Vertical turbulence structure and second-moment budgets in convection with rotation: A large-eddy simulation study

By D. V. Mironov1*, V. M. GryaniK1.2, C.-H. Moeng3, D. J. Olbers1 and T. H. Warncke1

1Alfred Wegener Institute for Polar and Marine Research, Germany
2A. M. Obukhov Institute of Atmospheric Physics, Russia
3National Center for Atmospheric Research, USA

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SUMMARY

The structure of the instantaneous flow fields and turbulence statistics and the second-order moment budgets in convection affected by rotation are analysed using a large-eddy simulation (LES) dataset. Three archetypes of convective flows driven by the surface buoyancy flux are generated. One is the reference case of the non-rotating convective boundary layer (CBL) growing into a quiescent stably stratified fluid. The other two are CBLs affected by rotation. In the geophysical turbulence context, these non-rotating and rotating CBLs mimic an early stage and a mature stage, respectively, of the vertical mixing phase of open-ocean deep convection.

Instantaneous flow structures reveal strong localization of the buoyancy anomalies and the non-hydrostatic pressure anomalies near the surface in rotating CBLs and their dilution as one moves towards the CBL outer edge. These anomalies are associated with the localized cyclonic vortices which are the centres of intense vertical motions. Most of the cyclones never reach the outer edge of the CBL.

Increasing rotation results in less mixing, reducing the entrainment flux at the CBL outer edge and maintaining a negative buoyancy gradient throughout the CBL. The effect of counter-gradient transport, which occurs in free convection, is largely reduced. The vertical-velocity variance and the layer-averaged turbulence kinetic energy are reduced by rotation, while the variances of buoyancy and pressure are enhanced. The vertical velocity and buoyancy fields are positively skewed in both rotating and free convection. The buoyancy skewness is considerably larger in the bulk of the rotating CBL than in the non-rotating CBL, reflecting strong localization of positive buoyancy anomalies.

The pressure transport term in the turbulence kinetic-energy budget becomes more important as the rotation rate increases, whereas the contribution of the third-order transport term is reduced. All terms in the buoyancy variance budget grow in amplitude as the rotation rate increases. The mean-gradient term and the turbulent transport term are both gains that are offset by a loss to dissipation in the bulk of the CBL. This is different from free convection where the buoyancy variance budget in mid-CBL is maintained mainly by turbulent transport since the mean-gradient term is small there. The budget of the vertical buoyancy flux in convection with rotation is strongly dominated by the pressure-gradient/buoyancy covariance and the buoyancy production terms.

Evaluation of closures for the turbulence energy dissipation against the LES data supports the idea of imposing a limitation on the dissipation length scale due to the background rotation. This limitation is required to account for the reduced turbulence energy in convection with rotation. A similar limitation on the length scale for the dissipation of buoyancy variance is not found to be important. Analysis of parametrized budgets of the third-order moments reveals the dominance of the direct effects of buoyancy. These effects are enhanced with increasing rotation rate. They must be included in parametrizations for the third-order moments. The conventional down-gradient approximations neglecting the buoyancy effects would greatly underestimate the turbulent transport.

KEYWORDS: Large-eddy simulation Rotating convection Second-moment budgets Turbulence

1. INTRODUCTION

Rotating convection is encountered in many geophysical and astrophysical fluid systems (Golitsyn 1991; Boubnov and Golitsyn 1995) and in some technical applications (Fontaine et al. 1989). An important geophysical example of rotating convection is open-ocean deep convection. It is known to occur in a few localized areas of the world's oceans; the Mediterranean, Labrador, Greenland and Weddell Seas being the best documented areas, and is suspected to play a key role in the ocean thermohaline circulation and hence in the climate system. Since it was first documented in the Gulf of Lions (MEDOC Group 1970), deep convection has received much attention. Although numerous observational, laboratory and numerical studies have given insight into many

* Corresponding author: Deutscher Wetterdienst, Abteilung Meteorologische Analyse und Modellierung, Referat FE14, Postfach 100465, Frankfurter Str. 135, D-63067 Offenbach am Main, Germany. e-mail: Dmitrii.Mironov@dwd.de, dmironov@awi-bremerhaven.de

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features of the phenomenon, it is still not well understood. There is a need for a usable parametrization of the effect of rotation on the structure of convective turbulence and its transport properties. The present study makes a step forward in this direction.

Using a dataset generated with a large-eddy simulation (LES) model, we compare mean and turbulence structure in three convective flows driven by the surface buoyancy flux. One is the reference case of the non-rotating convective boundary layer (CBL) growing into a quiescent stably stratified fluid. The other two are CBLs affected by rotation. In the context of the open-ocean deep convection, the non-rotating case can be considered as a numerical analogue of an early stage of its development, when the CBL is too shallow to feel the background rotation. Rotating cases mimic a mature stage of deep convection, when the CBL is deep and its structure is affected by rotation. These rotating CBLs differ by their Rossby numbers, a similarity parameter that characterizes the effect of rotation on convective turbulence (see section 3), and by the strength of the density interfaces at their outer edges. Thus, the focus of the present study is on the upright turbulent convection and the vertical mixing. Large-scale processes, such as lateral transport of convected water, as well as small-scale processes controlled by molecular transfer mechanisms, are beyond the scope of this study.

We analyse the instantaneous flow structures, vertical profiles of mean buoyancy and the second- and third-order statistical moments of turbulence, and evaluate terms in the second-order moment budgets (variance and flux budgets). These budgets are used in the second-order approach to develop closure models for turbulent flows. Various terms in the equations governing the evolution of variances and fluxes are parametrized in order to derive a closed set of equations describing the flow structure. We examine the validity of some closure assumptions, commonly used in the second-order modelling approach, for convection with rotation.

2. BACKGROUND

Convection affected by the background rotation has been observed during open-ocean deep convection events and studied in laboratory conditions. Comprehensive reviews of observational and laboratory studies are presented by Killworth (1983), Paluszkievicz et al. (1994), Boubnov and Golitsyn (1995), Maxworthy (1997) and Marshall and Schott (1999). We will not discuss these issues here. We briefly touch upon a number of numerical studies pertinent to the present analysis.

A number of non-hydrostatic models were applied to study rotating convection. Jones and Marshall (1993) simulated thermal convection in a neutrally stratified ocean where the horizontal component of the earth rotation vector is zero and the water density is a linear function of temperature. The sub-grid-scale processes were parametrized through the use of the eddy-transfer coefficients held constant in space and time, and the surface cooling was applied over the central part of the domain in order to allow horizontal spreading of convected water. Results from simulations proved to be helpful in quantifying the break-up of an open-ocean convective chimney. However, the resolution was insufficient to describe the vertical structure of the convective region in detail. Further studies with the same model aimed at understanding and classifying regimes, scaling relations and integral effects of open-ocean convection were reported by Klinger and Marshall (1995) and Send and Marshall (1995). Sander et al. (1995) simulated open-ocean deep convection using constant eddy diffusivity but the complete form of the Coriolis acceleration and a nonlinear equation of state. An analysis of the kinetic-energy budget showed that buoyancy production, dissipation and pressure redistribution are leading terms. The horizontal component of the Coriolis acceleration
was found to facilitate the transfer of vertical kinetic energy to horizontal kinetic energy. The inclusion of the thermobaric effect (the pressure dependence of the thermal-expansion coefficient) leads to extra acceleration of the sinking plume and a deficit of buoyancy in deep layers. Convective adjustment as used in large-scale ocean models was found to be unable to properly represent the vertical transport of tracers.

Direct numerical simulation of penetrative convection into a stably stratified fluid was performed by Julien et al. (1996). The focus of that study was on the effect of rotation on the entrainment zone at the CBL outer edge. It was shown that rotation reduces the energy of the plume reaching the entrainment zone and thus reduces the buoyancy flux due to entrainment.

LES models with the sub-grid closure based on the balance equation for the sub-grid-scale (SGS) turbulence kinetic energy (TKE) were applied by Raasch and Etling (1991), Garwood et al. (1994) and Denbo and Skyllingstad (1996). Raasch and Etling (1991) compared simulations of free and rotating convection in a surface-heating-driven boundary layer entraining into the overlying quiescent layer with the height-constant stable potential-temperature lapse rate. Only the vertical component of the Coriolis parameter was retained. They analysed vertical profiles of mean potential temperature and second-order turbulence moments and performed a visualization study of the flow structures. Results from the study are in agreement with laboratory experiments on rotating turbulent convection, indicating an increase in the potential-temperature gradient and a decrease in the root mean square (r.m.s.) vertical velocity and the scales of motions in convection with rotation. The entrainment buoyancy flux at the CBL top decreased with the increasing rotation rate, as in the direct numerical simulation of Julien et al. (1996).

Garwood et al. (1994) included both the vertical and horizontal components of the Coriolis parameter and the thermobaricity into their ocean large-eddy model. The LES solutions were used to consider the three-dimensional structure of thermobaric-enhanced turbulence. It was shown that the thermobaric acceleration may cause sinking plumes to penetrate deep into the pycnocline and possibly to the ocean bottom.

Denbo and Skyllingstad (1996) performed a series of large-eddy simulations of oceanic convection driven by surface buoyancy flux. Results from simulations of rotation-free and rotating CBLs with no thermobaric effects and constant salinity corroborate previous laboratory and numerical results, indicating a decrease of the scales of motion, of the r.m.s. vertical velocity and of the entrainment buoyancy flux, and a slowdown of the CBL growth in cases with rotation. The inclusion of the horizontal component of the Coriolis parameter has negligible effect on the structure of the second-order turbulence moments, although it may cause asymmetries in the circulation around an individual plume. It should be pointed out that the flow structures and turbulence statistics in the Denbo and Skyllingstad (1996) LES are very similar (qualitatively and also quantitatively) to those in the Raasch and Etling (1991) LES in spite of the difference in surface boundary conditions for the horizontal velocity components. In the shear-free CBL, with or without rotation, changing from no-slip to free-slip surface boundary conditions appears to have no appreciable effect on the mean and turbulence structure of the CBL. Results from simulations using the temperature and salinity profiles from the central Greenland Sea for model initialization showed the importance of the thermobaric effect at some stages of the evolution of the convective layer. The thermobaric instability enhances vertical motions, thus opposing the damping effect of rotation.

