \quad (27)$$

d. Integrated budgets

The budget analysis provides an abundance of information: there are separate, height-dependent budget equations for each covariance and for each EOF. The EOFs themselves are a function of horizontal wave-number and index n . Since it is not possible to display all of the available information, we will examine some representative examples of individual EOF covariance budgets, as well as properties that have been integrated in various ways.

All of the linear terms in the budgets [Eqs. (19) and (23)], except for pressure, can be computed directly from the EOFs and eigenvalues. To compute the pressure term, one needs to calculate the covariance between the pressure field and the EOF projections. This presents no great difficulties. The nonlinear (interscale transfer–turbulent transport) term, however, is computationally prohibitive to determine directly. By assuming stationarity of the flow, so that time derivatives of all statistical quantities are zero, we can estimate the nonlinear term indirectly as the residual of the budget.

The first analysis we will consider consists of budget equations that have been integrated over the entire EOF space [more precisely, integration over k_x and k_y , and summation over n , as shown in Eq. (12)]. This operation leaves us with budgets for the entire resolved part of the turbulence field. Although such a budget analysis could be accomplished without ever having performed an EOF analysis, it does provide us with a useful reference point for understanding the EOF budgets of individual structures to be discussed later.

Figure 13 shows the resolved TKE budget. In this simulation, since the surface heat flux is very small, shear production of TKE dominates over buoyant pro-

FIG. 13. Resolved part of the TKE budget. “Shear” is the mean velocity gradient (momentum flux) term; “pressure” is the pressure–velocity gradient correlation term; “buoyancy” is the heat flux term; and “interscale” is the interscale transfer–flux divergence term. Viscous dissipation is negligible for the resolved scales.

FIG. 14. Comparison of shear production terms in the TKE budget. The contribution from the first EOF, the sum of the first three EOFs, the total resolved field, and the resolved plus modeled subgrid fields are shown. Also shown is the negative of the modeled LES molecular dissipation term.

duction. (In the *total* TKE budget, the normalized buoyancy term has a value of unity at the surface. The reason why the buoyancy term in Fig. 13 is so small near the surface is that most of the flux is subgrid.) Below the inversion, the pressure term is also small, so that the only other significant term in the budget is interscale transfer–turbulent transport, which simply balances shear production. Although the effect of viscosity on the resolved scales is negligible, the energy lost by the resolved scales via interscale transfer eventually is dissipated by viscous forces. Above $z/z_i = 1$, the pressure term becomes a significant loss mechanism, and it is largely balanced by the interscale–transport term. Buoyancy plays a small role above the inversion, acting as a sink.

The resolved shear production term is compared to the total (resolved plus subgrid) shear production in Fig. 14. Also shown is the negative of the molecular dissipation term, as modeled by the LES (Moeng 1984). It is seen that molecular dissipation closely balances the total shear production locally. Above $z/z_i \approx 0.2$, most of the shear production of TKE is resolved by the LES.

To assess the validity of the statistical stationarity assumption, we show the TKE as a function of time in Fig. 15. The height is $z/z_i = 0.5$. The resolved TKE tends to decrease with time over the interval shown. In Fig. 16, we calculate the difference between the TKE at the beginning and ending of the run interval from which the EOF calculations were made ($1.8 < t/t_* < 4.1$) and divide by the time elapsed. This can be thought of as an estimate of $\partial T/\partial t$ for the resolved part of the flow. Comparison to Fig. 13 shows that this quantity is smaller than (generally an order of magni-

FIG. 15. TKE as a function of time (normalized by the large-eddy turnover time) at $z = z_i/2$.

tude less than) the residual term, which is designated interscale transfer–turbulent transport. This provides assurance that it is valid to approximate the interscale term as a residual in the budget.

Figure 17 shows the resolved momentum flux budget. (In making this figure, the budget equation has been multiplied through by -1 since the momentum flux is *normally negative*. After this multiplication, positive values represent a source of momentum flux, and negative values a sink.) The shear, pressure, and buoyancy terms are all sources for the production of resolved momentum flux near the ground. The pressure term becomes a sink near mid-BL and then becomes a source again near the inversion. The interscale transport term is a sink throughout the BL, although it be-

FIG. 16. Estimate of the temporal derivative of the resolved TKE as a function of height.

FIG. 17. Resolved part of the momentum flux budget.

comes small around mid-PBL. The contribution from the Coriolis force is nonzero but negligible throughout the BL.

