Comparative Analysis of Four Second-Moment Turbulence Closure Models for the Oceanic Mixed Layer

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ABSTRACT

In this comparative study, four different algebraic second-moment turbulence closure models are investigated in detail. These closure schemes differ in the number of terms considered for the closure of the pressure−strain correlations. These four turbulence closures result in the eddy-diffusivity principle such that the closure assumptions are contained in dimensionless so-called stability functions. Their performance in terms of Prandtl number, Monin−Obukhov similarity theory, and length scale ratios are first tested against data for simple flows. The turbulence closure is then completed by means of a $k-e$ two-equation model, but other models such as the two-equation model by Mellor and Yamada could also be used. The concept of the steady-state Richardson number for homogeneous shear layers is exploited for calibrating the sensitivity of the four models to shear and stable stratification. Idealized simulations of mixed layer entrainment into stably stratified flow due to surface stress and due to free convection are carried out. For the latter experiment, comparison to recent large eddy simulation data is made. Finally, the well-known temperature profile data at OWS Papa are simulated for an annual cycle. The main result of this paper is that the overall performance of the new second-moment closure model by Canuto et al.—expressed as nondimensional stability functions—is superior compared to the others in terms of physical soundness, predictability, computational economy, and numerical robustness.

1. Introduction

The intention of this paper is to construct a turbulence closure model that can be recommended for implementation into a wide range of three-dimensional numerical ocean models. The following criteria will be applied for the evaluation of such a model: (i) derivation from second-moment transport equations, (ii) physical soundness, (iii) high predictability, (iv) computational economy, and (v) numerical robustness. The physics relevant for ocean dynamics is included in the Navier–Stokes equations and the molecular transport equations for heat and salt. Due to the importance of numerically unsolvable small-scale turbulence to large-scale processes in the ocean, model assumptions are necessary in order to achieve an applicable ocean model. Two main schools can be differentiated in the literature: statistical closure models and empirical approaches. Statistical models are based on the Reynolds decomposition of momentum and scalar fields into mean (ensemble average) and fluctuating (due to turbulence) fields. A system of infinitely many differential equations for higher statistical correlations that is equivalent to the Reynolds equations and the heat and salt equations can be derived. It has been the major work of turbulence modelers in the last decades to suggest closures of this system of equations on various levels of sophistication. Milestones in this process of finding practical solutions for marine and atmospheric modeling were the work of Launder and colleagues (Launder and Spalding 1972; Launder 1975; Launder et al. 1975) and the work of Mellor and Yamada (1974, 1982). To date, numerous modifications to these models have been suggested (see, e.g., Galperin et al. 1988; Mellor 1989; Kantha and Clayson 1994; Burchard and Baumert 1995; D’Alessio et al. 1998; Canuto et al. 2001). This shows that entirely satisfying solutions have not been found yet and that they might never be found. Due to this fact, empirical approaches have been popular throughout recent decades. Even the most simple parameterizations such as constant eddy viscosity and diffusivity are still applied with some success (see, e.g., Roussenov et al. 1995). In oceanography, the present most widely spread empirical turbulence closure is the K-profile parameterization (KPP) model introduced by
Large et al. (1994) (see also Large and Gent 1999) in which profiles for eddy viscosity and eddy diffusivity are constructed based on the Monin–Obukhov similarity theory and Deardorff’s countergradient fluxes without any consideration of statistical moments. The success of this model can only be explained by the fact that statistical models still do not fulfil some basic requirements: They mix too little (see Martin 1985), they do not generally reproduce nonlocal processes [D’Alessio et al. (1998) try to solve this problem by introducing nonlocal fluxes empirically on top of their statistical local model], they rarely consider rotation, and they do not sufficiently consider breaking surface [the breaking surface wave parameterization suggested by Craig and Banner (1994) has not yet been successfully implemented into two-equation models] or internal waves (generally, internal waves are reduced to background diffusivity in ocean models).

In this paper we carry out a comparative analysis of four algebraic second-moment closure models and their quasi-equilibrium versions. Their characteristics are furthermore compared to empirical data for the turbulent Prandtl number, the Monin–Obukhov similarity, and length scale ratios.