The present study extends previous numerical studies to describe the vertical turbulence structure, the second-order moment budgets, and implications for parametrizing the turbulent convection with rotation. The second-order budgets in rotation-free
TABLE 1.  INPUT PARAMETERS OF THE SIMULATED CASES

<table>
<thead>
<tr>
<th>Case</th>
<th>$L_x$</th>
<th>$L_y$</th>
<th>$N_x \times N_y \times N_z$</th>
<th>$Q_s$ (K m s$^{-1}$)</th>
<th>$B_s$ (m$^2$ s$^{-3}$)</th>
<th>$f$ (s$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>FC</td>
<td>5000</td>
<td>2000</td>
<td>96 $\times$ 96 $\times$ 96</td>
<td>0.24</td>
<td>7.85 $\times$ 10$^{-3}$</td>
<td>0</td>
</tr>
<tr>
<td>R2</td>
<td>1728</td>
<td>1200</td>
<td>144 $\times$ 144 $\times$ 120</td>
<td>0.10</td>
<td>3.27 $\times$ 10$^{-3}$</td>
<td>5 $\times$ 10$^{-3}$</td>
</tr>
<tr>
<td>R3</td>
<td>2250</td>
<td>1500</td>
<td>150 $\times$ 150 $\times$ 150</td>
<td>0.24</td>
<td>7.85 $\times$ 10$^{-3}$</td>
<td>2 $\times$ 10$^{-2}$</td>
</tr>
</tbody>
</table>

$L_x$, $L_y$, and $L_z$ are the numerical domain sizes in $x$, $y$, and $z$ directions, respectively. $N_x$, $N_y$, and $N_z$ are the numbers of grid points in these directions. $Q_s$ is the surface potential-temperature flux (heat flux divided by the density and specific heat at constant pressure), and $B_s = \beta Q_s$ is the surface buoyancy flux. $f$ is the Coriolis parameter.

Turbulent convection and parametrizations for various terms in the budgets have been thoroughly investigated using observational and LES data (e.g. Lenschow et al. 1980; Moeng and Wyngaard 1989). The case of rotating turbulent convection is considered in the present study. We use an LES model to generate three convective boundary-layer flows ranging from free to rotationally dominated convection. In our configuration the surface-heating-driven boundary layer grows into the overlying stably stratified fluid. We carry potential temperature as the only thermodynamic variable, use a linear equation of state, and take the rotation vector aligned with the vector of gravity. The three-dimensional large-eddy fields explicitly calculated by the LES model provide the data required to analyse details of the turbulence. We realize that our configuration is somewhat simplified. We believe, however, that the flow structure and budgets in more complex regimes (e.g. those including thermobaricity and the tilting of the rotation vector as in a real ocean) could hardly be understood until simpler cases are understood and satisfactorily described. Furthermore, as far as physical parametrizations are concerned, it is the simplified clear-cut cases that often reveal their deficiencies, whereas in complex configurations the situation may be obscured by a sophisticated interplay of various forces that may partly counterbalance the effects of each other.

3. LARGE-EDDY SIMULATION DATASET

The LES code used in the present study is described in detail in Moeng (1984) and Moeng and Wyngaard (1988). A brief overview of the LES equations, used later to elucidate the relation between the LES and the ensemble-mean second-moment budgets, is given in appendix A.

One rotation-free CBL, referred to as case FC, and two flows affected by rotation, referred to as cases R2 and R3, were generated. The input parameters of the simulated cases are summarized in Table 1.

In all simulated cases periodic boundary conditions are applied in both $x$ and $y$ directions. The top and bottom boundary conditions are as follows. At the upper boundary, zero SGS TKE, free-slip for the horizontal velocity components, the potential-temperature lapse rate and the radiative upper boundary conditions that allow internal gravity waves to leave the system, are applied. At the surface, velocities are zero, potential-temperature flux is prescribed, and the vertical fluxes of the horizontal momentum are evaluated from the surface-layer similarity.

The initial potential-temperature profile has a three-layer structure. In cases FC and R3, a mixed layer of depth 1000 m and potential temperature 300 K is capped by a strongly stratified interfacial layer where potential temperature increases linearly by 8 K over six grid intervals. The lapse rate is $\Gamma = 3 \times 10^{-3}$ K m$^{-1}$ above the interfacial layer. In case R2, the potential-temperature difference across the interfacial layer is smaller,
1.2 K over four grid intervals, the initial mixed-layer depth is 780 m, and the lapse rate above the interfacial layer is $\Gamma = 6 \times 10^{-3}$ K m$^{-1}$.

The simulations start with the mixed layer at rest. To facilitate the growth of convective turbulence, small random disturbances are added to the initial temperature and velocity fields in the lower part of the mixed layer, and the SGS energy is set to a small value. The model is then run for several large-eddy turnover times at which point the sampling of three-dimensional fields is started. The sampling time, the number of samples and internal parameters of the simulated cases are given in Table 2. Here, $h$ is the CBL depth defined from the surface to the level where the heat flux is a minimum, and $w_*$ and $\theta_*$ are the Deardorff (1970a, 1970b) velocity and temperature scales,

$$w_* = (h\beta Q_s)^{1/3}, \quad \theta_* = Q_s/w_*.$$

The time scale $\tau_* = hw_*^{-1}$ is the turnover time scale based on the Deardorff convective velocity scale. The time scale $\tau_c = hw_c^{-1}$ is the turnover time scale based on the rotational velocity scale, $w_c = (\beta Q_s)^{1/2} f^{-1/2}$, which is perhaps more relevant to cases with rapid rotation. The cube of the ratio of the two time scales is a Rossby number,

$$Ro_* = (\beta Q_s)^{1/2} f^{-3/2} h^{-1},$$

often called the ‘natural’ Rossby number (Maxworthy and Narimousa 1991, 1994; Jones and Marshall 1993; Marshall et al. 1994). It has been introduced as a measure of the effect of rotation on convective processes. Viewed as a ratio, $Ro_* = l_c/h$, of the rotational depth scale, $l_c = (\beta Q_s)^{1/2} f^{-3/2}$, to the CBL depth, $h$, a small $Ro_*$ shows that convection would be affected by rotation when $h$ exceeds $l_c$ (perhaps by a factor of ten, as argued by Ivey et al. (1995)). This concept of a critical Rossby number was first introduced by Hopfinger and Browand (1981); see also Maxworthy and Narimousa (1991). Alternatively, the natural Rossby number can be viewed as the (cube of the) ratio of the rotational-velocity scale, $w_c$, to the Deardorff convective-velocity scale, $w_*$. The former scale was first proposed by Golitsyn (1980, 1981) who derived it from the dimensional arguments on the assumption that the CBL depth is unimportant and drops out of the problem as long as it is sufficiently large compared with the rotational length scale, $l_c$. The rotational length scale appeared (perhaps independently) in several publications (see Boubnov and Golitsyn 1990; Golitsyn 1991; Fernando et al. 1991; Maxworthy and Narimousa 1991, 1994; Jones and Marshall 1993).

Marshall and Schott (1999) find that values of the Rossby number from 0.01 to 1 are most relevant to oceanic deep convection. Although the values of $Ro_*$ in our simulations with rotation fall in the above range, $Ro_* = 0.03$ is perhaps too low for typical oceanic conditions. We deliberately designed the case R3 in such a way as to highlight the effect of rotation on the structure of convective turbulence. The case R2 with $Ro_* = 0.2$ mimics typical oceanic conditions. An important point however, as we shall see later, is that the turbulence structure in this moderate Rossby number case
appears to be closer to that in the small Rossby number case, R3, than in case FC. This suggests that the 'average' oceanic conditions represent the most 'difficult' intermediate regime, where the effect of rotation cannot be neglected but the turbulence structure is not yet entirely dominated by rotation.

In what follows, all quantities are presented in dimensionless form. They are made dimensionless with the CBL depth, \( h \), and the Deardorff velocity and temperature scales, Eq. (1), which are now commonly used in studies of convective flows. The discussion below is presented in terms of potential temperature. Buoyancy could be used instead as the two quantities are taken to be linearly related.

4. Analysis of Large-Eddy Simulation Data

(a) Instantaneous flow structures

The flow structures in our simulations should differ due to the effect of rotation. In order to reveal these differences and to identify coherent structures present in the flows, we carried out a visualization study using the instantaneous flow fields. We compare two simulations, case FC and case R3 which is characterized by a small Rossby number. Except for the Coriolis parameter (and differences in domain and grid sizes, which we believe have very little effect on our solutions), all governing parameters and initial and boundary conditions in these simulations are identical. The vertical velocity, the vertical component of the relative vorticity, \( \omega = \partial u / \partial x - \partial v / \partial y \), and the potential temperature and kinematic pressure in the \( x-y \) plane at vertical locations \( z/h = 0.1, 0.3, 0.5, 0.7 \) and 0.9 are shown in Figs. 1–6. These figures are snapshots taken at the final times of the simulations. All quantities are shown as fluctuations about their horizontal means at each level (horizontal-mean vertical velocity and relative vorticity are zero). They are made dimensionless with the Deardorff scales, i.e. with \( h \), \( w_u \) and \( \theta_u \) given in Table 2.

The vertical velocity field shown in Fig. 1 is typical of the surface-flux-driven convective boundary layer with no rotation. In the lower part of the CBL, characteristic 'spoke' patterns of rising motions are readily identified. The 'hubs' of these spoke patterns are the centres of most energetic ascents. Although some elongated features are still seen in the vertical-velocity field in mid CBL, there is a clear tendency towards more isolated plumes springing from the hubs of the spoke patterns. Those plumes that survive the journey to the CBL top penetrate into the stably stratified fluid aloft, causing the entrainment. The entire picture is comprehensively described by Schmidt and Schumann (1989) and Mason (1989).

The structure of the vertical-velocity field in the rotating CBL, Fig. 2, is essentially different; the spoke patterns are missing. Instead, very distinct vortical structures are formed in the lower CBL. Intense ascending motions, rising plumes, are associated with the centres of these vortices. Note that only a few plumes survive the journey to the CBL top, many die in mid layer and can hardly be identified in the upper CBL.

Associated with the regions of intense rising motions are the regions of strong localization of cyclonic vorticity in the lower half of rotating CBLs, Fig. 3. Only some of these cyclones are readily identified in the mid layer, and no distinct localized vortices are seen near the CBL top. More elongated vortex structures are present near the CBL top which can loosely be called 'vortex sheets'. The vorticity field in rotation-free flow (not shown) reveals a chaotic 'speckled' picture all the way through the boundary layer, where no distinct structures can be seen.

