Pressure–potential-temperature covariance in convection with rotation

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SUMMARY

The pressure–potential-temperature covariance in free and rotating turbulent convection with no mean velocity shear is analysed, using a dataset generated with a large-eddy simulation (LES) model. The pressure field is resolved into turbulence–turbulence, buoyancy and Coriolis components, and the contributions from these components to the pressure-gradient–potential-temperature covariance in the budget equation for the potential-temperature flux are examined.

In non-rotating convection, the buoyancy contribution compensates for about one half of the buoyant production term in the flux budget equation, and the turbulence–turbulence contribution is well approximated by the Rotta-type return-to-isotropy model with the relaxation time-scale set proportional to the turbulence energy dissipation time-scale.

In convection with rotation, neither the simplest Rotta-type model with the relaxation time-scale proportional to the energy dissipation time-scale nor the more sophisticated two-component-limit (TCL) nonlinear model are able to accurately describe the LES data. A somewhat better agreement is found when a limitation is imposed on the relaxation time-scale due to the background rotation. The simplest model for the buoyancy contribution, where it is set proportional to the buoyant production term in the flux budget equation, fares poorly. The TCL model shows better agreement with LES data although some uncertainties remain. However, the relative importance of the buoyancy contribution to the pressure-gradient–potential-temperature covariance decreases with increasing rotation rate.

In contrast, the Coriolis contribution becomes more important as the rotation rate increases. Neither the simplest linear model for the Coriolis contribution nor the much more complex nonlinear TCL model are found to be adequate. Neither model appropriately accounts for the component of the angular velocity of rotation that is parallel to the component of the pressure gradient in question. In the seemingly simplest case considered in the present paper, when the rotation vector is aligned with the vector of gravity, no Coriolis contribution to the vertical-pressure-gradient–potential-temperature covariance is predicted by these models. This results in a strong undersatation of the pressure term in the flux budget equation and may lead to an erroneous prediction of the vertical potential-temperature flux in convection with rotation. In an attempt to remedy the situation, an extension of the TCL model that contains only one extra empirical coefficient is developed and checked against LES data.

KEYWORDS: Large-eddy simulation Pressure–scalar covariance Rotating convection Turbulence

1. INTRODUCTION

One of the key issues in the second-order turbulence closure modelling is the parametrization of the pressure terms in the second-moment budget equations. Following the early work of Rotta (1951), who proposed the so-called return-to-isotropy parametrization for the pressure–velocity-gradient covariance in turbulent shear flows, a number of more sophisticated parametrizations for the pressure–velocity covariances in the Reynolds stress equations and the pressure–scalar covariances in the budget equations for turbulent fluxes of scalars (potential temperature, moisture, salinity, or any passive admixture) were developed.

The pressure field is often not known in sufficient detail from field observations and laboratory experiments. Datasets generated through large-eddy simulation (LES) have been used to evaluate parametrizations for the pressure terms (e.g. Moeng and Wyngaard 1986; Andrén and Moeng 1993). The pressure field is decomposed into turbulence–turbulence, shear, buoyancy, and Coriolis components, the Poisson equation for each component is solved, and contributions from each of the components to the pressure–velocity covariance and the pressure–scalar covariance are evaluated.

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In the present paper, an LES dataset is used to analyse the pressure–potential-temperature covariance in convective flows strongly affected by the background rotation. Rotating convection is important for many geophysical and astrophysical (e.g. Boublnov and Golitsyn 1995) and technical (e.g. Fontaine et al. 1989) applications. A prominent geophysical example is open-ocean deep convection (Marshall and Schott 1999). It occurs in a few areas of the world’s oceans and is believed to play a key role in the ocean thermohaline circulation and hence in the climate system. The objective of the present study is to evaluate current parametrizations and to attempt to develop an improved parametrization for the pressure term in the budget equation for the potential-temperature flux. As was shown by Mironov et al. (2000), the pressure-gradient–potential-temperature covariance is one of the dominating terms in the flux budget in the convective boundary layer (CBL) affected by rotation. This places stringent requirements upon the accuracy of the parametrization of the pressure term. Using an LES dataset, we show that the Coriolis contribution to the pressure-gradient–potential-temperature covariance becomes more important as the rotation rate increases. We find that neither the simplest linear model for the Coriolis contribution, nor a more complex two-component-limit (TCL) nonlinear model, are adequate. We then attempt to develop an improved model and check it against LES data.

We restrict our consideration to the one-point second-moment closures. In spite of their numerous shortcomings, these closures remain the most widely used turbulence models that offer fairly accurate solutions to a large variety of problems at a bearable computational cost. The so-called realizible models (e.g. Schumann 1977; Lumley 1978; Shih 1996) have become increasingly popular in recent years. By their very construction, realizible models cannot yield physically impossible solutions (e.g. negative variances). A prominent example of an intrinsically realizable model is the TCL model of Craft et al. (1996). The model is designed to satisfy the TCL, i.e. the limit which turbulence approaches when the velocity component in one direction vanishes. This occurs, for example, at a rigid wall or at a very sharp density interface. The model is shown to perform satisfactorily over a variety of shear and buoyant flows. Because of its expected broad range of applicability, and considering that rotation has the effect of driving the turbulence towards the TCL, the Craft et al. (1996) TCL model is taken in this study as a basis for further development.

2. Background

Rotta (1951) was apparently the first to propose a return-to-isotropy parametrization for the pressure–velocity-gradient covariance in turbulent shear flows. He assumed that the rate of return of turbulence to isotropy is proportional to the degree of anisotropy and inversely proportional to a certain time-scale called the ‘return-to-isotropy’ time-scale. This formulation was extended to the pressure-gradient–potential-temperature covariance on the assumption that the rate of destruction of the turbulent flux of potential temperature can be related to the flux in question through a certain relaxation time-scale,

$$\left\{ \frac{\partial p}{\partial x_i} \right\} = \frac{\langle u_i \theta \rangle}{\tau}.$$  \hspace{1cm} (1)

Here, $x_i$ are the right-hand Cartesian coordinates, $u_i$ are the velocity components, $p$ is the kinematic pressure (pressure divided by the reference density, $\rho_r$), $\theta$ is the potential temperature, and $\tau$ is the relaxation ‘return-to-isotropy’ time-scale for potential temperature. To simplify notation, we omit primes and use small letters to denote turbulent fluctuations, while capital letters stand for mean quantities. The angle brackets
denote the ensemble means. In the present paper we restrict our consideration to potential temperature. For the sake of brevity, it will also be referred to as simply ‘temperature’ in what follows (the term ‘buoyancy’ could be used instead as the two quantities are taken to be linearly related). Any other conservative scalar could be considered in a similar way.

Some modellers applied the return-to-isotropy parametrization to the entire pressure-gradient–temperature covariance, thus lumping all the uncertainties on the return-to-isotropy time-scale. A standard approach nowadays is to decompose \( \langle \theta \partial p / \partial x_i \rangle \equiv \Pi_i \) into the contributions due to the nonlinear turbulence–turbulence interactions, \( \Pi_i^T \), mean shear, \( \Pi_i^S \), buoyancy, \( \Pi_i^B \), and the Coriolis effects, \( \Pi_i^C \), and to model these contributions separately. This decomposition is briefly introduced in appendix A. Then, the return-to-isotropy parametrization is applied to the turbulence–turbulence contribution only. The simplest linear approximations for the above four contributions to \( \Pi_i \) can be written in the form (e.g. Zeman 1981)

\[
\Pi_i^T = C_T \frac{\langle u_i \theta \rangle}{\tau},
\]

\[
\Pi_i^S = C_{S1} \langle u_j \theta \rangle \frac{\partial U_i}{\partial x_j} + C_{S2} \langle u_j \theta \rangle \frac{\partial U_j}{\partial x_i},
\]

\[
\Pi_i^B = C_B \beta_i \langle \theta^2 \rangle,
\]

\[
\Pi_i^C = C_C \delta_{ij} f_p \langle u_j \theta \rangle.
\]

where \( C_T, C_{S1}, C_{S2}, C_B \) and \( C_C \) are dimensionless coefficients (other symbols are introduced in appendix A). The turbulence kinetic energy (TKE) dissipation time-scale, \( \tau_\epsilon = \langle \epsilon \rangle / \langle \epsilon \rangle \), where \( \langle \epsilon \rangle = \langle u_i u_i \rangle / 2 \) is the TKE and \( \langle \epsilon \rangle \) is the TKE dissipation rate, is typically used in Eq. (2) instead of the return-to-isotropy time-scale, assuming that the two time-scales are proportional to each other.