The resolved temperature flux budget is shown in Fig. 18. Because the surface heat flux is so small in this simulation, the budget terms are large only around the capping inversion. Above the inversion, the budget is very similar to Carruthers and Moeng's (1987) previous results for a more highly convective BL. At $z/z_i \approx 1.1$, buoyancy is the dominant production mechanism. The pressure and temperature gradient terms are both sinks. Interscale transfer (the vertical integral of the interscale-transport term) is an order of magnitude smaller than the buoyancy, pressure, and gradient terms, indicating that the phenomenon responsible for temperature flux at the inversion is linear.

e. Individual structures

In this section, we use Eqs. (23) and (19) to examine the TKE and flux budgets of individual EOF modes. The budgets were computed by averaging over a sequence of ten flow snapshots, as discussed in W96. The snapshots were spread over 2.3 large-eddy turnover times. Averaging must be performed in time, rather than in space, since each flow snapshot provides only a single data point for each EOF. True ensemble averaging would be computationally prohibitive. Of course, temporal averaging requires that the flow is approximately stationary; results given in the previous section suggest stationarity holds reasonably well in our case.

The figures in this section show only the significant terms in the respective budgets; in particular, the molecular dissipation terms, since they scale inversely as the Reynolds number, are an insignificant component of the budgets for large-scale structures and thus are not shown.

Vertical profiles of the TKE, momentum, and temperature flux budgets for B1 are shown in Fig. 19. Profiles for B2 are shown in Fig. 20. Recall that B1 and B2 both involve motions at and around the inversion, with B1 concentrated above the inversion and B2 below (Fig. 5b).

The most striking difference between the TKE budgets for B1 and B2 is in the sign of the shear term. It is a source for B1 and a sink for B2. This strongly suggests that B1 and B2 are dynamically distinct motions. It is interesting to compare this result to the observations of Finnigan et al. (1984), who developed budget for the wavelike motions in a stably stratified nocturnal boundary layer. These authors found the shear term to be either a source or sink, depending on the height. This is also the case in our results, when the motions at wavenumber B are viewed in aggregate (Fig. 5c). But the EOF analysis has separated the aggregate wave motions into two structures having opposite signs in the shear term. Another important distinction between B1 and B2 is that buoyancy is a source for B1 and a sink for B2. The buoyancy term was a source for the gravity waves observed by Finnigan et al. (1984). The negative heat flux observed in the B2 mode suggests that it entrains warm air at the inversion and transports it downward.

The main source term in the TKE budget for B1 is interscale transfer-turbulent transport. This is primarily a sink term for B2. Hence B1 gains energy from other structures in the flow, whereas B2 loses energy. It would be interesting to learn which structures transfer energy to B1. This would require an explicit breakdown of the triad interactions (nonlinear term), something we do not attempt in this paper. It is plausible that the transfer comes from structures near to B1 both in space and in wavenumber, such as B2.

The longitudinal momentum flux budget for B1 essentially balances production by the shear and pressure

FIG. 18. Resolved part of the temperature flux budget.

FIG. 19. Budgets for EOF B1. (a) TKE. (b) Momentum flux. (c) Temperature flux.

FIG. 20. Budgets for EOF B2. (a) TKE. (b) Momentum flux. (c) Temperature flux.

terms with destruction by buoyancy. In the B1 heat flux budget, buoyancy becomes the dominant source and is roughly balanced by losses through the temperature gradient and pressure terms. The heat flux budget for B1 is quite similar to the overall budget (Fig. 18), indicating that B1 and dynamically similar modes are responsible for most of the heat transport around the inversion level. The flux budgets for B2 are somewhat similar to B1, although they have a much noisier character. Smoother profiles would probably result from averaging over more field snapshots.

There are only two significant terms in the temperature variance budgets: gradient production (the product of the temperature gradient and the heat flux), and interscale transfer–flux divergence. Although these budgets are not shown here, we summarize the results. Gradient production is a loss term for B1. Hence temperature variance is gained through nonlinear interactions. The temperature variance budget of B2 is rather noisy, with gradient production sometimes a gain and sometimes a loss. However, the absolute value of the gradient production term at all heights is a full order of magnitude less than for B1.

Vertical profiles for the budgets of E1 and E2 are shown in Figs. 21 and 22, respectively. For both structures, shear production of TKE is nearly balanced by interscale losses. Presumably these losses are to smaller scales, although a detailed analysis of the nonlinear term would be required for a definitive conclusion. The pressure and buoyancy terms are small in the TKE budgets for E1 and E2, particularly in the lower BL. Hence the energetics of these roll-like structures appears rather simple: they derive their energy from mean shear, primarily near the surface, and lose energy via a Reynolds-type cascade to smaller-scale structures. Besides deriving energy from surface shear, E1 has a second local peak in shear production about $z/z_i = 0.7$. Note also that, above the inversion, the TKE balance of E1 is very similar to the gravity wave mode B1.