The potential-temperature fluctuations in rotation-free CBLs (not shown) correlate well with the vertical velocity. The spoke-like patterns in the lower part of the CBL and plume-like patterns in the mid layer are readily identified. In rotating CBLs, Fig. 4,
Figure 1. Horizontal cross-sections of the dimensionless vertical velocity \((w/w_a)\) at \(z/h = 0.1, 0.3, 0.5, 0.7\) and \(0.9\) (\(h\) is the convective boundary-layer depth) for simulation FC (see text). \(L\) is the numerical domain size in the \(x\) and \(y\) directions. Light (dark) colours correspond to high (low) values of the vertical velocity as shown on the colour scale bar. Lines are contours of zero vertical velocity.
Figure 2. Same as in Fig. 1 for simulation R3. See text for further explanation.
Figure 3. Horizontal cross-sections of the dimensionless vertical component of the relative vorticity ($\omega h/w_*$) at $z/h = 0.1, 0.3, 0.5, 0.7$ and $0.9$ ($h$ is the convective boundary-layer depth) for simulation R3 (see text). $L$ is the numerical domain size in the $x$ and $y$ directions. Light shadings correspond to positive (cyclonic) vorticity, dark shadings, to negative (anticyclonic) vorticity, as shown on the shading scale bar.
Figure 4. Horizontal cross-sections of the dimensionless fluctuation of potential temperature about its horizontal mean \( (\theta - \theta_m)/\theta_k \) at \( z/h = 0.1, 0.3, 0.5, 0.7 \) and \( 0.9 \) \( (h \) is the convective boundary-layer depth) for simulation R3 (see text). \( L \) is the numerical domain size in the \( x \) and \( y \) directions. Light (dark) shadings correspond to high (low) values of the temperature fluctuation as shown with the shading scale bar. Lines are contours of zero temperature fluctuation.
Figure 5. Horizontal cross-sections of the dimensionless fluctuation of pressure about its horizontal mean \((p - p_m)/w^2\), at \(z/h = 0.1, 0.3, 0.5, 0.7\) and 0.9 (\(h\) is the convective boundary-layer depth) for simulation FC (see text). \(L\) is the numerical domain size in the \(x\) and \(y\) directions. Light (dark) shadings correspond to high (low) values of the pressure fluctuation as shown with the shading scale bar. Lines are contours of zero pressure fluctuation.
Figure 6. Same as in Fig. 5 for simulation R3. See text for further explanation.
positive temperature anomalies are very strong, several times stronger than negative anomalies, and are associated with the cyclonic vortices. Note that the localization of positive temperature anomalies in the lower CBL is stronger than the localization of positive vertical velocities, indicating higher skewness of the temperature field. Higher up in the boundary layer, the temperature anomalies are smeared out horizontally. Note also that the temperature anomalies clearly indicate the reduction in the number and strength of rising plumes as one moves away from the heated surface towards the outer edge of the boundary layer.

Perhaps the most striking difference between rotating and non-rotating flows is in the structure of the pressure field. In rotation-free CBLs, Fig. 5, no strong correlation between the temperature and the pressure patterns immediately catches the eye. In the bulk of rotating CBLs, Fig. 6, strong correlation between negative pressure anomalies and positive potential-temperature anomalies is immediately apparent. Both anomalies are very localized and are associated with cyclonic vortices and intense rising motions. This feature is manifested in the differences in vertical profiles of the second- and third-order statistical moments of turbulence between free and rotating CBLs. The issue is discussed in what follows.

(b) Mean potential temperature, variances and fluxes

An average over horizontal planes and over a number of recorded time steps (Table 2) is treated as an approximation to the ensemble average. These ensemble means are denoted by angle brackets. To simplify notation, we omit primes and use small letters to denote turbulent fluctuations. Capital Θ stands for mean potential temperature. The second-order moments are the sum of the resolved and SGS contributions. As the CBL depth slightly increases during the sampling period, we normalize all data with the Deardorff convective scales prior to time averaging.

The vertical profile of mean potential temperature (not shown) in simulation FC is typical of the surface-flux-driven rotation-free CBL. A large negative potential-temperature gradient develops near the surface, whereas the central part of the convective layer is comparatively well mixed. Rotation suppresses mixing, leaving a negative potential-temperature gradient throughout most of the convective layer. It also reduces the negative potential-temperature flux due to entrainment at the CBL outer edge (see solid curves in Fig. 11). The part of the CBL characterized by the counter-gradient buoyancy transport shrinks as the Rossby number decreases. The buoyancy transport in convection with rapid rotation is, therefore, primarily down-gradient. The result is in agreement with previous results from laboratory experiments (e.g. Boubnov and Golitsyn 1990), LESs (e.g. Raasch and Etling 1991, Denbo and Skjellingstad 1996) and direct numerical simulation (e.g. Julien et al. 1996), and is well-known.

Vertical-velocity variances are shown in Fig. 7(a). \( \langle w^2 \rangle \) is strongly inhibited by rotation. Other noteworthy features of the \( \langle w^2 \rangle \) profiles are that at small values of the Rossby number, the \( \langle w^2 \rangle \) maximum is pressed down against the surface and that the \( \langle w^2 \rangle \) profile in simulation R3 is nearly flat over a sizable portion of the CBL. This lends some support to the view of Golitsyn (1980) that the r.m.s. vertical velocity in convection with rapid rotation increases only in a thin layer adjacent to the heated surface and remains constant above. Note, however, that this is not the case in simulation R2, where \( \langle w^2 \rangle \) decreases continuously above the level of its maximum.

The horizontal-velocity variances are also modified by rotation as shown in Fig. 7(b) (because of the symmetry between x- and y-directions only \( \langle u^2 \rangle \) is displayed). Compared with case FC, \( \langle u^2 \rangle \) in cases with rotation is larger in the lower part of the CBL,
Figure 7. Vertical profiles ($h$ is the convective boundary-layer depth) of the vertical-velocity variance ($\langle w^2 \rangle / w^2$) (a), horizontal-velocity variance ($\langle u^2 \rangle / w^2$) (b), total and subgrid-scale turbulence kinetic energy ($\langle e \rangle / w^2$) (c), potential-temperature variance ($\langle \theta^2 \rangle / \theta^2$) (d) and square root of the kinematic-pressure variance ($\langle p^2 \rangle^{1/2} / w^2$) (e) for simulations FC—solid curves, R2—dashed curves, and R3—dotted curves. See text for further explanation.
but is smaller aloft. Profiles of turbulence kinetic energy presented in Fig. 7(c) show a similar behaviour (as is seen from this figure, the contribution of the SGS TKE to the total TKE is appropriately small over most of the layer). The reduced energy in the upper part of the rotating CBL is due to a reduced vertical TKE transport. This point is discussed below in relation to the TKE budget.

As illustrated in Figs. 7(d) and 7(e), both the temperature variance and the pressure variance are strongly enhanced by rotation. The increase is larger close to the surface. This is consistent with the strong localization of the temperature anomalies and the pressure anomalies in the lower part of the rotating CBL, as seen in Figs. 4 and 6. In the upper part of the CBL, the temperature anomalies are smeared out, and so are the pressure differences between the plume interior and the ambient fluid. Notice, however, that due to the large difference in $\Theta$ across the entrainment layer the temperature variances near the CBL top in simulations FC and R3 are very large (not shown at the scale of Fig. 7(d) adjusted to better illustrate the CBL interior).

We compare our LES results with the available laboratory data and predictions from the rotational scaling of Golitsyn (1980) who proposed that in the limit of rapid rotation an appropriate scale for the r.m.s. fluctuating velocity is the rotational-velocity scale, $w_t$, defined in section 3. This suggests the expression of the r.m.s. vertical velocity in the form

$$\langle w^2 \rangle^{1/2} = C_w w_t = C_w (\beta Q_s)^{1/2} f^{-1/2},$$

(3)

where $C_w$ is a dimensionless coefficient. A very crude estimate of $C_w = 3$ was obtained by Golitsyn (1981) from an experiment with carbonated water. Data from the bottom-heated water-tank experiment of Fernando et al. (1991) suggest a lower value of $C_w = 2.4$. A value of order one was obtained by Coates et al. (1995). In the latter experiment, however, convection was agitated by a localized source of bottom heating, not by a homogeneous heating over the entire bottom of the tank. Using the maximum $\langle u^2 \rangle^{1/2}$ values in the CBL, we obtain $C_w = 1.3$ in simulation R3 and $C_w = 1.0$ in R2. These values are close to a lower bound of the range of laboratory estimates, possibly because the limiting small-Rossby-number regime of convection is not achieved in our simulations. On the other hand, it is not clear at present whether laboratory data are not adversely affected by the configuration of the tank, e.g. by its limited size, and which of the estimates should be favoured. Notice further that the above scaling relation is strictly valid only if the r.m.s. vertical velocity remains depth-independent in the bulk of the CBL. This is the case in mid CBL in simulation R3, but is not in simulation R2.

A scaling relation, Eq. (3), has been applied to the r.m.s. horizontal velocity, $\langle u^2 \rangle^{1/2}$, as well. Empirical estimates of the proportionality-factor average at about 2 (a summary is given by Boubnov and Golitsyn (1995)). Coates and Ivey (1997) applied the scaling relation, Eq. (3), to the r.m.s. fluctuating velocity defined as $q = (\langle u^2 \rangle + \langle w^2 \rangle)^{1/2}$. They estimated the proportionality factor at 2.2 using data from their water-tank experiment. Again, it is difficult to apply the above scaling relation to our simulated CBLs in a straightforward way, since the horizontal-velocity variances in rotating CBLs also show considerable variation with height. It would, perhaps, be more appropriate to consider the Golitsyn (1980) bulk scaling as applicable to the CBL mean r.m.s. velocity components (or to the CBL mean turbulence kinetic energy), and to use more sophisticated $z$-dependent scaling for the vertical profiles of turbulence quantities (see e.g. Sorbjan (1991), and Zilitinkevich (1994), for the $z$-dependent scalings for free and sheared CBL). Nevertheless, if we use the scaling relation Eq. (3) with the layer-averaged r.m.s. fluctuating velocity, we find a proportionality factor of 2.4 in case R3, very close to the estimate of Coates and Ivey (1997).
Figure 8. Vertical profiles ($h$ is the convective boundary-layer depth) of the vertical fluxes of the vertical-velocity variance ($\langle w'^3 \rangle / w'^3$) (a), of the horizontal-velocity variance ($\langle w'u'^2 \rangle / w'^3$) (b), of the vertical potential-temperature flux ($\langle w'^2 \theta \rangle / w'^3 \theta$) (c) and of the potential-temperature variance ($\langle w\theta'^2 \rangle / w'^3 \theta^2$) (d) for simulations FC—solid curves, R2—dashed curves, and R3—dotted curves. See text for further explanation.

(c) Third-order moments

The third-order moments discussed in this section are computed from the resolvable-scale fields; SGS contributions to the third- and higher-order moments are not available from our LES and thus cannot be included.

Vertical fluxes of the vertical- and horizontal-velocity variances, $\langle w^3 \rangle$ and $\langle w'u^2 \rangle$, respectively, are shown in Figs. 8(a) and 8(b) (because of the symmetry between the horizontal directions $\langle w'u^2 \rangle$ is not shown). In rotation-free CBLs, $\langle w^3 \rangle$ is an order of magnitude greater than $\langle w'u^2 \rangle$ and is the dominant contribution to the vertical flux of turbulence energy. This is no longer the case in rotating CBLs, where a strong reduction
of the vertical-velocity fluctuations results in a dramatic reduction in \( \langle w^3 \rangle \). The vertical flux of the horizontal-velocity variance is, on the contrary, enhanced in the lower CBL due to rotation (as well as the horizontal-velocity variance itself, see Fig. 7(b)) with its maximum pressed down against the surface. The increase in \( \langle uw^2 \rangle \) is, however, not as large as the decrease in \( \langle w^3 \rangle \), indicating the decay of the vertical turbulent flux of TKE in convection with rotation.