Generally speaking, \( \Pi_i^T, \Pi_i^S, \Pi_i^B \) and \( \Pi_i^C \) depend non-linearly on the flow variables, such as the distance to the nearest wall and the departure-from-isotropy tensor defined as

\[
a_{ij} = \frac{\langle u_i u_j \rangle}{\langle \epsilon \rangle} - \frac{2}{3} \delta_{ij}.
\]

A number of elaborate nonlinear models for various contributions to \( \Pi_i \) have been developed to date (summaries are given by Lumley (1978), Zeman (1981), and Hallbäck et al. (1996), among others). The nonlinear models perform better than the simplified linear models, particularly in the flows with large departures from isotropy. The nonlinear models are inevitably complex, however, and are inconvenient to use. Many modellers, therefore, accept the deficiencies of linear approximations and use Eqs. (2)–(5) where the dimensionless coefficients \( C_T, C_{S1}, C_{S2}, C_B \) and \( C_C \) are adjusted so as to provide a better fit to empirical data. This is the case, for example, for a popular family of turbulence closure schemes known as the Mellor–Yamada closures (Mellor and Yamada (1974, 1982); see also Nurser (1996) for a comprehensive overview) that have been extensively used in geophysical applications.

The work of Jones and Musogna (1983), (see also Dakos and Gibson 1987) should be mentioned. These authors considered the pressure–scalar covariance in non-rotating turbulent flows. Along with the \( \Pi_i^T \) and \( \Pi_i^S \) terms, they included an additional term, \( \Pi_i^M \), proportional to the gradient of mean scalar concentration, into their model of \( \Pi_i \). Their
expression for $\Pi_i^M$ reads

$$\Pi_i^M = C_M \langle e \rangle a_{ij} \frac{\partial \Theta}{\partial x_j},$$

(7)

where $C_M$ is a dimensionless coefficient. Jones and Musonge (1983) showed that the inclusion of the above term produces a good agreement between the model results and data from laboratory experiments on nearly homogeneous strongly sheared flow. The Jones and Musonge approach was further developed by Craft et al. (1996) who incorporated the term proportional to $\partial \Theta / \partial x_j$ into the expression for $\Pi_i^T$.

3. The Large-Eddy-Simulation Dataset

The large-eddy simulation model used in the present study was developed by Moeng (1984) and modified by Moeng and Wyngaard (1988). The model solves filtered Navier-Stokes equations using a mixed finite-difference pseudo-spectral method. The sub-grid scale (SGS) parametrization is based on a prognostic equation for the SGS TKE. The SGS fluxes are computed through the down-gradient approximation. Derivatives in the horizontal directions are evaluated pseudo spectrally. The upper 1/3 of wave numbers are truncated in Fourier space for de-aliasing. Centred finite differences on a uniform vertical grid are used with the vertical velocity and SGS turbulence energy staggered with respect to other variables. 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.

Four shear-free convective flows were generated. The simulations of the surface-heating-driven convective boundary layers (CBLs) that grow into quiescent stably stratified fluids are referred to as case R0 (no rotation) and R2 (strong rotation). Two simulations of convection between the two rigid boundaries where the lower boundary is heated at the same rate as the upper is cooled are referred to as case D0 (no rotation) and D2 (strong rotation). The latter flows have no complications related to the entrainment at the CBL outer edge. In our configuration, potential temperature is the only thermodynamic variable, the equation of state is linear, and the rotation vector is aligned with the vector of gravity (both are aligned with the $x_3$-axis). The input parameters of the simulated cases are given in Table 1, where $L_1$, $L_2$ and $L_3$ are the numerical domain sizes in $x_1$, $x_2$ and $x_3$ directions, respectively, $N_1$, $N_2$ and $N_3$ are the number of grid points in these directions, and $f = (f_1 f_i)^{1/2}$ is the modulus of the Coriolis vector.

In all simulated cases periodic boundary conditions are applied in both $x_1$ and $x_2$ horizontal directions. The boundary conditions at the horizontal (upper and lower) boundaries are as follows. In cases R0 and R2, zero SGS TKE, free-slip for the horizontal velocity components, the potential-temperature lapse rate, $\Gamma = 6 \times 10^{-3}$ K m$^{-1}$, and the radiative upper-boundary conditions, that allow internal gravity waves
TABLE 2. INTERNAL PARAMETERS FROM THE SIMULATED CASES

<table>
<thead>
<tr>
<th>Case</th>
<th>Sampling time (s)</th>
<th>No. of samples</th>
<th>$h$ (m)</th>
<th>$w_*$ (m s$^{-1}$)</th>
<th>$\theta_*$ (K)</th>
<th>$\tau_*$ (s)</th>
<th>$\tau_*$ (s)</th>
<th>$\Omega_*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>R0</td>
<td>4000</td>
<td>40</td>
<td>842</td>
<td>1.40</td>
<td>0.071</td>
<td>600</td>
<td>0</td>
<td>$\infty$</td>
</tr>
<tr>
<td>R2</td>
<td>4000</td>
<td>40</td>
<td>861</td>
<td>1.41</td>
<td>0.071</td>
<td>610</td>
<td>0</td>
<td>2230</td>
</tr>
<tr>
<td>D0</td>
<td>10800</td>
<td>90</td>
<td>800</td>
<td>1.38</td>
<td>0.073</td>
<td>580</td>
<td>0</td>
<td>$\infty$</td>
</tr>
<tr>
<td>D2</td>
<td>8000</td>
<td>80</td>
<td>1000</td>
<td>1.48</td>
<td>0.067</td>
<td>670</td>
<td>0</td>
<td>2470</td>
</tr>
</tbody>
</table>

to leave the system, are applied at the upper boundary of the domain. At the lower boundary, velocities are zero, the potential-temperature flux (heat flux divided by the reference density and specific heat at constant pressure) is prescribed, and the vertical fluxes of the horizontal momentum are evaluated from the surface-layer similarity. In cases D0 and D2, the bottom of the domain is heated at the same rate as its top is cooled, and no-slip conditions for the horizontal velocity are applied at both upper and lower boundaries. The surface potential-temperature flux is $Q_s = 0.1$ K m s$^{-1}$ in all simulations. This corresponds to the surface buoyancy flux, $B_s = \beta Q_s = 3.27 \times 10^{-3}$ m$^2$ s$^{-3}$, where $\beta = \beta_3 = g/\Theta_r$ is the buoyancy parameter, $g = 9.81$ m s$^{-2}$ is the (magnitude of) acceleration due to gravity, and $\Theta_r = 300$ K is the reference temperature.