Furthermore, we demonstrate how these closure schemes can be embedded into a two-equation turbulence model (here the well-known $k$–$\varepsilon$ model) in such a way that mixing in stratified shear flows is well reproduced. The concept of steady-state Richardson numbers for homogeneous shear layers has already been used by Burchard and Baumert (1995) for calibrating an empirical buoyancy parameter in $k$–$\varepsilon$ models. This approach is modified here in the same way that Burchard (2001) recently did for the $k$–$kL$ model by Mellor and Yamada (1982). The well-known entrainment experiment by Kato and Phillips (1969) is used here as a simple performance test for these second-moment closures, all embedded into a $k$–$\varepsilon$ model. All models are furthermore applied for simulating the free convection experiment by Willis and Deardorff (1974) and the results are compared to recent large eddy simulation (LES) data by Mironov et al. (2000).

In a final performance test, the second-moment closures suggested by Kantha and Clayson (1994), which is a slight improvement of the models of Mellor and Yamada (1982) and Galperin et al. (1988), and Canuto et al. (2001) are compared by means of applying them to the well-known mixed layer dataset OWS Papa (northern Pacific). This clearly shows the improvements achieved by the closure of Canuto et al. (2001).

The paper is structured as follows: After presenting the mean flow equations (section 2), the procedure for various second-moment closures is discussed (section 3). Two-equation models are introduced in section 4 and their stationary solutions are investigated in section 5. Idealized and ocean mixed layer studies are presented in sections 6a–c. Final conclusions are discussed in section 7. In section a of the appendix our notation is explained. To our experience, differences in notation have long been a major obstacle for exchange between various schools of statistical modeling. In the appendix sections d–f, exact forms of the stability functions suggested by Kantha and Clayson (1994), Rodi (1980), and Hossain (1980) are given. This should help the reader to better understand these functions. In section 8g, the exact formulations for the $k$ and the $\varepsilon$ equation are given, as derived from the Navier–Stokes equations and the Reynolds decomposition.

#### 2. Basic mean flow equations

The basic model assumption for obtaining the so-called Reynolds equations is that any flow property $X$ may be decomposed into a mean and a fluctuating part:

$$X = \overline{X} + \hat{X}.$$  \hspace{1cm} (1)

Here, $\overline{X}$ is called the ensemble average [see, e.g., Lesieur (1997)] and will alternatively be denoted by $\langle X \rangle$. It is assumed that $\langle \overline{X} \hat{X} \rangle = 0$, $\langle \overline{X} \rangle = \overline{X}$, and $\langle \overline{X} \overline{Y} \rangle = \overline{XY}$ (see e.g., Haidvogel and Beckmann 1999).

After application of this Reynolds decomposition and the boundary layer approximation, the Navier–Stokes equations and transport equations for active tracers (temperature $T$ and salinity $S$), can be formulated as the so-called Reynolds equations for mean quantities:

$$\partial_t \overline{u} + \partial_x (\overline{u} \overline{v}) + \partial_y (\overline{u} \overline{w}) + \partial_z (\overline{u} \overline{w}) - \partial_z (\nu \partial_z \overline{u}) = -\frac{1}{\rho_0} \partial_x p + f \overline{v},$$

$$\partial_t \overline{v} + \partial_x (\overline{v} \overline{u}) + \partial_y (\overline{v} \overline{w}) + \partial_z (\overline{v} \overline{w}) - \partial_z (\nu \partial_z \overline{v}) = -\frac{1}{\rho_0} \partial_y p - f \overline{u},$$

$$\partial_t \overline{w} + \partial_x (\overline{w} \overline{u}) + \partial_y (\overline{w} \overline{v}) + \partial_z (\overline{w} \overline{v}) + \partial_z (\nu \partial_z \overline{w}) - \partial_z (\nu' \partial_z \overline{w}) = \frac{1}{c_f \rho_0} \partial_y I,$$

$$\partial_t \overline{S} + \partial_x (\overline{S} \overline{u}) + \partial_y (\overline{S} \overline{v}) + \partial_z (\overline{S} \overline{w}) + \partial_z (\nu \partial_z \overline{S}) - \partial_z (\nu' \partial_z \overline{S}) = 0.$$  \hspace{1cm} (2)