The flux of the potential-temperature flux, \( \langle w^2 \theta \rangle \), shown in Fig. 8(c), tends to become linear with height over most of the CBL as the rotation rate increases. Its maximum is located very close to the surface, and its magnitude in mid CBL appears to be only slightly smaller in cases with rotation. The flux of potential-temperature variance, \( \langle w \theta^2 \rangle \), shown in Fig. 8(d), and the vertical-velocity/pressure covariance, \( \langle wp \rangle \), shown in Fig. 9, are strongly enhanced by rotation (cf. the increase of the potential-temperature variance and the pressure variance in rotating CBLs). Noteworthy also is the decrease of the third-order transport moments and the vertical-velocity/pressure covariance in the entrainment zone. This seems consistent with the suppression of the entrainment activity in rotating convection.

Figures 10(a) and 10(b) compare the vertical-velocity skewness, \( S_w \), and the temperature skewness, \( S_\theta \) (computed using only the resolvable-scale fields). In simulation FC, \( S_w \) shows an increase towards the CBL top where it peaks just below \( z = h \). The shape of the profile and the magnitude of skewness is in agreement with previous LES results (e.g. Mason 1989; Schmidt and Schumann 1989; Nieuwstadt et al. 1993). For a detailed discussion of \( S_w \) in free convective flows we refer to Moeng and Rotunno (1990). In simulations R2 and R3, \( S_w \) is slightly smaller than in simulation FC over most of the CBL, the shape of the profile being similar in all cases. Large values of \( S_w \) very close to the surface in cases with rotation as well as negative \( S_w \) in cases with no rotation (not shown in Fig. 10(a)) are spurious. As discussed by Schmidt and Schumann (1989), they reflect the deficiency of LES in the near vicinity of the surface, which, however, does not deteriorate the results over the bulk of the CBL. The fact that \( S_w \) does
Figure 10. Vertical profiles (h is the convective boundary-layer depth) of vertical-velocity skewness \( S_w = \langle w^3 \rangle / \langle w^2 \rangle^{3/2} \) (a) and potential-temperature skewness \( S_\theta = \langle \theta^3 \rangle / \langle \theta^2 \rangle^{3/2} \) (b) for simulations FC—solid curves, R2—dashed curves, and R3—dotted curves. See text for further explanation.

A not increase in rotating CBLs in spite of localization of strong ascending motions in the centres of cyclonic vortices may be explained by taking a closer look at the structure of the vertical-velocity field illustrated in Fig. 2. As seen from the figure, the centres of strong ascents are surrounded by long curled ‘tails’ where the vertical velocity is very weak but still positive. These tails occupy a large area. As the skewness is indicative of the ratio of the areas covered by updraughts and downdraughts, it does not increase with rotation, although the vertical-velocity field remains positively skewed. The temperature skewness, \( S_\theta \), in cases with rotation proves to be about twice as large as in free convection over most of the convective layer, except near the CBL top. This behaviour of \( S_\theta \) reflects strong localization of positive temperature anomalies in the lower part of rotating CBLs and their dilution as one moves towards the boundary-layer top. Notice that these anomalies do not have long ‘tails’ as illustrated in Fig. 4, thus making the fractional cover of positive temperature anomalies small compared with the fractional cover of negative anomalies.

(d) Variance and flux budgets

Having discussed some general features of the statistical moments of turbulence, we now analyse the second-order moment budgets, hoping to get some insight for closure modelling. We consider budgets of the turbulence kinetic energy, potential-temperature variance and potential-temperature flux. It should be particularly emphasized that the second-moment budgets derived from LES are not the same as the ensemble-mean budgets. As the relation between the LES and the ‘formal’ ensemble-mean budgets is not entirely straightforward (furthermore, different interpretations of the effects of the SGS model are possible, and the approach used is not always made clear), we find it appropriate to discuss this important issue in some detail. The relation between the two sets of budgets is elucidated in appendix B. It should be remembered that we deal with the LES estimates that (presumably) approximate the ensemble-mean budgets progressively more closely as the resolution is increased.
(i) **Turbulence kinetic energy.** The budget equation for turbulence kinetic energy, $\langle e \rangle$, reads

$$
\frac{\partial \langle e \rangle}{\partial t} = \beta \langle w \theta \rangle - \frac{\partial}{\partial z} \langle we \rangle - \frac{\partial}{\partial z} \langle wp \rangle - \epsilon.
$$

(4)

where the terms on the right-hand side (r.h.s.) are the LES approximations to the buoyancy, turbulent transport, pressure transport, and dissipation terms, respectively. As no mean flow is present in our simulations, the shear production is zero throughout the CBL. The time-rate-of-change term is zero provided that the ensemble-mean TKE budget has reached a steady state. To check this we analysed the time history of the TKE averaged over the CBL depth (not shown). The energy remains fairly steady during the course of the sampling period although small oscillations about the time mean are present. Time averaging over the sampling period should lead to the TKE budget, which is stationary to a good approximation. As seen in Fig. 11, in all simulations the budget imbalance is negligibly small over most of the CBL, except very close to the surface. This lends support to our treatment of the TKE budget derived from the LES equations, as discussed in appendix B.

The TKE budget in case FC, shown in Fig. 11(a), indicates that all terms are of the same size and are all important in maintaining the budget in the CBL with no rotation. The vertical buoyancy flux is a major gain over most of the CBL and is a loss in the entrainment zone. The dissipation is a loss throughout. The turbulent transport vertically redistributes the TKE from the lower half of the CBL to the upper half. The pressure transport redistributes the TKE from the mid CBL towards its lower and upper parts. It has a smaller magnitude than the turbulent transport term. Results from our FC simulation are in agreement with data from measurements in the atmospheric CBL (Lenschow et al. 1980) and with LES of shear-free (Mason 1989) and slightly sheared (Moeng and Wyngaard 1989) CBLs.

The TKE budget in simulations with rotation is shown in Figs. 11(b) and 11(c). Not unexpectedly, all terms decrease in magnitude in the entrainment zone, where the buoyancy flux and dissipation are sinks and the budget is maintained by the pressure transport and turbulent transport of TKE. Over most of the CBL, the buoyancy production remains a major source and the dissipation remains a major sink. Compared with case FC, the dissipation shows an increase in the lower part of the CBL. A similar behaviour of the dissipation was found by Julien et al. (1996) in their direct numerical simulation of rotating CBLs.

The main difference between the TKE budget in free and rotating convection is in the relative contribution of the two transport terms. While the turbulent transport is of primary importance in redistributing the TKE vertically in the rotation-free CBL, its role in the rotating CBL is drastically reduced. The pressure transport, on the contrary, plays an important role in rotating convection. Notice that the total TKE transport, i.e. the sum of the turbulent transport and pressure transport, is largely reduced in the upper part of rotating CBLs. A reduced transport provides less energy to the upper CBL, as indicated in Fig. 7(c), thus also reducing the entrainment. Our results corroborate previous findings from the direct numerical simulations of Julien et al. (1996) and their explanation of the reduced entrainment in rotating CBLs.

One further comment should be made. The transport terms in the TKE budget must integrate to zero over the CBL. This is readily seen in Fig. 11(a) showing the TKE budget for simulation FC. Rotation alters the budget such that the pressure transport is a (large) gain and the turbulent transport is a (large) sink only in the near vicinity of the surface. As the details of the surface layer are not highly resolved in our simulations with
rotation, this might give the impression that the transport terms do not integrate to zero over the CBL. In fact they do, as indicated in Figs. 8(a), 8(b) and 9. Both the vertical flux of turbulence energy and the vertical-velocity/pressure correlation are zero at the surface and above the interfacial layer, and both vary rapidly with height, near the surface. Taking vertical derivatives of rapidly varying quantities results in additional sampling errors. To avoid this, higher resolution and longer sampling periods are required. We do not pursue this issue further, as the bulk of the CBL is our major concern.

(ii) **Potential-temperature variance.** The budget equation for the potential-temperature variance reads

\[
\frac{1}{2} \frac{\partial \langle \theta^2 \rangle}{\partial t} = -\langle w \theta \rangle \frac{\partial \Theta}{\partial z} - \frac{1}{2} \frac{\partial}{\partial z} \langle w \theta^2 \rangle - \epsilon_\theta, \tag{5}
\]
where the terms on the r.h.s. represent the effects of mean potential-temperature gradient, turbulent transport, and dissipation, respectively. As illustrated in Fig. 12, the budget imbalance is small over most of the CBL, except near the surface and in the interfacial layer.

The temperature-variance budget from simulation FC with no rotation is shown in Fig. 12(a). The mean-gradient term is a loss in mid CBL due to the counter-gradient temperature flux. As this term is small there, the budget in the mid CBL is maintained by the turbulent transport and the dissipation. This is in agreement with the atmospheric measurements (Lenschow et al. 1980) and LESs of slightly sheared CBLs (Moeng and Wyngaard 1989).

As viewed in Figs. 12(b) and 12(c), both the dissipation and the turbulent transport term grow in amplitude as the rotation rate increases (the very large negative transport term near the surface, which compensates for all the positive values in the CBL, is not
shown in Fig. 12). The mean-gradient term becomes a gain over most of the CBL. It is a loss only in a small portion of the CBL, just below the interfacial layer. This portion tends to shrink, indicating the disappearance of the counter-gradient heat transport in convection with rapid rotation. Although the dissipation and turbulent transport terms are the leading terms in the mid CBL, the mean-gradient term is not negligible there, playing an important part in maintaining the temperature-variance budget in rotating convection. Notice also the smaller budget terms near the CBL top in simulations with rotation.

(iii) **Vertical potential-temperature flux.** The budget equation for the vertical potential-temperature flux is

\[
\frac{\partial\langle w\theta \rangle}{\partial t} = -(w^2) \frac{\partial \Theta}{\partial z} + \beta \langle \theta^2 \rangle - \frac{\partial}{\partial z} \langle w^2 \theta \rangle - \left\{ \frac{\partial P}{\partial z} \right\} - P_{sg},
\]

(6)

where the terms on the r.h.s. represent the effects of the mean potential-temperature gradient, buoyancy, turbulent transport, and pressure, respectively. The budget imbalance (not shown in Fig. 13) is negligibly small over most of the CBL. As discussed in appendix B, the sum of the sub-grid scale and resolvable-scale pressure terms can reasonably be treated as the LES approximation to the pressure-gradient/temperature covariance term in the ensemble-mean temperature-flux budget. For the purposes of illustration the SGS pressure term, \( P_{sg} \), is written separately on the r.h.s. of Eq. (6). As Fig. 13 suggests, \( P_{sg} \) is smaller than the other terms in the budget but is not negligible. Presumably a very high resolution is required for this term to vanish. When data from low to moderate resolution LESs are used, the SGS pressure term should be added to the resolvable-scale pressure term to close the flux budget to a good order.