The initial potential-temperature profile in simulations R0 and R2 has a three-layer structure. A mixed layer of depth 780 m and potential temperature $\Theta_r$ is capped by an interfacial layer where potential temperature increases linearly by 1.2 K over four grid intervals. The lapse rate is $\Gamma$ above the interfacial layer. In simulations D0 and D2, the initial temperature is $\Theta_r$ throughout the domain.

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 (lower and upper parts for runs with two rigid boundaries), and the SGS TKE 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 the internal parameters of the simulated cases are given in Table 2.

Here, $h$ is the CBL depth (which is equal to the vertical domain size in cases D0 and D2, and is defined from the surface to the level where the temperature flux is a minimum in cases R0 and R2), and $w_* = (h\beta Q_s)^{1/3}$ and $\theta_* = Q_s/w_*$ are the Deardorff (1970a, b) velocity and temperature scales, respectively. The time-scale $\tau_* = hw_*^{-1}$ is the turnover time-scale based on the Deardorff convective-velocity scale. The time-scale $\tau_* = hw_*^{-1}$ is the turnover time-scale based on the rotational velocity scale $w_0 = (\beta Q_s)^{1/2} f^{-1/2}$ (Golitsyn 1980). The cube of the ratio of the two time-scales is a Rossby number, $\Omega_*$ = $(\beta Q_s)^{1/2} f^{-3/2} h^{-1}$. The Rossby number can also be considered as the cube of the ratio of the rotational velocity scale, $w_0$, to the Deardorff convective-velocity scale, $w_*$, or as the ratio of the rotational depth scale, $l_0 = (\beta Q_s)^{1/2} f^{-3/2}$, to the CBL depth, $h$. A small $\Omega_*$ shows that convection is affected by rotation, as is the case in simulations R2 and D2.

In what follows, all quantities are presented in dimensionless form. They are made dimensionless with the CBL depth, $h$, and the Deardorff velocity $w_*$ and temperature $\theta_*$ scales, which are now routinely used in studies of convective flows. The turbulence statistics are computed by means of averaging over horizontal planes and over a number of recorded time steps (Table 2). These horizontal and time means are treated as approximations to the ensemble means denoted by the angle brackets. As the CBL depth
in cases R0 and R2 slightly increases during the sampling period, we normalize all data with the Deardorff convective scales prior to time averaging.

4. ANALYSIS

(a) Components of the pressure field

The fluctuating pressure computed by an LES model is a result of several processes. It may be decomposed into the components due to the nonlinear turbulence–turbulence interactions, mean shear, buoyancy, Coriolis effects, and the SGS stress effects, as discussed briefly in appendix A. The component due to the mean shear is zero in our simulations.

The components of the root mean square (r.m.s.) fluctuating pressure are shown in Fig. 1. As seen from the figure, the total r.m.s. pressure is enhanced by rotation. The increase in \( (p^2)^{1/2} \) is larger close to the boundaries. The turbulence–turbulence component is the largest over most of the convective layer in cases D0 and R0 with no rotation. The buoyancy component is about the same close to the surface (upper and lower surfaces in case D0). It shows a maximum in the interfacial layer near the CBL top in case R0. In cases D2 and R2 with strong rotation, the Coriolis component dominates over most of the convective layer, except near the surface in case R2. The turbulence–turbulence component is the second largest, while the relative importance of the buoyancy component is reduced. In all simulations, the component due to the SGS stress is small over most of the CBL except close to the rigid boundaries. It should be mentioned that the square root of the sum of the four pressure variances (not shown) is slightly different from the square root of the total pressure variance, indicating that the pressure components are correlated.

(b) Components of the pressure-gradient–temperature covariance

The various contributions to the pressure field computed from Eqs. (A.3) and (A.4) are used to compute the corresponding contributions to the covariance of the vertical pressure gradient and temperature (see appendix A). The result is shown in Fig. 2 (in this and other figures, covariances with the sign reversed are shown as they appear in the temperature flux budget). In the bulk of non-rotating CBLs, the turbulence–
turbulence component, \( \Pi_3^T \), and the buoyancy component, \( \Pi_3^B \), are of the same order of magnitude, \( \Pi_3^B \) being slightly larger than \( \Pi_3^T \) in case D0 and vice versa in case R0. The buoyancy component dominates in the interfacial layer in case R0. In simulation D2 with rotation, the turbulence–turbulence component is still the largest over most of the CBL. The Coriolis component, \( \Pi_3^C \), is the second largest and is very close in magnitude to \( \Pi_3^T \). The relative importance of \( \Pi_3^B \) is reduced. In case R2, \( \Pi_3^T \) and \( \Pi_3^C \) dominate in the mid CBL, while \( \Pi_3^B \) is the largest component in the interfacial layer near the CBL top. The SGS component, \( \Pi_3^{SG} \), is small in all cases over most of the convective layer except close to the rigid boundaries, thus making the LES estimates of the ensemble-mean quantities less useful there. The interfacial layer is also known to present serious problems for LESs, and care must be exercised in the interpretation of results. However, considering that \( \Pi_3^{SG} \) appeared to be small there in cases R0 and R2, it is believed that a useful insight can still be gained.

One important issue pertaining to the relation between the LES and the ‘formal’ ensemble-averaged second-moment budgets, and, therefore, to the estimation of \( \Pi_3 \) from LES data, should be considered. Although this issue is discussed in some detail by Mironov et al. (2000), we feel that a brief account would be appropriate here. The LES
estimates of the various terms in the budgets of the second-order turbulence moments should contain the resolved-scale and the SGS contributions. It is then hoped that the SGS contributions become progressively smaller as the resolution is increased. Since our LES model carries the transport equation for the SGS turbulence energy, the SGS contributions to the various terms in the TKE budget can be evaluated directly. This is not the case for the temperature variance and the temperature flux. When the budgets of these quantities are constructed from the LES fields, the SGS contributions to various terms in the budgets are often entirely neglected. Using data from moderate resolution
LESs, Mironov et al. (2000) showed that the neglect of the SGS contribution to the third-order transport terms does not result in a noticeable imbalance in the second-moment budgets, while the SGS contribution to the pressure-gradient-temperature covariance should be retained in order to close the temperature flux budget to a good order. The question then arises as to whether the temperature flux budget derived from low to moderate resolution LESs is useful for the second-order modelling with Reynolds averaging, and if so, how the LES data should be interpreted. A plausible interpretation is considered in appendix B. Based upon arguments adduced in appendix B, we propose that an estimate of the SGS pressure term be added to the turbulence–turbulence part.
of the pressure-gradient–temperature covariance derived from the resolved-scale LES fields. This sum is used as an approximation for \( \Pi_i^T \) in what follows.

\[ (c) \quad \text{Slow part of } \Pi_i \]

In this section, we examine the turbulence–turbulence (slow) contribution to the pressure-gradient–temperature covariance. We first consider the simplest Rotta-type parametrization of \( \Pi_i^T \) given by Eq. (2). Values of dimensionless constant \( C_T \) in Eq. (2) recommended by various authors for free convective flows average at about 3. As seen from Fig. 3, the approximations to \( \Pi_i^T \) computed from the right-hand side (r.h.s.) of Eq. (2) with this commonly accepted value of \( C_T = 3.0 \) exhibit very good fit to LES data over the CBL interior in cases D0 and R0. The model, Eq. (2), underestimates LES data in the interfacial layer in case R0 and close to the rigid boundaries in case D0.