In W96, E1 was called an inflection-point roll mode, whereas E2 was called a thermal roll mode. One of the main reasons for making this distinction was that E2 (unlike E1) had temperature and vertical velocity in phase over the depth of the BL, creating a positive heat flux up to the inversion. (The heat flux for E1 changed signs at mid-BL.) But Fig. 22a, showing that convective instabilities (as represented by the buoyancy term) play only a small role in the generation of TKE for the E2 structure, makes our association between E2 and traditional thermal roll modes more tenuous. The reason why E2 has positive heat flux throughout the BL, and yet is not convectively driven, must be that warm air is *passively* ejected away from the surface, nearly to the top of the BL.

The shear, pressure, buoyancy, and nonlinear terms all play significant roles in the momentum flux budgets for E1 and E2. These budgets make it particularly clear that E1 involves motions throughout the BL and above

the inversion, whereas E2 is concentrated in the lower BL. The pressure term is a strong gain for both E1 and E2 near the ground, and also for E1 at the inversion, but becomes a sink in the middle BL. Shear is a source throughout the BL for both structures. Interscale transfer is an important loss mechanism for the structures, particularly in the lower BL. Buoyancy is the dominant loss for E1 around inversion level, as it was for B1.

The terms in the temperature flux budget for E1 and E2 become largest around inversion level. However, the E2 budget is an order of magnitude smaller than E1. In E1, buoyancy is the dominant source; the pressure and temperature gradient terms are significant losses. Once again, the behavior of E1 around inversion level is quite similar to B1, a gravity wave mode. This reinforces the conclusion that E1 is a BL roll mode coupled to an inversion-borne gravity wave.

f. Classification scheme and summary

The discussion in the previous section dealt with the budgets at only two representative locations in the wavenumber domain, designated B and E. Structure B1 has been classified as a gravity wave mode, B2 as an inversion-level entraining (breaking) mode, E1 as an inflection-point instability roll, and E2 as a passive thermal roll. We now consider the contributions of these different mode classes to the overall BL energetics and summarize their occurrence as a function of horizontal wavenumber. This task is made difficult by the tremendous variety observed in the EOF modes. Nonetheless, we have tried to develop a reasonably simple method for classifying the modes that agrees with the physical interpretations discussed in W96 and earlier in this text. Perhaps more general, satisfactory classification schemes can be developed in the future by examining EOF analyses of other flow regimes.

The first step in classifying the EOF modes was to rank them terms of their TKE. Two separate rankings were done, one for TKE integrated from the inversion downward, and one for TKE integrated from the inversion upward. After performing these rankings, enough modes were retained so that about 90% of the resolved TKE above and below the inversion was retained. [Since the LES resolves about 90% of the TKE (Fig. 2), the retained modes represent about 80% of the total TKE.]

Next, the retained modes for $z < z_i$ were sorted according to their net heat flux in the upper BL; that is, the heat flux integrated over $0.5 < z/z_i < 1$. (Recall that the heat flux for the simulation changes sign at $z/z_i = 0.5$.) If the net heat flux in the upper BL was positive, the modes were classified as passive thermal rolls. Negative heat flux modes were classified as inflection-point rolls. The retained modes for $z > z_i$ were classified according to their net heat flux around the inversion level, $0.8 < z/z_i < 1.2$. Positive heat flux modes were classified as gravity waves, and negative heat flux modes were classified as entraining motions.

FIG. 21. Budgets for EOF E1. (a) TKE. (b) Momentum flux. (c) Temperature flux.

FIG. 22. Budgets for EOF E2. (a) TKE. (b) Momentum flux. (c) Temperature flux.

Figure 23 shows the results of the classification scheme. The solid lines in Figs. 23a,b enclose the regions where inflection-point and passive thermal modes were found, respectively. The shading indicates where there is coupling to a strong inversion-level mode, either to a gravity wave or an entraining motion. One striking feature of the plots is that the rolls are broadly distributed over the wavenumber space. It is difficult to assign a particular aspect ratio to either of the roll modes.