All terms on the r.h.s. of Eq. (6) are important in maintaining the budget of potential-temperature flux in rotation-free CBLs, as revealed in Fig. 13(a) (\( P_{sg} \) being smaller than other terms over most of the layer). Buoyancy production is the major source of \( \langle w\theta \rangle \). The mean-gradient term is a gain in the lower part of the layer and is a loss aloft. The turbulent transport term provides a substantial gain in mid CBL and a loss near the surface and in the interfacial layer at the CBL outer edge. The budget is balanced by a loss due to the pressure-gradient/temperature covariance.

The budgets from simulations with rotation, shown in Figs. 13(b) and 13(c), are strongly dominated by the buoyancy production and the pressure-gradient/temperature covariance terms. These two large terms almost balance each other over most of the rotating CBL. The other terms are many times smaller. The mean-gradient term is a gain over most of the CBL (again indicating that the counter-gradient transport vanishes as the rotation rate increases). The turbulent transport term is positive over most of the CBL and is negative very near the surface and in the upper part of the interfacial layer.

5. **Parametrization issues**

It is common practice to use LES solutions for evaluating turbulence closure models. Moeng and Wyngaard (1989), for example, considered parametrizations for turbulent transport and dissipation in second-order models, using LESs of strongly convective, slightly sheared boundary layers virtually unaffected by rotation (the Rossby number, Eq. (2), in their simulation was about 100). Closure assumptions for the dissipation and the pressure correlations in a neutrally stratified Ekman layer were evaluated by Andrén and Moeng (1993). In this section we examine the validity of some closure assumptions, used in second-order modelling, for convection with strong rotation. We
focus on closures for the dissipation and the third-order transport terms in the second-order budget equations.

(a) **Dissipation terms**

The dissipation of turbulence kinetic energy, $\epsilon$, and of potential-temperature variances, $\epsilon_\theta$, are usually parametrized as

$$
\epsilon = \frac{\langle e \rangle}{\tau_\epsilon} = \frac{\langle e \rangle^{3/2}}{l_\epsilon},
$$

$$
\epsilon_\theta = \frac{\langle \theta^2 \rangle}{\tau_\theta} = \frac{\langle e \rangle^{1/2} \langle \theta^2 \rangle}{l_\theta},
$$
where $\tau_\epsilon$ and $\tau_{\theta}$ are the dissipation time scales, and $l_\epsilon$ and $l_{\theta}$ are the dissipation length scales. Using $\epsilon$, $\epsilon_{\theta}$, $\langle \epsilon \rangle$ and $\langle \theta^2 \rangle$ from LESs, we computed the time and length scales from Eqs. (7) and (8), shown in Fig. 14. Both $\tau_\epsilon$ and $l_\epsilon$ are clearly reduced in mid CBL in cases with rotation. Since the TKE dissipation rate is only slightly affected by rotation in mid CBL as indicated in Fig. 11, a reduction of time and length scales reflects a reduction of the turbulence kinetic energy in rotating CBLs, Fig. 7(c). The total TKE dissipation is constrained by the net buoyancy input (the layer-integrated vertical buoyancy flux) and hence remains unaffected by rotation. Notice that the time, $\tau_\theta$, and length, $l_\theta$, scales for the dissipation of potential-temperature variance do not show a decrease with the increasing rotation rate.

In the majority of the second-order closure models the various time and length scales are assumed to be proportional to each other. If closure assumptions are formulated in terms of length scales, the various length scales are set proportional to the so-called master length scale, $l_M$. Then, the expressions for $l_\epsilon$ and $l_{\theta}$ read

$$l_M = \frac{l_\epsilon}{C_\epsilon} = \frac{l_{\theta}}{C_{\theta}},$$

(9)

where $C_\epsilon$ and $C_{\theta}$ are dimensionless constants. The master length scale is determined either from an algebraic relation or from a transport equation for a quantity that includes $l_M$ (e.g. for $\langle \epsilon \rangle/l_M$ as proposed by Mellor and Yamada (1982)).

A second-order model for neutral and unstable rotating boundary layers with an algebraic formula for $l_M$ was proposed by Hassid and Galperin (1994). These authors found it crucial to impose a limitation on the turbulence length scale due to the background rotation. Their expression for $l_M$ in the asymptotic case of rapid rotation (small Rossby number) reads

$$l_M = C_r \langle \epsilon \rangle^{1/2}/|f|,$$

(10)

where $C_r$ is a dimensionless constant. In Fig. 14(c), the dissipation length scale, computed from Eqs. (9) and (10) with the estimates of $C_\epsilon = 5.9$ and $C_r = 1.4$ recommended by Hassid and Galperin (1994), is compared with the LES data from cases R2 and R3. The overall agreement between LES data and model prediction in case R3 is satisfactory. This counts in favour of the limitation on the turbulence length scale due to the background rotation as given by Eq. (10). The model overestimates $l_\epsilon$ in case R2 because the Rossby number in this simulation is not sufficiently small.

Figure 15 compares the turbulence kinetic energy, diagnosed from Eqs. (7), (9) and (10) with $C_\epsilon = 5.9$ and $C_r = 1.4$, with the LES data from cases R2 and R3. Again, the overall agreement between LES data and model prediction in case R3 is good, while the model overestimates the TKE in case R2.

Figure 14(d) shows that the length scale for the dissipation of potential-temperature variance, $l_{\theta}$, does not decrease with the increasing rotation. Unlike the TKE dissipation, the dissipation of temperature variance increases with the increasing rotation rate, as shown in Fig. 12, as does the temperature variance itself, shown in Fig. 7(d). The model of Hassid and Galperin (1994), as well as many other Mellor–Yamada-type closure models (Mellor and Yamada (1974, 1982); see Galperin et al. (1988), and Kantha and Clayson (1994), for more recent modifications, and Nurser (1996), for a comprehensive review), does not carry a transport equation for $\langle \theta^2 \rangle$. Instead, they employ a local formulation, $\langle \theta^2 \rangle = -\tau_{\theta}(w\theta)\partial\Theta/\partial z$, that is obtained from the stationary form of Eq. (5) by neglecting the turbulent transport term and using Eq. (8) to
parametrize the dissipation term. However, as Fig. 12 suggests, the turbulent transport is crucial in maintaining the budget of \( \langle \theta^2 \rangle \). Its neglect would result in large errors in \( \langle \theta^2 \rangle \). Notice also that the local formulation neglecting the third-order transport term should not allow for the counter-gradient potential-temperature flux (when \( \langle w\theta \rangle \) and \( \partial \Theta / \partial z \) have the same sign) as this would lead to totally spurious negative values of the temperature variance.
Third-order transport terms

Parametrizations for the third-order terms in the second-order budget equations vary from the simplest down-gradient approximations (e.g., Mellor and Yamada 1982) to the complex closures based on the complete set of budget equations for the third-order moments (e.g., Zeman and Lumley 1976). The third-order budgets are usually closed by applying the quasi-normal approximation (Millionshchikov 1941) to the fourth-order terms, and the return-to-isotropy approximation, similar to the Rotta (1951) approximation for the pressure-velocity covariance, to the sum of the pressure and molecular terms. Moeng and Wyngaard (1989) used the third-order budgets parametrized in this way in order to examine the validity of closure assumptions for the third-order transport in the second-order models of the rotation-free CBL. We focus on rotating CBLs using data from runs R2 and R3. We will not consider case FC but will make a comparison with the results of Moeng and Wyngaard (1989) to highlight the differences due to rotation.

The parametrized budget of the vertical TKE flux, $\langle we \rangle$, where the quasi-normal approximation for the fourth-order moment is used, and the sum of the pressure and molecular terms is parametrized through the return-to-isotropy approximation, i.e., expressed as $-\langle we / \tau_{we} \rangle$, $\tau_{we}$ being a relaxation time scale, reads

$$\frac{\langle we \rangle}{\tau_{we}} = -(w^2) \frac{\partial (e)}{\partial z} - (w^2) \frac{\partial (w^2)}{\partial z} + \beta ((e \theta) + (w^2 \theta)).$$

Moeng and Wyngaard (1989) found that in rotation-free CBLs the $\langle we \rangle$ budget is dominated by the buoyancy and the $\langle w^2 \rangle$ gradient terms, the third and the second terms on the r.h.s. of Eq. (11), respectively. Therefore, the conventional down-gradient approximation which retains only the first term on the r.h.s. of Eq. (11), the smallest of the three terms on the r.h.s., is inappropriate. Vertical profiles of (the LES approximations to) the terms on the r.h.s. of Eq. (11) from simulations R2 and R3 are shown in Fig. 16. Due to strong attenuation of the vertical motions in rotating CBLs, the contribution from
the \( \langle w^2 \rangle \)-gradient term is very small while the relative importance of the \( \langle e \rangle \)-gradient term is increased. The budget is, however, still dominated by the buoyancy contribution (notice that the buoyancy term is multiplied by 0.5 to fit into the plot). This means that conventional down-gradient approximations, retaining only the \( \langle e \rangle \)-gradient term, are poor for rotating CBLs.

The usual way to model the pressure transport term, \( \langle wp \rangle \), in the TKE budget equation is to set it proportional to the third-order transport term, \( \langle we \rangle \). As Fig. 11 suggests, the role of the pressure transport in maintaining the TKE budgets increases with the increasing rotation rate. This indicates that the ratio of the two transport terms in rotating CBLs is not merely a constant but a function of rotation rate. To model the TKE in rotating CBLs, the pressure transport term needs to be carefully parametrized, which is beyond the scope of the present paper.

The budget of the flux of potential-temperature flux, parametrized through the use of the quasi-normal and the return-to-isotropy approximations for the fourth-order terms and for the sum of the pressure and molecular terms, respectively, reads

\[
\frac{\langle w^2 \theta \rangle}{\tau_{w^2 \theta}} = -\langle w^3 \rangle \frac{\partial \Theta}{\partial z} - \langle w \theta \rangle \frac{\partial \langle w^2 \rangle}{\partial z} - 2\langle w^2 \rangle \frac{\partial \langle w \theta \rangle}{\partial z} + 2\beta \langle w^2 \theta \rangle,
\]

(12)

where \( \tau_{w^2 \theta} \) is a relaxation time scale. The terms on the r.h.s. of the above equation describe the effects of the gradient of mean potential temperature, the gradient of vertical-velocity variance, the gradient of potential-temperature flux, and buoyancy, respectively. These terms are plotted in Fig. 17. The budget in the central part of rotating CBLs is completely dominated by the buoyancy term which is multiplied by 0.1 to fit into the plot. So the flux of potential-temperature flux in mid CBLs may be approximated as \( \langle w^2 \theta \rangle = 2\tau_{w^2 \theta} \beta \langle w^2 \theta \rangle \). The down-gradient approximation, which retains only the \( \langle w \theta \rangle \)-gradient term on the r.h.s. of Eq. (12), would greatly underestimate \( \langle w^2 \theta \rangle \) and is, therefore, inappropriate. The same is true for the interfacial layer, where the dominant contribution comes from the mean-temperature gradient term, the first term on the r.h.s. of the above equation.
Figure 17. Vertical profiles (h is the convective boundary-layer depth) of terms in the parametrized \( \langle w^2 \theta \rangle \) budget, Eq. (12), from simulations R2 (a) and R3 (b). Long-dashed curves represent the effect of the \( \Theta \) gradient, dot-dashed—the \( \langle w^2 \rangle \) gradient, dotted—the \( \langle w \theta \rangle \) gradient, and solid—buoyancy. Terms are normalized with \( h^{-1} w^2 \partial_\theta \). The buoyancy term is multiplied by 0.1. See text for further explanation.