In cases D2 and R2, the approximation through Eq. (2) with \( C_T = 3.0 \) considerably underestimates the LES data. One possible way to remedy the situation (probably not well justified theoretically, but attractive from the standpoint of practical applications) is to keep the simple form given by Eq. (2), but to alter the relaxation time-scale. To this end, we invoke the idea of Hassid and Galperin (1994) who impose a limitation on the TKE dissipation length scale, \( l_e \equiv \langle e \rangle^{3/2}/\langle \epsilon \rangle \), due to the background rotation. These authors proposed a second-order turbulence model for neutral and unstable rotating boundary layers. The various length scales of the model were set proportional to the so-called master length scale, \( l_M \), and an algebraic formula for \( l_M \) was developed to close the problem. The Hassid and Galperin (1994) expression for \( l_M \) in the asymptotic case of rapid rotation (small Rossby number) reads

\[ l_M = \left( \frac{\langle e \rangle}{\langle \epsilon \rangle} \right)^{1/2} f, \tag{8} \]

where a constant on the r.h.s. is arbitrarily set to one as this constant always occurs in combination with other constants. Mironov et al. (2000) evaluated this formulation against data from LESs of CBLs strongly affected by the background rotation. The LES data lend support to the idea of imposing a limitation on the TKE dissipation length scale, \( l_e = C_{el} l_M \), \( C_{el} \) being a dimensionless constant. This limitation is required to account for the reduced TKE in convection with rotation.

It is a straightforward exercise to reformulate the above parametrization in terms of the 'master' time-scale. The result is \( \tau = (C_{\tau} f)^{-1} \), where \( C_{\tau} \) is a dimensionless constant. Then, the simplest interpolation formula for the relaxation time-scale that accounts for the asymptotic limits of rotation-free and rotationally dominated turbulence reads

\[ \tau = \frac{\langle e \rangle/\langle \epsilon \rangle}{1 + C_{\tau} f \langle e \rangle/\langle \epsilon \rangle}. \tag{9} \]

The relaxation approximation Eq. (2) with \( C_T = 3.0 \) and the time-scale given by Eq. (9) is shown in Fig. 3 by dot-dashed curves for cases with rotation. In case R2, a reasonable fit to LES data in mid CBL (but not in the interfacial layer) is obtained with \( C_{\tau} = 0.15 \). In case D2, a reasonable overall fit is obtained with \( C_{\tau} = 0.1 \), but the shapes of the LES and theoretical curves are different.

Craft et al. (1996) developed an elaborate nonlinear second-moment closure model that satisfies the TCL, i.e. the limit which turbulence approaches when the velocity component in one direction (and, therefore, also a scalar flux in this direction) vanishes.
Figure 3. Dimensionless turbulence–turbulence component of the pressure-gradient–temperature covariance, $-\Pi_3^T h/w^2 \theta_s$, versus dimensionless height, $x_3/h$, for simulations D0 (a), D2 (b), R0 (c), and R2 (d). Short-dashed curves show total $-\Pi_3^T h/w^2 \theta_s$ from the LES data. Solid curves are computed from the right-hand side of Eq. (2) with $r = \langle e \rangle / \langle e \rangle$ and $C_T = 3.0$. Dot-dashed curves are computed from Eq. (2) with $r$ given by Eq. (9), $C_T = 3.0$, and $C_r = 0.1$ for case D2 and $C_r = 0.15$ for case R2. Long-dashed curves show the Craft et al. (1996) TCL formulation, Eq. (10). See text for further explanation.

Details of the TCL model are discussed in what follows. The Craft et al. (1996) formulation for the slow part of $\Pi_i$ reads

$$\Pi_i^T = C_{T1} \frac{R^{1/2}}{\tau_e} \{ \langle u_i \theta \rangle (1 + C_{T2} A_2) + C_{T3} a_{ij} \langle u_j \theta \rangle + C_{T4} a_{ij} a_{jk} \langle u_k \theta \rangle \}$$

$$+ C_{T5} R \langle e \rangle a_{ij} \frac{\partial \Theta}{\partial x_j}. \quad \text{(10)}$$
Here, \( C_{T1} = 1.7(1 + 1.2(A_2A)^{1/2}) \), \( C_{T2} = 0.6 \), \( C_{T3} = -0.8 \), \( C_{T4} = 1.1 \) and \( C_{T5} = 0.2A^{1/2} \) are dimensionless coefficients, \( R = (2(\epsilon_\theta)/\langle \theta^2 \rangle) \tau_e \) is the time-scale ratio, \( \epsilon_\theta \) is the dissipation rate of the temperature variance, \( A = 1 - (9/8)(A_2 - A_3) \) is the ‘flatness parameter’, and \( A_2 = a_{ij}a_{ij} \) and \( A_3 = a_{ij}a_{jk}a_{kl} \) are the invariants of the departure-from-isotropy tensor. The quantity \( A \) has the property that it vanishes in the two-component limit (Lumley 1978). Notice the term proportional to the gradient of the mean potential temperature on the r.h.s. of Eq. (10).

In Fig. 3, \( \Pi_3^T \) computed through Eq. (10) is shown by long-dashed curves. In cases R0 and D0 with no rotation, the Craft et al. (1996) TCL model fits LES data fairly well. Notice that in case R0 the TCL model shows a considerably better agreement with LES data in the interfacial layer than a simple Rotta-type return-to-isotropy model. It overestimates data close to the rigid boundaries, however. In cases D2 and R2 with rotation, the TCL model underestimates LES data over most of the CBL. It would not be an exaggeration to say that all models tested are far from perfect when applied to rotating CBLs.

\[ \Pi_3 \]

\[ \text{(d) Buoyancy contribution to } \Pi_i \]

Isotropic tensor modelling (e.g. Lumley 1978) leads to the estimate \( C_B = 1/3 \) of the dimensionless coefficient in the parametrization, Eq. (4), of the buoyancy contribution to the pressure-gradient–temperature covariance. As this isotropic value appears to be inconsistent with most boundary-layer data, other estimates were suggested. For CBLs, the estimate of \( C_B = 0.5 \) was used by many authors. Moeng and Wyngaard (1986) demonstrated that this value is consistent with data from LESs of slightly sheared strongly convective boundary layers.

In Fig. 4, \( \Pi_3^B \) from LESs is compared with its parametrization through Eq. (4) with \( C_B = 0.5 \). In cases D0 and R0 with no rotation, the agreement between the parametrization and the data is good over most of the CBL. In case R0, the parametrization somewhat underestimates the data in the interfacial layer. Notice that the value of \( C_B = 0.4 \), used by some authors (e.g. Zilitinkevich et al. 1999), would provide even closer agreement with data over the CBL interior but would depart from it in the interfacial layer. The situation is considerably worse in cases D2 and R2 with rotation. In case D2, Eq. (4) with the ‘free convection’ value of \( C_B = 0.5 \) strongly overestimates the LES data. A value of \( C_B \) a few times smaller (of order 0.1) is required to provide a reasonable overall fit to data over mid CBL. In case R2, Eq. (4) with \( C_B = 0.5 \) provides a nearly perfect fit to the LES data in the interfacial layer, but greatly overestimates the data over the CBL interior. It should be emphasized that in case R2 a reasonably good fit to data throughout the CBL cannot be obtained by simply varying the value of \( C_B \) in Eq. (4). This is because the shapes of the \( \Pi_3^B \) curve (Fig. 4) and of the \( \beta(\langle \theta^2 \rangle) \) curve (Fig. B.1) are different.