In these equations, $u$, $v$, and $w$ are the $x$ (eastward), the $y$ (northward), and the $z$ (upward) velocity components, respectively, and $t$ is time; $\nu$ is calculated diagnostically from the incompressibility condition

$$\partial_t \overline{u} + \partial_x \overline{v} + \partial_y \overline{w} = 0.$$  \hspace{1cm} (3)

The pressure $p$ is hydrostatic with

$$\partial_x \overline{p} + g \overline{z} = 0$$  \hspace{1cm} (4)

with gravitational acceleration $g$ and density $\rho$. Earth
rotation is considered through the Coriolis frequency \( f = 2 \omega \sin \phi \) with the earth’s angular velocity \( \omega \) and latitude \( \phi \) (positive for Northern Hemisphere). In the temperature (or local heat balance) equation, further terms are solar radiation \( I \) (in W m\(^{-2}\)) in the water column (generally calculated from the given surface radiation as an exponentially decreasing function with depth), the specific heat capacity of seawater \( C_w \), and a mean density \( \rho_0 \). The molecular diffusivities for momentum, temperature, and salinity are given by \( \nu, \nu' \) and \( \nu'' \), respectively.

Together with an equation of state giving density as function of \( T, S, \) and \( p \) and suitable boundary conditions, Eq. (2) is the physical basis for most marine models ranging from estuarine, over coastal, shelf sea, basin, and global ocean scale.

The ocean circulation modeler might miss terms for horizontal mixing in Eq. (2). They do not appear here due to the boundary layer approximation. All mesoscale activity is already included in the equations above through the advective terms. Mesoscale activity only needs to be parameterized because of the generally rather coarse horizontal resolution in ocean models and has therefore to be considered as part of the discretization. In contrast, vertical turbulent transport needs to be parameterized due to the Reynolds decomposition and the hydrostatic approximation even for the (theoretical) limit of arbitrarily fine model resolution. Therefore, in hydrostatic ocean models, vertical and horizontal mixing must not be parameterized with the same model approach.

The main differences among these models are due to boundary conditions, coordinate transformations, numerical aspects, and, of course, the closure assumptions for the unknown second-order correlators \( \langle \tilde{u} \tilde{v} \rangle, \langle \tilde{w} \tilde{v} \rangle, \langle \tilde{w} \tilde{T} \rangle, \) and \( \langle \tilde{v} \tilde{S} \rangle \), which are the Reynolds stresses, the turbulent heat flux, and the turbulent salinity flux.

For the derivation of these fluxes, we apply a major simplification that is used by almost all turbulence closure models: during the closure procedure, only one active tracer is considered. Afterward, the derived flux parameterization for one active tracer is applied to the other tracers in analogy. By means of this simplification, consideration of correlators such as \( \langle \tilde{T} \tilde{S} \rangle \) is avoided.

3. Second-moment closure

Here, three different approaches for closing the second-order moments \( \langle \tilde{u} \tilde{v} \rangle, \langle \tilde{w} \tilde{v} \rangle, \) and \( \langle \tilde{w} \tilde{T} \rangle \) will be presented. They have been published by:

- Kantha and Clayson (1994, hereafter KC),
- Burchard and Baumert (1995) [based on the work of Rodi (1980) and Hossain (1980); hereafter RH], and
- Canuto et al. (2001 hereafter CA).

All of these approaches are based on the exact forms of the Reynolds stress and the heat flux equation. These forms can be derived from the Navier–Stokes and the local heat balance equations by applying the aforementioned algebraic rules for the ensemble averaging of tensors. The exact forms for the Reynolds stress and the heat flux equation can be found, for example, in Launder et al. (1975) or Canuto (1994).

The equations are presented here in a closed form with the exception of third-order correlators occurring on the left-hand sides causing turbulent transport of the second-order correlators. The three approaches discussed here differ mainly in the manner how the pressure–strain correlators \( \Pi_p = \langle \tilde{u} \tilde{e} \tilde{p} \rangle + \langle \tilde{u} \tilde{p} \tilde{p} \rangle \) and \( \Pi_f = \langle \tilde{F}_0 \tilde{p} \rangle \) are parameterized. All approaches neglect rotational terms, although they are known to be important for free convection (see Mironov et al. 2000).