Applying the quasi-normal and the return-to-isotropy approximations to the fourth-order terms and to the sum of the pressure and molecular terms, respectively, the budget of the flux of potential-temperature variance is

\[
\frac{\langle w^2 \theta^2 \rangle}{\tau_{w\theta^2}} = -2\langle w^2 \partial_\theta \rangle \frac{\partial \Theta}{\partial z} - \langle w^2 \rangle \frac{\partial \langle \theta^2 \rangle}{\partial z} - 2\langle w \theta \rangle \frac{\partial \langle w \theta \rangle}{\partial z} + \beta \langle \theta^3 \rangle,
\]

where \( \tau_{w\theta^2} \) is a relaxation time scale. The terms on the r.h.s. of Eq. (13) describe the effects of the gradient of mean potential temperature, the gradient of potential-temperature variance, the gradient of potential-temperature flux, and buoyancy, respectively. Terms on the r.h.s. of Eq. (13) are shown in Fig. 18, where the buoyancy term is multiplied by 0.1 to fit into the plot. Again, the budget is completely dominated by the buoyancy term, so that the approximation \( \langle w^2 \theta^2 \rangle = \tau_{w\theta^2} \beta \langle \theta^3 \rangle \) should be fairly accurate over most of the rotating CBL.

According to the analysis of Moeng and Wyngaard (1989), the down-gradient closures underestimate the third-order transport in CBLs, simply because they neglect the direct effects of buoyancy. The implication of our analysis is that their result remains in force for the CBL affected by rotation. Furthermore, the dominance of the buoyancy contributions is so overwhelming that the formulations retaining only the pressure and buoyancy terms in the budget equations for the third-moments in question, as is illustrated above for \( \langle w^2 \theta \rangle \) and \( \langle w \theta^2 \rangle \), should fare well over most of the CBL. Notice, however, that such formulations rely on the approximations (closure hypotheses) that are employed to derive the budget equations (11)–(13). These are the quasi-normal approximation for the fourth-order terms and the return-to-isotropy approximation for the sum of the pressure and molecular terms. Although these approximations are common, caution is required when they are applied to buoyancy-dominated flows. Thus, a part of the pressure term that comes from the buoyancy contribution to the pressure field may directly compensate a part of the buoyancy term in the budget. Then the return-to-isotropy approximation should be applied only to the part of the pressure term that comes from the turbulence–turbulence contribution to the pressure field, not to the entire
term (cf. the analysis of Moeng and Wyngaard (1986), of the pressure-scalar covariance in rotation-free CBLs).

6. CONCLUSIONS

An LES model has been applied to generate three archetypes of CBL flows driven by the surface buoyancy flux. One is the reference case of the non-rotating CBL growing into a quiescent stably stratified fluid. The other two are the CBLs affected by rotation. The two rotating CBLs are characterized by different values of the natural Rossby number, Eq. (2). The LES data have been used to analyse instantaneous flow structures and vertical profiles of mean potential temperature (buoyancy is taken to be linearly related to the potential temperature) and second- and third-order statistical moments of turbulence, to evaluate terms in the budgets of turbulence kinetic energy, potential-temperature variance and potential-temperature flux, and to examine some commonly used closure assumptions for the dissipation and third-order transport terms in the second-order budget equations. The main outcomes of the analysis may be summarized as follows.

The instantaneous flow structures reveal strong localization of the potential-temperature anomalies and the non-hydrostatic pressure anomalies near the surface in the rotating CBL and their dilution as one moves towards the CBL outer edge. These anomalies are associated with the localized cyclonic vortices which are the centres of intense vertical motions. Most of the cyclones never reach the outer edge of the CBL. Strong localization of the vorticity, potential-temperature, and pressure anomalies are the distinctive features that set the rotating CBL apart from its non-rotating counterpart.

Increasing rotation results in less mixing, reducing the entrainment flux at the CBL outer edge and maintaining a negative buoyancy gradient throughout the CBL. Hence, the effect of counter-gradient transport, which occurs in free convection, is largely reduced.
The vertical-velocity variance is attenuated by rotation, while the variances of potential temperature and pressure are enhanced in the lower and middle parts of the CBL. The horizontal-velocity variance is increased near the surface and is decreased above. Rotation reduces the layer-averaged turbulence kinetic energy. The vertical-velocity and potential-temperature fields are positively skewed in both rotating and free convection. The vertical-velocity skewness does not increase with the increasing rotation rate, while the potential-temperature skewness is considerably larger in the lower and middle parts of the rotating CBL than in the non-rotating CBL. This reflects stronger localization of positive potential-temperature anomalies than of positive vertical velocities in rotating CBLs.

The pressure transport term in the turbulence kinetic-energy budget becomes more important as the rotation rate increases, whereas the contribution of the third-order turbulent transport term is reduced. The joint contribution of the two transport terms to the TKE budget in the upper CBL decreases with the increasing rotation rate, which leads to the reduction in the entrainment activity there.

All terms in the budget of potential-temperature variance grow in amplitude as the rotation rate increases. The mean-gradient term and the turbulent transport term are both gains that are offset by a loss to dissipation in the bulk of the CBL. This is different from free convection where the budget of potential-temperature variance in mid CBL is maintained mainly by turbulent transport, since the mean-gradient term is small there.

The budget of the vertical potential-temperature flux in convection with rotation is strongly dominated by the pressure-gradient/temperature covariance and the buoyancy-production terms. These two big terms almost balance each other over most of the CBL.

Evaluation of the commonly used closures for the TKE dissipation against LES data lends support to the idea of Hassid and Galperin (1994) who impose a limitation on the TKE dissipation length scale due to the background rotation, Eq. (10). This limitation is required to account for the reduced TKE in convection with rotation. A similar limitation on the length scale for the dissipation of potential-temperature variance is not found necessary, at least for the range of rotation rates considered in the present study.

Analysis of parametrized budgets of the third-order moments, namely the fluxes of the TKE, of the potential-temperature variance and of the potential-temperature flux, reveals the dominance of the direct effects of buoyancy. The implication of this result is that the simple down-gradient approximations would strongly overestimate the third-order transport contributions to the second-order budgets and that the inclusion of the direct effects of buoyancy into parametrizations for the third-order moments is crucial.

The analysis of the second-order budgets in section 4(d) suggests that modelling the pressure-correlation terms is an important issue. The pressure-gradient/temperature covariance, for example, is one of the dominating terms in the budget of potential-temperature flux in convection with rotation. This places stringent requirements upon the accuracy of its parametrization. A comprehensive analysis of the pressure-scalar covariances, aiming first of all at evaluating closures for pressure terms, should be performed for the CBL strongly affected by rotation. The task is beyond the scope of the present study; it will be a subject for future work.

The LES velocity variances are compared with predictions of the rotational scaling of Golitsyn (1980), Eq. (3). The idea of Golitsyn (1980) was that the r.m.s. vertical velocity in convection with rapid rotation increases only in a thin layer adjacent to the heated (cooled) surface and remains constant above (below) until the upper (lower) boundary is felt by the flow. The r.m.s. vertical velocity in simulation R3 is nearly flat over a sizable portion of the CBL, thus lending some support to Golitsyn’s idea. In simulation R2, however, the r.m.s. vertical velocity continuously decreases above the
level of its maximum, close to the surface. Following previous authors, who used Eq. (3) to scale their laboratory data, we have also applied the rotational scaling to the r.m.s. horizontal velocity and the square root of TKE. We find it difficult to use this scaling in a straightforward way, as both the horizontal-velocity variances and the TKE show considerable variation with height in our simulated CBLs. Perhaps a more sophisticated z-dependent scaling for the vertical profiles of turbulence quantities is required.

Finally, we emphasize that the turbulence structure in case R2 with \( R_o = 0.2 \), which is typical for oceanic conditions, proves to be strongly modified by rotation and is closer to the turbulence structure in the small Rossby number case, R3, than in case FC. This underlines the need to include the effect of rotation in the turbulence closure schemes applied to oceanic deep convection. Strictly speaking, results from our analysis of turbulence parametrizations immediately apply to non-eddy-resolving models that neglect the horizontal components of the Coriolis parameter (which is generally the case in practical applications). Notice, however, that physically realistic parametrizations should describe both general cases and particular cases. Hence, results from our analysis may be considered as generally valid. A more complex case, including both the vertical and horizontal components of the Coriolis parameter, calls for further investigation. Results from the present study are a necessary prerequisite for such an investigation which should be a subject for future work.

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APPENDIX A

The large-eddy simulation code

By filtering the Navier-Stokes equations, turbulent motions are separated into the resolved-scale and sub-grid-scale parts. Using the Boussinesq approximation, the conservation equations for the resolved-scale fields are

\[
\frac{\partial \bar{u}_i}{\partial t} = -\frac{\partial \bar{u}_j \bar{u}_i}{\partial x_j} - \frac{\partial}{\partial x_i} \left( \bar{p} + \frac{2}{3} \bar{\varepsilon} \right) + \delta_{i3} \beta (\bar{\theta} - \theta_0) - 2 \varepsilon_{ijk} \Omega_j \bar{u}_k - \frac{\partial \tau_{ij}}{\partial x_j},
\]

(A.1)

\[
\frac{\partial \bar{\theta}}{\partial t} = -\frac{\partial \bar{u}_j \bar{\theta}}{\partial x_j} - \frac{\partial \tau_{\theta j}}{\partial x_j},
\]

(A.2)

\[
\frac{\partial \bar{u}_j}{\partial x_j} = 0.
\]

(A.3)

Here, \( t \) is time and \( (x_1, x_2, x_3) = (x, y, z) \) are the right-hand Cartesian coordinates. An overbar denotes a filtered resolved-scale variable, \( (\bar{u}_1, \bar{u}_2, \bar{u}_3) = (\bar{u}, \bar{v}, \bar{w}) \) are the velocity components, \( \bar{\theta} \) and \( \theta_0 \) are the potential temperature and its reference value, \( \bar{p} \) is the kinematic pressure (pressure divided by the reference density), and \( \bar{\varepsilon} \) is the SGS TKE. The anisotropic parts of the SGS stresses are denoted by \( \tau_{ij} \) and the SGS temperature flux, by \( \tau_{\theta j} \). A linear equation of state, \( \bar{\rho} = \rho_0 [1 - \alpha (\bar{\theta} - \theta_0)] \) (\( \bar{\rho} \) and \( \rho_0 \)
are the density and its reference value), is used in this study, where the buoyancy parameter \( \beta = \alpha g \) (\( \alpha \) is the thermal expansion coefficient and \( g \) is the acceleration of gravity) is constant. Only the vertical component of the Coriolis acceleration is retained, \( \Omega_j = (0, 0, f/2) \), where \( f \) is the Coriolis parameter.