Lumley (1978) proposed a nonlinear model for \( \Pi_i^B \) in the form

\[
\Pi_i^B = \left\{ \frac{1}{3} \delta_{ij} + \frac{1}{2} a_{ij} - \frac{3}{4(\epsilon_\theta) \langle \theta^2 \rangle} \left( u_i \theta \langle u_j \theta \rangle - \frac{1}{3} \delta_{ij} \langle u_k \theta \rangle \langle u_k \theta \rangle \right) \right\} \beta_j (\langle \theta^2 \rangle). \tag{11}
\]

The buoyancy components of the pressure-gradient–temperature covariance computed from Eq. (11) are shown in Fig. 4 by dot-dashed curves. As seen from the figure, the Lumley parametrization underestimates the LES data in case D0 (notice the different shapes of the short-dashed and dot-dashed curves). In case R0, it provides a good fit to the data over mid CBL but underestimates the data in the interfacial layer. In case D2, Eq. (11) overestimates the LES data over most of the CBL except close to the
Figure 4. Dimensionless buoyancy component of the pressure-gradient-temperature covariance, $-\Pi_3^B h/w^2 \theta$, versus dimensionless height, $x_3/h$, for simulations D0 (a), D2 (b), R0 (c), and R2 (d). Short-dashed curves show $-\Pi_3^B h/w^2 \theta$, from the LES data. Solid curves are computed from the r.h.s. of Eq. (4) with $C_B = 0.5$. Dot-dashed curves show the Lumley (1978) formulation, Eq. (11), and long-dashed curves, the Craft et al. (1996) TCL formulation, Eq. (12). The insert shows profiles in the interfacial layer. See text for further explanation.

Boundaries. In case R2, Eq. (11) fits the LES data slightly better in mid CBL than the linear parametrization, Eq. (4), with the 'free convection' value of $C_B = 0.5$. It strongly underestimates the data in the interfacial layer, however.

Craft et al. (1996) proposed the TCL model for $\Pi_3^B$ in the form

$$\Pi_i^B = (\frac{1}{2} \delta_{ij} - a_{ij}) \beta_j (\theta^2).$$

(12)

Long-dashed curves in Fig. 4 show $\Pi_3^B$ computed through Eq. (12). In cases D2 and R2 with rotation, the Craft et al. (1996) TCL model reveals a much better fit to the LES
data than the linear model, Eq. (4), and the Lumley (1978) nonlinear model, Eq. (11). Although uncertainties remain, an overall fit to data should be considered satisfactory. In cases R0 and D0 with no rotation, Eq. (12) performs worse than both Eq. (4) and Eq. (11). Being superior for complex flows with rotation, the TCL model appears to be unable to satisfactorily describe seemingly simpler free-convection flows. It is interesting to note that the simplest linear model, Eq. (4), with $C_B = 0.5$, which does not have many desired properties (it does not even satisfy the isotropic limit), shows better agreement with data in cases D0 and R0 than both nonlinear models Eqs. (11) and (12).

(e) Coriolis contribution to $\Pi_i$

The linear parametrization, Eq. (5), for the Coriolis contribution to the pressure-gradient–temperature covariance does not account for the component of the angular velocity of rotation that is parallel to the component of the pressure gradient in question. For the simplest configuration considered in the present paper, where the rotation vector is aligned with the vector of gravity, Eq. (5) yields no Coriolis contribution to $\Pi_i$. As the Coriolis contribution is large in cases D2 and R2 (Fig. 2), this would lead to a strong underestimation of the pressure term in the budget equation for the temperature flux. The result is not surprising, however. The linear model, Eq. (5), is by its very nature meant for the flows with small departures from isotropy, whereas convection with rotation is an example of strongly anisotropic flow.

In an attempt to remedy the above defect of the linear model, we have taken the TCL approach of Craft et al. (1996). Although these authors did not explicitly consider the Coriolis contribution to $\Pi_i$, this contribution can be incorporated in a straightforward way by analogy with the contribution to $\Pi_i$ due to the mean shear. Using the Craft et al. (1996) approach, $\Pi_i^C$ is represented in the form

$$\Pi_i^C = -b_{kji} \epsilon_{jpk} f_p,$$

that follows from the integral expression for $\Pi_i^C$ formed through the formal solution to the Poisson equation for the fluctuating pressure in terms of the Green function (see Zeman and Tennekes 1975; Zeman and Lumley 1976; Craft et al. 1996 for details). The tensor $b_{kji}$ satisfies the following conditions:

$$\text{symmetry} \quad b_{kji} = b_{kij},$$
$$\text{continuity} \quad b_{kki} = 0,$$
$$\text{normalization} \quad b_{kjj} = (u_k \theta).$$

Assuming that $b_{kji}$ is a function of the temperature flux $\langle u_i \theta \rangle$ and the departure-from-isotropy tensor, $a_{ij}$, Craft et al. (1996) employed the linearity principle which suggests that the expression for $b_{kji}$, while possibly nonlinear in $a_{ij}$, should be linear in $\langle u_i \theta \rangle$. Then, the expression of the third order in $a_{ij}$ that satisfies the symmetry in $i$ and $j$ reads

$$b_{kji} = \alpha_1 \langle u_k \theta \rangle \delta_{ji} + \alpha_2 \langle u_j \theta \rangle \delta_{ki} + \langle u_i \theta \rangle \delta_{kj}$$
$$+ \alpha_3 \langle u_k \theta \rangle a_{ji} + \alpha_4 \langle u_j \theta \rangle a_{ki} + \langle u_i \theta \rangle a_{kj}$$
$$+ \alpha_5 \langle u_i \theta \rangle a_{ik} \delta_{ji} + \alpha_6 \langle u_i \theta \rangle (a_{ij} \delta_{ki} + a_{ki} \delta_{ij})$$
$$+ \alpha_7 \langle u_i \theta \rangle a_{ik} a_{ji} + \alpha_8 \langle u_i \theta \rangle (a_{ij} a_{ki} + a_{kl} a_{ij})$$
$$+ \alpha_9 \langle u_i \theta \rangle a_{ij} a_{li} + \alpha_{10} a_{ik} (\langle u_j \theta \rangle \delta_{ki} + \langle u_i \theta \rangle \delta_{kj})$$
$$+ a_{ml} a_{ml} [\alpha_1 \langle u_k \theta \rangle \delta_{ji} + \alpha_2 \langle u_j \theta \rangle \delta_{ki} + \langle u_i \theta \rangle \delta_{kj}$$
$$+ \langle u_m \theta \rangle a_{ml} [\alpha_{11} \langle u_k \theta \rangle \delta_{ji} + \alpha_{12} \langle u_j \theta \rangle \delta_{ki} + \langle u_i \theta \rangle \delta_{kj}],$$

(17)
where \( \alpha_i \) are dimensionless constants. These constants are determined by applying the continuity and normalization constraints, Eqs. (15) and (16), and the TCL constraint. The TCL constraint as applied by Craft et al. (1996) requires that, when one of the velocity components vanishes, the net Coriolis contribution to the transport equation for the corresponding component of the temperature flux also vanishes. For \( \Pi_3^C \), this gives

\[
b_{kji} \varepsilon_{jpk} f_p - \varepsilon_{3pk} f_p \langle u_k \theta \rangle = 0.
\]

(18)

The situation is conveniently considered in principal axes of \( a_{ij} \), where \( a_{33} = -2/3 \) in the limit \( u_3 = 0 \), and the other two non-zero components of \( a_{ij} \) can be written as \( a_{11} = 1/3 + \gamma \) and \( a_{22} = 1/3 - \gamma \).