The inflection-point modes include E1, F2, and similar motions. The distribution of these modes in wavenumber space closely follows the power spectral contours of the longitudinal velocity field at $z/z_i = 0.8$, as given in W96. Apparently the modes we have designated inflection-point rolls dominate the horizontal velocity fields in the upper BL.

The passive thermal modes, which include the likes of D1, E2, and F3, are observed to have a larger angle relative to the geostrophic wind than the inflection-point modes (about 20° and 10° , respectively). The region in which the thermal modes are strong roughly follows the contour lines of the power spectrum for u at $z/z_i = 0.2$, shown in W96. Therefore, the thermal mode can be associated with processes occurring near the surface. Further support for this view comes from the flow realizations for E2 shown in W96, which show the large velocity fluctuations near the surface gradually dying out as the inversion is approached. Hence we might associate E2 with the streaky structure observed near the surface. Apparently powerful bursting events in the surface layer propel parcels of warm air to heights well above mid-BL. The strong, surface-layer wind shear stretches out these bursts in the direction of the flow.

The inversion-level motions, shown in Fig. 23c, include entraining modes (regions enclosed by the dashed contours) and gravity waves (the shaded regions). Energetic entraining modes are distributed over a broader region of the wavenumber space than the gravity waves. This distribution could reflect the nonlinearity of wave breaking events. Much of the energy in the gravity wave modes is oriented at roughly 45° to the right of the geostrophic wind.

5. Concluding remarks

The EOF TKE and flux profiles demonstrated that although large-scale structures account for most of the TKE throughout the boundary layer, their direct role in transporting heat and momentum through the atmospheric surface layer is small. This is not particularly surprising since these large structures cannot have substantial vertical velocities near the surface. Some of the profiles also revealed how roll-like modes found in W96 actually couple to inversion-borne gravity waves. Apparently we have detected an example of convection waves, such as discussed by Kuettner et al. (1987). EOFs are a very useful technique for detecting these convection waves and for studying their energetics and coupling to BL structures.

We also discussed an indirect EOF method for calculating skewness and kurtosis as a function of vertical scale in the flow. Using this method, positive skewness at mid-BL was associated with the large, BL-scale structures. Kurtosis, a measure of intermittency, could not be associated with a particular spatial scale. Intermittency therefore results from interactions between large- and small-scale structures. One shortcoming in the calculations of higher-order statistics was the im-

FIG. 23. Locations of the different structural types within the wavenumber domain. (a) Inflection-point instability roll modes. Shading indicates regions where the rolls are coupled to a gravity wave. (b) Thermal instability roll modes. Shading indicates regions where the rolls are coupled to a gravity wave. (c) Gravity waves (dark shading and solid contour) and breaking waves (dashed contour).

perfect association that exists between EOF index and vertical spatial scale. The calculations of higher-order statistics would perhaps be more informative if the EOF modes were classed according to their physical characteristics, rather than simply by their EOF index, prior to the filtering operation.

The EOF TKE budget analysis provided evidence that shear instabilities near the surface cause bursting events (ejections) that passively drive warm air parcels well up into the boundary layer. These bursting events and their corresponding sweeps appear in flow snapshots as long streaks, aligned with the mean surface-layer wind. Perpendicular cross sections of the EOF modes responsible for the streaks look quite similar to the thermal roll modes discussed in the literature (e.g., Haack and Shirer 1992; Etling and Brown 1993). However, these particular EOF modes are driven by shear, rather than convective, instabilities. The actual relationship between the EOF thermal roll modes observed in this study and thermal rolls previously described in the literature remains to be worked out.

Viewing this paper and W96 as a whole, the EOF method clearly has proven itself a valuable tool for decomposing a complex, high Reynolds number, boundary-layer flow into its characteristic motions. Part of the reason why the EOF analysis was able to yield such a rich variety of structural information was simply because it was applied to highly sampled, three-dimensional fields obtained by LES. A 1D or 2D EOF analysis would not have captured most of the interesting structure obtained from the 3D analysis. As discussed in W96, this makes direct comparison with observations difficult since such highly sampled, 3D fields are unobtainable experimentally.

By using the EOF technique, we were not limited to studying a particular type of structure, such as thermal plumes, because the analysis does not require specification of a sampling condition. EOF analysis is particularly well suited to studying quasi-periodic motions such as rolls and gravity waves. There is still much to be learned from applying the EOF method to LES covering a wide range of surface heat fluxes, wind profile shapes, and inversion-layer temperature gradients. There is also room for further development of the analysis tools. Besides the EOF covariance and energy budgets studied in this paper, it would be worthwhile to develop an equation for the EOF vorticity budget. This would be particularly helpful in shedding further light on the mechanisms responsible for the roll generation in complex PBL flows.