The SGS fluxes are related to the resolved-scale fields as

\[
\tau_{ij} = -K_M \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right), \quad \tau_{\theta j} = -K_H \frac{\partial \theta}{\partial x_j},
\]

(A.4)

where \( K_M \) and \( K_H \) are the SGS eddy viscosity and temperature conductivity. The SGS eddy coefficients are related to the SGS TKE through

\[
K_M = \text{Pr} K_H = C_K l \varepsilon^{1/2},
\]

(A.5)

where \( \text{Pr} \) is the Prandtl number, \( l \) is a mixing length and \( C_K = 0.1 \) is a constant. In unstable and neutral conditions, the mixing length is equal to the effective mesh spacing \( l = \Delta = \left( \frac{9}{4} \Delta_x \Delta_y \Delta_z \right)^{1/3} \), where the coefficient \( 9/4 \) appears due to de-aliasing of the upper 1/3 of wave numbers in the horizontal directions. The mixing length is reduced in stable conditions as suggested by Deardorff (1980), \( l = \min(\Delta, 0.76 \varepsilon^{1/2} / N) \), where \( N \) is the buoyancy frequency. Following Deardorff (1980), the Prandtl number is also taken to be stability dependent, \( \text{Pr}^{-1} = 1 + 2l / \Delta \).

The LES model carries a prognostic equation to determine the SGS TKE. It reads

\[
\frac{\partial \varepsilon}{\partial t} = -\frac{\partial \bar{u}_j \varepsilon}{\partial x_j} - \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} + \beta \tau_{\theta j} - \frac{\partial T_{\varepsilon j}}{\partial x_j} - \varepsilon.
\]

(A.6)

Here, \( T_{\varepsilon j} \) symbolizes the sub-grid-scale flux of \( \varepsilon \) (the third-order velocity correlation and the pressure-velocity correlation together), and \( \varepsilon \) stands for the TKE dissipation rate. The down-gradient diffusion assumption, \( T_{\varepsilon j} = -2K_M \partial \varepsilon / \partial x_j \), and the Kolmogorov hypothesis with the stability-dependent coefficient, \( \varepsilon = (0.19 + 0.74l / \Delta) \varepsilon^{3/2} / l \), are employed to model these quantities. Dimensionless coefficients in the above relations are determined by Moeng and Wyngaard (1988) to give the best inertial sub-range spectrum.

The code uses centred finite differences on a uniform vertical grid with the vertical velocity and SGS TKE staggered with respect to other variables. The pseudo-spectral method is used to evaluate the horizontal derivatives. The upper 1/3 of wave numbers are truncated in Fourier space for de-aliasing. The Adams–Bashforth scheme is used for time advance, and the Poisson equation for pressure is solved through a mixed fast-Fourier and finite-difference technique.

**APPENDIX B**

*Relation between the large-eddy simulation and the ensemble-average second-moment budgets*

In the equations below, a tilde denotes an average over a horizontal plane, and a double prime denotes a deviation thereof. This rather cumbersome double-prime/tilde notation is only used in the appendix in order to elucidate the relation between the LES and the ‘formal’ budgets. A simpler notation is used in the body of the text, where angle brackets denote approximations to the ensemble-mean turbulence moments.
Turbulence kinetic energy

The budget equation for the resolved-scale TKE is obtained from the LES momentum equation (A.1) in the usual way. Subtracting from Eq. (A.1) its horizontal mean, then multiplying the resulting equation by the velocity fluctuation about its horizontal mean, \( \overline{\nu_i''} \), and averaging the result, we obtain

\[
\frac{1}{2} \left( \frac{\partial}{\partial t} + \overline{u_j} \frac{\partial}{\partial x_j} \right) \overline{\nu_i''^2} =
- \overline{u_i'' u_j''} \frac{\partial \overline{u_i}}{\partial x_j} + \delta_{i3} \beta \overline{u_i'' \nu_i'} - \frac{1}{2} \frac{\partial}{\partial x_j} \overline{u_i'' u_i''} \overline{\nu_i''^2} - \frac{\partial}{\partial x_i} \overline{u_i'' \nu_i'} \overline{\nu_j''} - \frac{2}{3} \frac{\partial}{\partial x_i} \overline{\nu_i''^2} - \overline{u_i''} \frac{\partial \overline{\nu_i''}}{\partial x_j}. \tag{B.1}
\]

Notice that the pressure, \( \overline{p} \), cannot be discriminated from the modified pressure \( \overline{p} + \frac{2}{3} \overline{\nu_i''} \) if the equation for the SGS TKE is not carried by the LES model (which is the case for many LES models). Then, the previous last term on the r.h.s. would not explicitly appear in the budget. However, the difference between the pressure and the modified pressure is expected to be small unless the resolution is very coarse. Using the results of comparatively low-resolution 40³ simulation of the neutrally stratified boundary layer, performed with Moeng's code, Andrén et al. (1994) showed that the inclusion of \( (2/3) \overline{\nu_i''} \) in the pressure variable changes the r.m.s. pressure by only about 5%.

The last term on the r.h.s. of Eq. (B.1) can be re-arranged to give

\[
- \overline{u_i''} \frac{\partial \overline{\nu_i''}}{\partial x_j} = - \frac{\partial}{\partial x_j} \overline{u_i'' \nu_i''} - \overline{\nu_i''} \frac{\partial \overline{u_i'}}{\partial x_j} + \overline{\nu_i''} \frac{\partial \overline{u_i'}}{\partial x_j}. \tag{B.2}
\]

The first term on the r.h.s. of Eq. (B.2) has the form of a transport term. It integrates vertically to zero. The second term is the mean-gradient term similar to the first term on the r.h.s. of Eq. (B.1). Taken together, these two terms represent the mean-gradient production/destruction of turbulence energy due to the interaction of the shear stress (resolved + sub-grid) with the mean velocity gradient. By virtue of Eq. (A.4) for the SGS stress, the last term on the r.h.s. of Eq. (B.2) is negative definite and is, therefore, a sink of the turbulence energy. In order to elucidate its relation to the TKE dissipation we invoke Eq. (A.6) for the SGS TKE. Averaging Eq. (A.6) over the horizontal yields

\[
\left( \frac{\partial}{\partial t} + \overline{u_j} \frac{\partial}{\partial x_j} \right) \overline{\epsilon} = - \tau_{ij} \frac{\partial \overline{u_i}}{\partial x_j} + \delta_{i3} \beta \overline{\nu_i'} \frac{\partial \overline{\nu_i'}}{\partial x_j} - \overline{\nu_i''} \frac{\partial \overline{\nu_i''}}{\partial x_j} - \overline{\epsilon} - \frac{\partial}{\partial x_j} \overline{\nu_i'' \epsilon}. \tag{B.3}
\]

Thus, the last term on the r.h.s. of Eq. (B.2) is equal in magnitude but opposite in sign to the mean-gradient production term in the horizontally averaged budget equation for the SGS TKE, Eq. (B.3). As the local equilibrium in the SGS TKE budget is approached and the SGS buoyancy flux vanishes, which presumably happens with the increasing resolution, this term would approximate the TKE dissipation progressively more closely. The last term on the r.h.s. of Eq. (B.3) originates from the averaging of the nonlinear advection terms in the SGS TKE equation (A.6). It represents the transport of the SGS TKE by the resolved-scale motions and can be lumped together with the third term on the r.h.s. of Eq. (B.1).

Adding Eqs. (B.1) and (B.3) and rearranging terms, we obtain the budget equation for the total, i.e. resolved + sub-grid, turbulence energy. As no mean flow is present in our simulations, \( \overline{u_i} = 0 \), the advection and the mean-gradient terms vanish. Then, with due regard to the periodic boundary conditions in the horizontal directions, the TKE
budget equation can be written in the form
\[
\frac{\partial}{\partial t} \left( \frac{1}{2} \tilde{u}_i' \tilde{u}_i'' + \tilde{w} \right) = \beta (\tilde{u}_3' \tilde{\theta}'' + \tau_{\tilde{\theta}3}) - \frac{\partial}{\partial x_3} \left( \frac{1}{2} \tilde{u}_3' \tilde{u}_3'' + \tilde{u}_3' \tilde{\theta} \right) - \frac{\partial}{\partial x_3} \tilde{u}_3' \tilde{p}' - \tilde{w} 
\]
\[= \frac{\partial}{\partial x_3} \left( \tilde{w}_{\tilde{u}3'} \tau_{3} + \frac{2}{3} \tilde{u}_3' \tilde{\theta} + \tau_{33} \right). \tag{B.4} \]

Further averaging of Eq. (B.4) over a number of recorded time steps gives the budget that is treated as an approximation to the ensemble-mean TKE budget (stationary, to a good approximation). Realizing that other interpretations are possible (e.g. Brown 1995), we propose to treat the time mean of the last term on the r.h.s. of Eq. (B.4) as the budget imbalance. The first four terms on the r.h.s. of the above equation can be reasonably treated as the approximations to the buoyancy, the third-order transport, the pressure transport and the dissipation terms, respectively, in the ensemble-mean TKE budget, Eq. (4). Such treatment of the terms \( \partial \tilde{w}_{\tilde{u}3'} \tau_{3} / \partial x_3 \) and \( \partial \tilde{u}_3' \tilde{\theta} / \partial x_3 \) that come from the sub-grid-scale effects is difficult. The term \( \partial \tau_{33} / \partial x_3 \) is a transport term which comes from the SGS TKE equation. We propose to add it to the imbalance, however. Since the entire transport term is parametrized through the down-gradient diffusion approximation in the SGS TKE equation (A.6), it is impossible to discriminate between the third-order transport and the pressure transport of the SGS TKE. Hence, it is impossible to decide whether this term should be combined with the second term or with the third term on the r.h.s. of Eq. (B.4). Certainly, the above treatment of the TKE budget derived from the LES equations is justified provided that the budget imbalance becomes progressively smaller as the resolution is increased. Some \textit{a posteriori} justification is given in Fig. 11. In all our simulations the TKE budget imbalance is small over most of the CBL.