Satisfying the above constraints, then substituting the resulting expressions for \( \alpha_i \) into Eq. (13) and grouping like terms, yields the following formulation:

\[
\Pi_i^C = -\frac{1}{2} \varepsilon_{ipj} f_p \langle u_j \theta \rangle + \frac{1}{2} \alpha_0 a_{kl} a_{ij} \varepsilon_{ipj} f_p \langle u_j \theta \rangle + \left( \frac{3}{4} a_{ij} \varepsilon_{jpk} f_p + \frac{3}{8} \varepsilon_{ipj} f_p a_{jk} \right) \langle u_k \theta \rangle + \left\{ \left( \frac{\alpha_0}{16} - \alpha_0 \right) a_{ij} \varepsilon_{jpk} f_p a_{kl} - \alpha_0 a_{ij} a_{jk} \varepsilon_{kpl} f_p - \alpha_0 \varepsilon_{ipj} f_p a_{jk} a_{kl} \right\} \langle u_i \theta \rangle,
\]

(19)

with only one free coefficient denoted by \( \alpha_0 \). We have omitted algebraic manipulations leading to Eq. (19) as they are cumbersome but fairly straightforward.

The first term on the r.h.s. of Eq. (19) is identically a linear model of \( \Pi_i^C \), Eq. (5). It is worth noting that the values of \( \alpha_1 = 2/5 \) and \( \alpha_2 = -1/10 \) that simply follow from the continuity and the normalization constraints result in the value of \( C_C = -1/2 \) in Eq. (5). The linear part of the implicit Coriolis term compensates for one half of the explicit Coriolis term in the flux budget equation and is not negligible as was assumed by some authors (e.g. Galperin et al. 1989; Kantha et al. 1989; Kantha and Clayson 1994). Notice, however, that if the second term on the r.h.s. of Eq. (19) is also retained, then the coefficient \(- (1/2)(1 - \alpha_0 A_2)\) that multiplies \( \varepsilon_{ipj} f_p \langle u_j \theta \rangle \) is not merely a constant but a function of the second invariant of the departure-from-isotropy tensor, \( A_2 = a_{ij} a_{ji} \). This coefficient may obviously take on different values in different flows.

It is easy to see that the above TCL model, Eq. (19), although quite sophisticated, is still inadequate. In the seemingly simplest case considered in the present paper, where the rotation vector is aligned with the vector of gravity, it predicts a \( \Pi_3^C \) that is identically zero. In the next section, we develop an extension of the TCL model that removes this deficiency.

5. AN IMPROVED MODEL OF THE CORIOLIS CONTRIBUTION TO \( \Pi_i \)

A straightforward extension of the TCL model considered above is developed by realizing that in turbulent flows strongly affected by the background rotation the tensor \( b_{kji} \), apart from being a function of \( \langle u_i \theta \rangle \) and \( a_{ij} \), may explicitly depend on the rotation tensor \( r_{ij} = \varepsilon_{ipj} f_p \langle e \rangle / \langle \epsilon \rangle \), where the TKE dissipation time-scale, \( \tau_e = \langle e \rangle / \langle \epsilon \rangle \), is used to make \( \varepsilon_{ipj} f_p \) dimensionless. With this hypothesis we then propose that, along with the terms given by Eqs. (17), \( b_{kji} \) contains terms that explicitly depend upon \( r_{ij} \). Including only the terms linear in \( \langle u_i \theta \rangle \), \( a_{ij} \) and \( r_{ij} \), the expression for the rotation-dependent part of \( b_{kji} \) (denoted by a tilde) that satisfies the symmetry in \( i \) and \( j \) reads

\[
\tilde{b}_{kji} = \tilde{a}_1 \langle u_i \theta \rangle r_{kj} + \langle u_j \theta \rangle r_{ki} + \tilde{a}_2 \langle u_i \theta \rangle r_{kl} \delta_{ji} + \tilde{a}_3 \langle u_i \theta \rangle (r_{jl} \delta_{ik} + r_{il} \delta_{jk}) + \tilde{a}_4 \langle u_i \theta \rangle r_{kl} a_{ji} + \tilde{a}_5 \langle u_j \theta \rangle (r_{jl} a_{ik} + r_{il} a_{jk})
\]
Figure 5. Dimensionless Coriolis component of the pressure-gradient–temperature covariance, \(-\Pi_3^C h/w^2 \theta\), versus dimensionless height, \(x_3/h\), for simulations D2 (a) and R2 (b). Short-dashed curves show \(-\Pi_3^C h/w^2 \theta\), from the LES data. Solid curves are computed from the r.h.s. of Eq. (22) with \(\tilde{\alpha}_1 = 0.02\). Dot-dashed curves are computed from the r.h.s. of Eq. (22), where \(\tilde{\alpha}_1 = 0.02\) and the dissipation time-scale, \(\tau_\epsilon = (\epsilon)/\langle \epsilon \rangle\), is replaced with the time-scale of the dissipation of the temperature variance, \(\tau_\theta = (\theta^2)/\langle \theta \rangle\). See text for further explanation.

\[
\begin{align*}
&+ \tilde{\alpha}_6 \langle u_i \theta \rangle (r_{jk} a_{il} + r_{ik} a_{jl}) + \tilde{\alpha}_7 \langle u_k \theta \rangle (r_{jl} a_{il} + r_{il} a_{jl}) \\
&+ \tilde{\alpha}_8 r_{kl} (\langle u_j \theta \rangle a_{il} + \langle u_l \theta \rangle a_{lj}) + \tilde{\alpha}_9 a_{kl} (\langle u_j \theta \rangle r_{il} + (u_l \theta) r_{jl}).
\end{align*}
\]

Dimensionless coefficients \(\tilde{\alpha}_i\) are determined by applying the continuity and the normalization conditions, Eqs. (15) and (16), and the TCL constraint which, for the rotation-dependent part of \(b_{kji}\), translates to \(\tilde{b}_{kji} = 0\). The resulting expression for \(\tilde{b}_{kji}\) contains only one free coefficient, \(\tilde{\alpha}_1\) (again, algebraic manipulations are omitted). Combining Eqs. (13), (19) and (20), the expression for the Coriolis contribution to the pressure-gradient–temperature covariance reads

\[
\Pi_3^C = \frac{\langle \epsilon \rangle}{\langle \epsilon \rangle} \left[ -\frac{1}{2} (1 - \alpha_0 a_{kl} a_{kl}) r_{ij} \langle u_j \theta \rangle + \frac{3}{4} a_{ij} r_{jk} + \frac{3}{8} r_{ij} a_{jk} \right] \langle u_k \theta \rangle \\
+ \left\{ \left( \frac{9}{16} - \alpha_0 \right) a_{ij} r_{jk} a_{kl} - \alpha_0 a_{ij} a_{jk} r_{kl} - \alpha_0 r_{ij} a_{jk} a_{kl} \right\} \langle u_l \theta \rangle \\
+ \frac{\tilde{\alpha}_1}{\langle \epsilon \rangle} \left[ r_{jk} r_{jl} \left( \langle u_l \theta \rangle + \frac{1}{4} a_{ij} \langle u_l \theta \rangle \right) + \frac{1}{4} r_{jk} r_{kl} a_{ij} \langle u_l \theta \rangle \\
+ \frac{1}{2} (r_{ij} r_{jk} \langle u_k \theta \rangle + a_{ij} r_{jk} r_{kl} \langle u_l \theta \rangle) - \frac{1}{4} (r_{ij} r_{jk} a_{kl} + r_{ij} a_{jk} r_{kl}) \langle u_l \theta \rangle \right\}.
\]

Notice that the terms multiplied by \(\tilde{\alpha}_1\) (namely, the first three terms in braces on the r.h.s. of the above expression) do account for the component of the rotation vector that is parallel to the \(i\)th component of the temperature flux and do not vanish when the two vectors are aligned.
In the case considered in the present study, where only the vertical component of the Coriolis parameter is present, Eq. (21) greatly simplifies to give

$$\Pi_3^C = 2\bar{a}_1 \frac{f^2\langle e \rangle}{\langle e \rangle} \left(1 + \frac{1}{4}a_{33} - \frac{1}{8}(a_{11} + a_{22})\right) \langle u_3 \theta \rangle = 2\bar{a}_1 \frac{f^2\langle e \rangle}{\langle e \rangle} \left(1 + \frac{3}{8}a_{33}\right) \langle u_3 \theta \rangle. \quad (22)$$

Figure 5 shows $\Pi_3^C$ computed from the proposed model versus LES data. The agreement between the LES data and the model predictions is good in case D2 and is fair in case R2 in the mid CBL. In case R2, the proposed model does not agree with the LES data in the interfacial layer.