Acknowledgments. H. Shirer first suggested the existence of convection waves in our results. The authors also benefitted from discussions with G. Young on plume budgets and A. Siegel on intermittency characterization. This work was sponsored by the ONR Marine Boundary Layer ARI, Grant N00014-92-J-1688.

APPENDIX

State Equation

An expression for the temporal change of a velocity component or the potential temperature was required in the body of the text in order to develop the EOF covariance budget. The derivation is given in this appendix. The main complication is that the equations for velocity and temperature have to be combined into a single, nondimensional state equation in order to be consistent with the EOF analysis.

Let us start with the Boussinesq system:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho_0} \frac{\partial p}{\partial x_i} + \frac{g}{\theta_0} [\theta - \langle \theta \rangle] \delta_{i3} - 2\epsilon_{ijk} \Omega_j u_k + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}, \quad (\text{A1})$$

$$\frac{\partial \theta}{\partial t} + u_j \frac{\partial \theta}{\partial x_j} = \kappa \frac{\partial^2 \theta}{\partial x_j \partial x_j}, \quad (\text{A2})$$

$$\frac{\partial u_j}{\partial x_j} = 0, \quad (\text{A3})$$

where ϵ_{ijk} is 0 if any of the indices ijk are equal, 1 if they are in cyclic order, and -1 if they are in anticyclic order. The earth's angular velocity is Ω , its components being $\Omega_1 = 0$, $\Omega_2 = \Omega \cos \alpha$, and $\Omega_3 = \Omega \sin \alpha$, where α is the latitude.

Next we nondimensionalize the Boussinesq equations using the substitutions $x_j = z_i \bar{x}_j$ (where z_i is the inversion height), $t = (z_i/w_*)t$, $u_i = w_* \beta_i$ ($i \neq 4$), $\theta = -(\theta_0/g)(w_*^2/z_i)\beta_4 = \theta_* \beta_4$, $p = \rho_0 w_*^2 \bar{p}$, and $\Omega_j = (f_0/2)\bar{\Omega}_j$, where $f_0 = 2\Omega \sin \alpha$ is the Coriolis parameter. The overbars indicate nondimensionalized quantities. With these definitions, the Boussinesq system becomes

$$\frac{\partial \beta_i}{\partial t} + \beta_j D_j \beta_i = -\frac{\partial \bar{p}}{\partial \bar{x}_i} - [\beta_4 - \langle \beta_4 \rangle] \delta_{i3} - \frac{1}{\text{Ro}} \epsilon_{ijk} \bar{\Omega}_j \beta_k + \frac{1}{\text{Re}} D_j D_j \beta_i, \quad (\text{A4})$$

for $i \neq 4$,

$$\frac{\partial \bar{\theta}}{\partial t} + \beta_j D_j \beta_4 = \frac{1}{\text{Pr}} \frac{1}{\text{Re}} D_j D_j \beta_4, \quad (\text{A5})$$

and

$$D_j \beta_j = 0, \quad (\text{A6})$$

where $\text{Ro} = w_*/f_0 z_i$ is the turbulent Rossby number, $\text{Re} = z_i w_*/\nu$ is the large-eddy Reynolds number, $\text{Pr} = \nu/\kappa$ is the Prandtl number, and $D_j = \partial/\partial \bar{x}_j$ for $j = 1, 2, 3$, and 0 for $j = 4$. It is also understood that $\epsilon_{ijk} = 0$ if any of the indices are 4. By defining a normalized "viscosity" as

$$\bar{\nu}_{ik} = \begin{cases} 1 & i = k = 1, 2, 3 \\ \frac{1}{\text{Pr}} & i = k = 4 \\ 0 & i \neq k \end{cases}, \quad (\text{A7})$$

the temperature and velocity equations in the Bousinesq system can be combined to yield

$$\frac{\partial \beta_i}{\partial t} + \beta_j D_j \beta_i = -D_i \bar{p} - [\beta_4 - \langle \beta_4 \rangle] \delta_{i3} - \frac{1}{\text{Ro}} \epsilon_{ijk} \bar{\Omega}_j \beta_k + \frac{1}{\text{Re}} \bar{\nu}_{ik} D_j D_j \beta_k. \quad (\text{A8})$$

For brevity, the overbars are dropped in the body of the text, although the reader should keep in mind that all dimensional quantities have been normalized.

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