In the following the Reynolds stress, the heat flux, and the temperature variance equations are given as prognostic equations (sections 3a and 3b), then an algebraization is discussed (section 3c) and finally the boundary layer approximation is applied (section 3d).

a. Reynolds stress equation

After neglecting viscous and rotational effects and parameterizing pressure–strain correlators, the Reynolds stress equations can be closed in the following form (see Canuto et al. 2001):

\[
\frac{\partial}{\partial t} \langle \tilde{u} \tilde{u} \rangle + \frac{\partial}{\partial x_j} \langle \tilde{u} \tilde{u} \tilde{v} \rangle + \frac{\partial}{\partial y} \langle \tilde{u} \tilde{v} \tilde{y} \rangle + \frac{\partial}{\partial z} \langle \tilde{u} \tilde{z} \tilde{v} \rangle = -c_1 \frac{\varepsilon}{k} \left( \langle \tilde{u} \tilde{u} \rangle - \frac{2}{3} \delta_{ij} \right) + (1 - c_1) \left( \frac{P_{ij} - \frac{2}{3} \delta_{ij} P}{3} + \frac{2}{3} \delta_{ij} P \right) + (1 - c_1) \left( \frac{B_{ij} - \frac{2}{3} \delta_{ij} B}{3} + \frac{2}{3} \delta_{ij} B \right)
\]

\[
- c_1 k S_{ij} - c_2 Z_{ij} - \frac{2}{3} \delta_{ij} \varepsilon \tag{R6}
\]

Here, the following definitions are used:

\[
P_{ij} = - \delta_{ij} \Pi \langle \tilde{u} \tilde{v} \rangle - \delta_{ij} \Pi \langle \tilde{u} \tilde{v} \rangle, \quad B_{ij} = \beta_i \langle \tilde{u} \tilde{T} \rangle + \beta_j \langle \tilde{u} \tilde{T} \rangle \tag{6}
\]

are production due to shear and buoyancy with \( \beta_1 = \beta_2 = 0 \), and \( \beta_3 = -g \tilde{u} \tilde{p} / \rho \), where the traces define the shear and the buoyancy production:

\[
P = \frac{1}{2} P_{ii}, \quad B = \frac{1}{2} B_{ii}. \tag{7}
\]

Further definitions are shear

\[
S_{ij} = \frac{1}{2} (\partial_j \Pi_i + \partial_i \Pi_j) \tag{8}
\]
and Yamada (1982) chose the same value for $c_{1T}$ that KC did, but used $c_{2T} = c_{3T} = 0$.

Finally a dynamic equation of the temperature variance $\langle T^2 \rangle$ has to be used:

\[
\begin{align*}
\partial_t \langle T^2 \rangle + \beta \langle \langle T \rangle \rangle + \langle \langle T^2 \rangle \rangle & = -2 \langle \langle u \rangle \rangle \partial_i \langle T \rangle \\
& - 2 \frac{1}{c_T k} \langle T^2 \rangle
\end{align*}
\]

Here the terms are production by mean gradient (T1) and dissipation (T2), which is often denoted as $\chi$. No basic difference can be found in the three approaches considered in this paper, and the parameter $c_T$ varies only little (see Table 1).

c. Algebrazation

The stability functions discussed in this paper are derived from the dynamic equations (5), (11), and (12) by means of two different approaches. The basic approach is to neglect time variation and advective and turbulent transports of Reynolds stresses $\langle \langle \vec{u} \rangle \rangle$, heat fluxes $\langle \langle \vec{u} \rangle \rangle$, and the autocorrelation $\langle \langle \vec{T} \rangle \rangle$. In order to retain the transport of turbulent kinetic energy $k$, the TKE equation multiplied with $\langle \langle T \rangle \rangle$ has to be subtracted from the Reynolds stress equation (5) first, and then the left-hand side of the resulting transport equation for $\langle \langle \vec{u} \rangle \rangle$ is set to zero. Furthermore, the left-hand sides of the heat flux equation and the equation for $\langle \langle \vec{T} \rangle \rangle$ are set to zero as well.