It should be recognized that in convective flows the TKE dissipation time-scale, $\tau_\epsilon = \langle e \rangle/\langle e \rangle$, is not the only relevant turbulence time-scale. The time-scale of the dissipation of the temperature variance, $\tau_\theta = \langle \theta^2 \rangle/\langle \theta \rangle$, can be used as an alternative to $\tau_\epsilon$ to form the dimensionless rotation tensor. Then, the quantities $\epsilon_{ipj} f_p \langle \theta^2 \rangle/\langle \theta \rangle$ and $\langle \epsilon \rangle/\langle \theta^2 \rangle$ would appear in Eq. (21) in place of $r_{ij}$ and $\langle \epsilon \rangle/\langle e \rangle$, respectively. Dot-dashed curves in Fig. 5 show $\Pi_3^C$ computed from the proposed model, where the time-scale of the dissipation of the temperature variance, $\tau_\theta$, is used instead of the TKE dissipation time-scale, $\tau_\epsilon$. The use of $\tau_\theta$ does not appreciably change the result in case D2. In case R2, the agreement between the model prediction and the LES data is somewhat improved in mid CBL. The model still fails in the interfacial layer, however. The interfacial layer seems to require special consideration. This task is beyond the scope of the present study.

6. CONCLUDING REMARKS

The pressure–potential–temperature covariance in free and rotating turbulent convection with no mean velocity shear has been analysed, using a dataset generated through LES. The LES data have been used to resolve the fluctuating pressure field into turbulence–turbulence, buoyancy, and Coriolis components, to evaluate contributions from these components to the pressure-gradient–potential-temperature covariance in the budget equation for the potential-temperature flux, and to test the performance of several closure models for the pressure term in the flux budget. An attempt has been made to develop an improved model for the Coriolis contribution to the pressure-gradient–potential-temperature covariance. The main findings from the analysis may be summarized as follows.

The slow part of the pressure-gradient–potential-temperature covariance in free convection is well approximated by the Rotta-type return-to-isotropy model with the relaxation time-scale set proportional to the turbulence energy dissipation time-scale. In convection with rotation, the slow part is not satisfactorily described by any of the models tested. Further development is required. However, if one of the models considered is still to be used for practical applications, one should put up with possible large uncertainties. Then, the Hassid and Galperin (1994) proposal to simply impose a limitation on the turbulence time-scale, i.e. to use the relaxation approximation Eq. (2) with the time-scale given by Eq. (9), is, perhaps, most attractive as it is computationally cheap.

In non-rotating convection, the buoyancy contribution compensates for about one half of the buoyant production term in the flux budget equation. In convection with rotation, the simplest model for the buoyancy contribution, where it is set proportional to the buoyant production term in the flux budget equation, fares poorly. The Craft
et al. (1996) TCL model, Eq. (12), shows better agreement with LES data, although some uncertainties remain. The relative importance of the buoyancy contribution to the pressure-gradient–potential-temperature covariance decreases with the increasing rotation rate.

In contrast, the Coriolis contribution becomes more important as the rotation rate increases. We find that neither the simplest linear model for the Coriolis contribution, Eq. (5), nor the much more complex nonlinear TCL model, Eq. (19), is adequate. Neither model appropriately accounts for the component of the angular velocity of rotation that is parallel to the component of the pressure gradient in question. In the seemingly simplest case considered in the present paper, when the rotation vector is aligned with the vector of gravity, no Coriolis contribution to the vertical-pressure-gradient–potential-temperature covariance is predicted by these models.

In an attempt to remedy the situation, we develop an extension of the TCL model, Eq. (21), that contains only one extra empirical coefficient. The proposed formulation appears to satisfactorily compare with the LES data in the core of the CBL. The model fails in the entrainment layer which seems to require special consideration. This task is left for future studies.

It should be remarked that the proposed formulation for the Coriolis contribution to the pressure-gradient–potential-temperature covariance, although being a step forward (it predicts non-zero Coriolis contribution when the other models entirely fail), is far from being perfect. It should be thoroughly tested, e.g. using data from convective flows with different values of the Rossby number, and, no doubt, further developed, e.g. by including terms of high order in the departure-from-isotropy tensor and the rotation tensor.

Finally, a word about possible applications of the results from the present study is appropriate here. The proposed formulation for the Coriolis part of the pressure-gradient–potential-temperature covariance is intended for modelling convective flows affected by rotation (it may also be applicable to other flows with rotation, e.g. to neutrally or stably stratified flows, but that remains to be seen). An obvious geophysical application is the open-ocean deep convection that is known to be affected by rotation (Marshall and Schott 1999). Notice, however, that the temperature flux budget in the CBL is dominated by the two terms, the pressure-gradient–potential-temperature covariance and the buoyancy term involving the temperature variance. The present study focuses on the pressure term. The temperature variance in rotating flows invites further research. The third-order transport term in the temperature variance budget presents major difficulties (Mironov et al. 2000), and contemporary models of this third-order term are barely applicable when the effect of rotation is important. This issue should be a subject for future work.

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APPENDIX A

Decomposition of the pressure-gradient–temperature covariance

It is common practice nowadays to decompose the pressure-gradient–temperature covariance, \( \langle \partial p / \partial x_i \rangle = \Pi_i \), into the contributions due to the nonlinear turbulence–turbulence interactions (denoted by the superscript T), mean shear (superscript S), buoyancy (superscript B), and the Coriolis effects (superscript C),

\[
\Pi_i = \Pi^T_i + \Pi^S_i + \Pi^B_i + \Pi^C_i. \tag{A.1}
\]

The above components of \( \Pi_i \) are built through the use of the corresponding components of the fluctuating pressure,

\[
p = p_T + p_S + p_B + p_C, \tag{A.2}
\]

which are found by solving the following set of Poisson equations:

\[
\frac{\partial^2 p_T}{\partial x_i^2} = -\frac{\partial}{\partial x_i} \left( u_j \frac{\partial u_i}{\partial x_j} \right), \quad \frac{\partial^2 p_S}{\partial x_i^2} = -2 \frac{\partial U_i}{\partial x_j} \frac{\partial u_j}{\partial x_i},
\]

\[
\frac{\partial^2 p_B}{\partial x_i^2} = \beta_i \frac{\partial \theta}{\partial x_i}, \quad \frac{\partial^2 p_C}{\partial x_i^2} = -\epsilon_{ij} f_i \frac{\partial u_j}{\partial x_i}, \tag{A.3}
\]

where \( \beta_i = \alpha g_i \) is the buoyancy parameter, \( \alpha \) is the thermal expansion coefficient, \( g_i \) is the vector of gravity, and \( f_i = 2 \Omega_i \) is the Coriolis vector, \( \Omega_i \) being the angular velocity of rotation.