Potential-temperature variance

With regard to the absence of mean flow and to the periodic boundary conditions, the budget of the resolved-scale potential-temperature variance is
\[
\frac{1}{2} \frac{\partial}{\partial t} \tilde{\theta}'' = -\frac{\tilde{u}_3' \tilde{\theta}''}{\partial x_3} - \frac{1}{2} \frac{\partial}{\partial x_3} \tilde{u}_3' \tilde{\theta}'' - \frac{\partial}{\partial x_j} \tilde{\theta}'' \frac{\partial}{\partial x_j}. \tag{B.5} \]

Rearrangement of the sub-grid term, the last term on the r.h.s. of Eq. (B.5), gives
\[
-\frac{\partial}{\partial x_j} \tilde{\theta}'' = -\frac{\partial}{\partial x_3} \tilde{\theta}'' \tau_{33} - \tilde{\theta}'' \frac{\partial}{\partial x_3} \tilde{\theta}'' + \tau_{33} \frac{\partial}{\partial x_3} \tilde{\theta}'' + \tau_{33} \frac{\partial}{\partial x_j}. \tag{B.6} \]

The first term on the r.h.s. of Eq. (B.6) has the form of a transport term and integrates vertically to zero. The second term has the form of the mean-gradient term and may be combined with the first term on the r.h.s. of Eq. (B.5). By virtue of Eq. (A.4), the last term on the r.h.s. of Eq. (B.6) is purely destructive. It can be referred to as the ‘SGS dissipation’ of the potential-temperature variance, recognizing that it is not true dissipation. The term in question cannot be expressed through the parametrized dissipation that appears in the transport equation for the SGS potential-temperature variance, denoted by \( \tilde{\vartheta} \), since this transport equation is not carried by our LES model (cf. the TKE budget considered above). It is instructive, however, to consider the budget of \( \tilde{\vartheta} \). On horizontal averaging of the transport equation for \( \tilde{\vartheta} \) (this and other transport equations for the SGS quantities are considered in detail by Deardorff (1973)), the
budget reads

\[ \frac{1}{2} \frac{\partial}{\partial t} \tilde{\vartheta} = - \tau_{\vartheta j} \frac{\partial \tilde{\vartheta}}{\partial x_j} - \frac{1}{2} \frac{\partial}{\partial x_3} \tilde{F}_{\vartheta 3} - \tilde{\varepsilon}_\vartheta - \frac{1}{2} \frac{\partial}{\partial x_3} \tilde{u}_3' \tilde{\vartheta}, \] (B.7)

where \( F_{\vartheta 3} \) is the vertical SGS flux of \( \vartheta \), and \( \varepsilon_\vartheta \) is the dissipation of the potential-temperature variance. The last term on the r.h.s. of Eq. (B.7), originating from the horizontal averaging of the advection terms in the transport equation for \( \vartheta \), represents the transport of the SGS temperature variance by the resolved-scale motions. Provided the local values of \( \vartheta \) are available (which is not the case with our LES model), this term could be put together with the second term on the r.h.s. of Eq. (B.5). As may be inferred from Eq. (B.7), the SGS dissipation of the potential-temperature variance is a close approximation to the true dissipation provided the transport terms in the above budget are small. We propose that the following budget equation for the potential-temperature variance be adopted:

\[ \frac{1}{2} \frac{\partial}{\partial t} (\tilde{\vartheta}^2 + \tilde{\vartheta}) = -(\tilde{u}_3' \tilde{\vartheta}'' + \tilde{\tau}_{\vartheta 3}) \frac{\partial \tilde{\vartheta}}{\partial x_3} - \frac{1}{2} \frac{\partial}{\partial x_3} \tilde{u}_3'' \tilde{\vartheta}'' - K_M \left( \frac{\partial \tilde{\vartheta}}{\partial x_j} \right)^2 - \frac{\partial}{\partial x_3} \tilde{\vartheta}'' \tilde{\tau}_{\vartheta 3}. \] (B.8)

The time mean of Eq. (B.8) is treated as an approximation to the ensemble-mean budget of the potential-temperature variance, where the first three terms on the r.h.s. of Eq. (B.8) are the approximations of the corresponding terms in Eq. (5), and the last term on the r.h.s. of Eq. (B.8) is considered as the budget imbalance.

**Potential-temperature flux**

The horizontally averaged budget equation for the resolved-scale potential-temperature flux is

\[ \frac{\partial}{\partial t} \left( \tilde{u}_3'' \tilde{\vartheta}'' \right) = -\tilde{u}_3'' \frac{\partial \tilde{\vartheta}}{\partial x_3} + \beta \tilde{\vartheta}'' - \frac{\partial}{\partial x_3} \tilde{u}_3'' \tilde{\vartheta}'' - \tilde{\tau}_{\vartheta 3} \frac{\partial \tilde{\vartheta}}{\partial x_3} - \frac{2}{3} \frac{\partial \tilde{\vartheta}''}{\partial x_3} \frac{\partial \tilde{\vartheta}''}{\partial x_j} - \tilde{u}_3'' \frac{\partial \tilde{\vartheta}}{\partial x_j}. \] (B.9)

Rearrangement of the last two terms on the r.h.s. of Eq. (B.9) gives

\[ -\tilde{\vartheta}'' \frac{\partial \tilde{\tau}_{\vartheta 3}}{\partial x_j} - \tilde{u}_3'' \frac{\partial \tilde{\tau}_{\vartheta 3}}{\partial x_j} = -\frac{\partial}{\partial x_3} \tilde{\vartheta}'' \tilde{\tau}_{33} - \frac{\partial}{\partial x_3} \tilde{u}_3'' \tau_{33} - \tilde{\tau}_{33} \frac{\partial \tilde{\vartheta}}{\partial x_3} + \left( \tilde{\tau}_{3j} \frac{\partial \tilde{\vartheta}}{\partial x_j} + \tau_{\vartheta j} \frac{\partial \tilde{u}_3}{\partial x_j} \right). \] (B.10)

The first term on the r.h.s. of Eq. (B.10) has the form of a transport term and integrates vertically to zero. The second term is the transport of the SGS potential-temperature flux by the resolved-scale motions. It can be combined with the third term on the r.h.s. of Eq. (B.9). The third term on the r.h.s. of Eq. (B.10) has the form of the mean-gradient term and may be combined with the first term on the r.h.s. of Eq. (B.9). As distinct from the TKE and the temperature-variance budgets, the sum of the terms in parentheses on the r.h.s. of Eq. (B.10) is not negative definite and cannot, therefore, be considered as the ‘SGS dissipation’ of the potential-temperature flux. In order to get some insight into the nature of these terms, we invoke the budget equation for the SGS potential-temperature
flux. Upon horizontal averaging of the transport equation for $\tau_{\theta 3}$, the budget is

$$\frac{\partial}{\partial t} \tilde{\tau}_{\theta 3} = - \left( \tilde{\tau}_{3j} \frac{\partial \tilde{\theta}}{\partial x_j} + \tilde{\tau}_{\theta j} \frac{\partial \tilde{\theta}}{\partial x_j} \right) - \frac{\partial \tilde{\tau}_{w\theta 3}}{\partial x_3} + \beta \tilde{\theta} - \tilde{P}_w - \frac{\partial}{\partial x_3} \tilde{u}_3'' \tau_{\theta 3}, \quad (B.11)$$

where $\tau_{w\theta 3}$ is the vertical SGS flux of $\tau_{\theta 3}$, and $P_w$ is the sub-grid-scale potential-temperature/pressure-gradient covariance. Thus, the terms in parentheses in Eq. (B.10) are equal in magnitude but opposite in sign to the mean-gradient production/destruction terms in the budget equation for the SGS potential-temperature flux, Eq. (B.11). Estimating the last term on the r.h.s. of Eq. (B.11) from the LES data, we find that in all our simulations it is much smaller than the sum of the mean-gradient terms in parentheses. Assuming that the SGS transport term, $\partial \tilde{\tau}_{w\theta 3}/\partial x_3$, is also small, Eq. (B.11) reduces to a local balance between the mean-gradient, the buoyancy and the pressure terms. Then, we propose the following form of the budget equation for the potential-temperature flux:

$$\frac{\partial}{\partial t} \left( \tilde{u}_3'' \tilde{\theta} + \tilde{\tau}_{\theta 3} \right) = - \left( \tilde{u}_3'' \tilde{\theta} + \tilde{\tau}_{\theta 3} \right) \frac{\partial \tilde{\theta}}{\partial x_3} + \beta \tilde{\theta} \tilde{\theta} + \tilde{\theta} \tilde{\theta}'' - \frac{\partial \tilde{\tau}_{w\theta 3}}{\partial x_3} - \frac{\partial \tilde{\tau}_{w\theta 3}}{\partial x_3} \tilde{\theta}'' \frac{\partial \tilde{\theta}}{\partial x_3} \tilde{\theta}'' \frac{\partial \tilde{\theta}}{\partial x_3} - \beta \tilde{\theta} \left( \frac{\partial \tilde{\theta}}{\partial x_3} \tilde{\tau}_{\theta 3} + \frac{\partial \tilde{\theta}}{\partial x_3} \tilde{\tau}_{\theta 3} + \frac{\partial \tilde{\theta}}{\partial x_3} \tilde{\tau}_{\theta 3} + \frac{\partial \tilde{\theta}}{\partial x_3} \tilde{\tau}_{\theta 3} \right). \quad (B.12)$$

The time mean of Eq. (B.12) is treated as an approximation to the ensemble-mean budget of the potential-temperature flux. The sum of the SGS terms in parentheses on the r.h.s. of Eq. (B.12) is labelled $-P_{SG}$ in Eq. (6). The above arguments suggest that it may be treated as an approximation to the SGS potential-temperature/pressure-gradient covariance and may, therefore, be combined with the resolved-scale pressure term. In order to be explicit, we write these terms separately. The sum of the terms in the second set of brackets on the r.h.s. of Eq. (B.12) is treated as the budget imbalance.

A rough estimate of the SGS potential-temperature variance, $\tilde{\sigma}$, is obtained by assuming local balance between the mean-gradient production and the dissipation of the temperature variance and local isotropy at the sub-grid scales. Then (e.g. Nieuwstadt et al. 1993), $\tilde{\sigma} = 5 \tilde{\theta} / \tilde{\sigma}$, where the numerical value of the coefficient follows from the consideration of the inertial sub-range temperature spectrum (Moeng and Wyngaard 1988). In all our simulations $\tilde{\sigma}$ is small over most of the CBL.

Results from the LES study of Kanna (1998) lend considerable support to the above treatment of the second-moment budgets. Kanna compared LESs of sheared CBLs, performed with the nested-grid version of Moeng’s large-eddy code, with the observational data from the Kansas field measurements. He found that neglect of the SGS contributions to the third-order transport of the TKE, of the potential-temperature variance and of the potential-temperature flux does not result in a noticeable underestimate of empirical data. The LES estimates of the TKE dissipation and of the dissipation of the temperature variance also compare well with empirical data. The resolved-scale potential-temperature/pressure-gradient covariance proves to significantly underestimate empirical data, suggesting that the SGS pressure term is important. This is consistent
with our interpretation of the SGS terms in the temperature-flux budget. As discussed in section 4(d), $P_{sg}$ is small compared with the major terms in the budget, but is not negligible.

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