Using LES data, approximations to the ensemble-mean turbulence statistics are usually built by means of averaging over horizontal planes (the fluctuations are thus fluctuations of the filtered quantities about their horizontal means) and further averaging over a number of recorded time steps. Notice that additional terms on the r.h.s. of Eqs. (A.1) and (A.2) are then considered, namely, the terms that stem from the SGS stress. The contribution to the fluctuating pressure due to the SGS stress is found by solving the following Poisson equation:

\[
\frac{\partial^2 p_{SG}}{\partial x_i^2} = -\frac{\partial^2 \tau_{ij}}{\partial x_i \partial x_j}, \tag{A.4}
\]

where \( \tau_{ij} \) is the SGS stress tensor. As seen from Figs. 1 and 2, both \( (p_{SG}^2)^{1/2} \) and \( \Pi_i^{SG} \equiv \langle \partial p_{SG} / \partial x_i \rangle \) are small over most of the CBL in all simulations performed. They are not negligible close to the rigid boundaries, where LES is known to be deficient. Further difficulties are associated with the estimation of the SGS part of the pressure-gradient–temperature covariance in the temperature flux budget (the term \( \hat{p}_{SG} \) in Eq. (B.3) that should not be confused with \( \Pi_3^{SG} \)). This issue is discussed in section 4(b) and in appendix B.
APPENDIX B

Relation between the large-eddy simulation and the ensemble-average budgets of the potential-temperature flux

In the equations below, an overbar denotes a filtered resolved-scale variable, a tilde denotes an average over a horizontal plane, and a double prime denotes a deviation therefrom. 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.

With due regard to the absence of mean flow and to the periodic boundary conditions in the horizontal directions, the budget equation for the resolved-scale temperature flux is

$$\frac{\partial}{\partial t} \bar{u}_3'' \bar{\theta}'' = -\bar{u}_3'' \bar{u}_3' \frac{\partial \bar{\theta}}{\partial x_3} + \beta \bar{u}_3'' \bar{\theta}'' \frac{\partial \bar{\theta}}{\partial x_3} - \bar{u}_3'' \bar{\theta}' \frac{\partial \bar{p}''}{\partial x_3} - \bar{u}_3'' \bar{\theta}'' \frac{\partial \bar{\tau}_{ij}''}{\partial x_j} - \bar{u}_3'' \bar{\theta}'' \frac{\partial \bar{\tau}_{ij}''}{\partial x_j}, \quad (B.1)$$

where $\bar{\tau}_{ij}$ is the SGS temperature flux. Notice that in our configuration the Coriolis term does not explicitly appear in the budget of the vertical temperature flux. The last two terms on the r.h.s. of Eq. (B.1) can be re-arranged to give

$$-\bar{u}_3'' \frac{\partial \bar{\tau}_{ij}''}{\partial x_j} - \bar{u}_3'' \frac{\partial \bar{\tau}_{ij}''}{\partial x_j} = -\bar{\tau}_{ij} \bar{u}_3'' \bar{\tau}_{ij} - \bar{u}_3'' \bar{\tau}_{ij} \bar{\tau}_{ij} - \bar{u}_3'' \bar{\tau}_{ij} \bar{\tau}_{ij} + \left( \bar{\tau}_{ij} \bar{u}_3'' \bar{\tau}_{ij} + \bar{\tau}_{ij} \bar{u}_3'' \bar{\tau}_{ij} \right). \quad (B.2)$$

The first term on the r.h.s. of Eq. (B.2) has the form of the mean-gradient term and may be combined with the first term on the r.h.s. of Eq. (B.1). The second term is the transport of the SGS temperature flux by the resolved-scale motions. It can be combined with the third term on the r.h.s. of Eq. (B.1). The third term on the r.h.s. of Eq. (B.2) has the form of a transport term and integrates vertically to zero. In order to get some insight into the nature of the terms in parentheses on the r.h.s. of Eq. (B.2), it is instructive to consider the budget equation for the SGS temperature flux. Upon horizontal averaging of the transport equation for $\bar{\tau}_{ij}$ (this, and other transport equations for the SGS quantities, are considered in detail by Deardorff (1973)), the budget is

$$\frac{\partial}{\partial t} \bar{\tau}_{ij} = - \left( \bar{\tau}_{ij} \frac{\partial \bar{\theta}}{\partial x_j} + \bar{\tau}_{ij} \frac{\partial \bar{u}_3}{\partial x_j} \right) - \bar{\tau}_{ij} \frac{\partial \bar{\tau}_{ij}}{\partial x_3} + \beta \bar{\tau}_{ij} \frac{\partial \bar{\tau}_{ij}}{\partial x_3} - \bar{\tau}_{ij} \frac{\partial \bar{\tau}_{ij}}{\partial x_3} \bar{\tau}_{ij} \frac{\partial \bar{\tau}_{ij}}{\partial x_3}, \quad (B.3)$$

where $\bar{\theta}$ is the SGS temperature variance, $\bar{T}_{ij}$ is the vertical SGS flux of $\bar{\tau}_{ij}$, and $\bar{P}_{ij}$ is the SGS pressure-gradient--temperature covariance. Thus, the terms in parentheses in Eq. (B.2) are equal in magnitude but opposite in sign to the mean-gradient production/destruction terms in the budget equation for the SGS temperature flux, Eq. (B.3). Estimating the last term on the r.h.s. of Eq. (B.3) 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, $\partial \bar{\tau}_{ij} / \partial x_3$, is also small (this term cannot be estimated as the transport equation for $\bar{\tau}_{ij}$ is not carried by our LES model), Eq. (B.3) 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
temperature flux:

\[
\frac{\partial}{\partial t} \left( \tilde{u}_3 \tilde{\theta}'' + \tilde{\tau}_{33} \right) = - \left( \tilde{u}_3'' + \tilde{\tau}_{33} \right) \frac{\partial \tilde{\theta}}{\partial x_3} + \beta \left( \tilde{\theta}'' + \tilde{\theta} \right) - \frac{\partial}{\partial x_3} \left( \tilde{u}_3'' \tilde{\theta}'' + \tilde{u}_3' \tilde{\tau}_{33} \right) \\
- \frac{\partial''}{\partial x_3} - \left( \beta \tilde{\theta} - \tilde{\tau}_{3j} \frac{\partial \tilde{\theta}}{\partial x_j} - \tilde{\tau}_{\theta j} \frac{\partial \tilde{u}_3}{\partial x_j} \right) - \frac{\partial}{\partial x_3} \tilde{\theta}'' \tilde{\tau}_{33}, \quad (B.4)
\]
The time mean of Eq. (B.4) is treated as an approximation to the ensemble-mean budget of the temperature flux. The above arguments suggest that the sum of the SGS terms in parentheses on the r.h.s. of Eq. (B.4) may be reasonably treated as an approximation to the SGS pressure-gradient–temperature covariance. The last term on the r.h.s. of Eq. (B.4) is treated as the budget imbalance.

Results from the LES studies of Khanna (1998) and Mironov et al. (2000) lend considerable support to the above treatment of the flux budget derived from the LES fields. These authors analysed the second-moment budgets in sheared, free, and rotating CBLs. They 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 imbalance in the corresponding budgets. The SGS pressure term in the temperature flux budget was found to be important. This is consistent with our interpretation of the SGS terms. Figure B.1 shows the potential-temperature flux budgets from our four simulations. The budget imbalance is not shown as it is negligibly small over most of the CBL. As seen from Fig. B.1, the SGS pressure term is small compared with the major 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.

A rough estimate of the SGS temperature variance 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),
\[ \bar{\overline{\theta}} = \text{3r}_Q^2 / e_{sg} \]
where \( e_{sg} \) is the SGS TKE, and 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 \( \bar{\overline{\theta}} \) is small over most of the CBL. With \( \bar{\overline{\theta}} \) small and the assumed local isotropy at the sub-grid scales, the SGS pressure term can be reasonably attributed to the turbulence–turbulence contribution to the pressure-gradient–temperature covariance.

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