Mellor and Yamada (1974, 1982) used this approach for their so-called level 2½ model. They justify the neglect of transports for $\langle \langle \vec{u} \rangle \rangle$ and $\langle \langle \vec{T} \rangle \rangle$ by a scaling procedure where terms are ordered by their degree of deviation from isotropy. This results in their level 3 model. The additional neglect of transport terms in the $\langle \langle \vec{T} \rangle \rangle$ equation then allows for a complete algebrazation.

In the present paper, a nonequilibrium version of the model suggested by Kantha and Clayson (1994) is derived by applying the above discussed algebrazation procedure to Eqs. (5), (11), and (12). This is an extension of the Mellor and Yamada (1974, 1982) level 2½ model in which the parameterization of the pressure correlations in the heat flux equation are simpler, because of $c_{2T} = c_{3T} = 0$. The quasi-equilibrium model by Kantha and Clayson (1994) is achieved from the nonequilibrium model by applying the equilibrium con-

<table>
<thead>
<tr>
<th>Model</th>
<th>$c_1$</th>
<th>$c_2$</th>
<th>$c_3$</th>
<th>$c_4$</th>
<th>$c_5$</th>
<th>$c_{1T}$</th>
<th>$c_{2T}$</th>
<th>$c_{3T}$</th>
<th>$c_{4T}$</th>
<th>$c_T$</th>
<th>$c_T^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KC</td>
<td>2.98</td>
<td>0.0</td>
<td>0.0</td>
<td>0.32</td>
<td>0.0</td>
<td>3.70</td>
<td>0.7</td>
<td>0.2</td>
<td>0.0</td>
<td>1.23</td>
<td>0.094</td>
</tr>
<tr>
<td>RH</td>
<td>1.8</td>
<td>0.6</td>
<td>0.5</td>
<td>0.0</td>
<td>0.0</td>
<td>3.0</td>
<td>0.33</td>
<td>0.33</td>
<td>0.0</td>
<td>1.6</td>
<td>0.121</td>
</tr>
<tr>
<td>CA</td>
<td>2.5</td>
<td>0.984</td>
<td>1.6</td>
<td>0.533</td>
<td>0.416</td>
<td>5.97</td>
<td>0.6</td>
<td>0.33</td>
<td>0.4</td>
<td>1.44</td>
<td>0.077</td>
</tr>
</tbody>
</table>
d. Boundary layer approximation

The solution of the systems of algebraic equations for \( \langle \bar{u} \bar{u} \rangle \), \( \langle \bar{u} \bar{T} \rangle \), and \( \langle \bar{T}^2 \rangle \) discussed above is simplified by applying the so-called boundary layer approximation first. This is justified since the resulting closure schemes are designed for use in estuarine and ocean models where the aspect ratio, that is, the ratio between vertical and horizontal scales, is sufficiently small. The boundary layer approximation is realized by setting all horizontal gradients inside the algebraic system of equations for \( \langle \bar{u} \bar{u} \rangle \), \( \langle \bar{u} \bar{T} \rangle \), and \( \langle \bar{T}^2 \rangle \) to zero. For easier notation, \( \bar{u} = (u, \bar{v}, \bar{w}) \), \( \bar{T} = (\bar{v}, \bar{T}) \), and \( \bar{R} = (\bar{v}, \bar{T}) \) is set to \( \bar{v}, \bar{T} \). Consequently, after applying the continuity equation (3), \( \bar{V} = 0 \) results as well. For the resulting relations for \( P_{uv}, B_{uv}, S_{uv}, \) and \( V_{uv} \), see section b of the appendix.

After this boundary layer approximation, an algebraic system of equations for the correlators \( \langle \bar{u} \bar{u} \rangle \), \( \langle \bar{v} \bar{v} \rangle \), \( \langle \bar{w} \bar{w} \rangle \), \( \langle \bar{u} \bar{w} \rangle \), \( \langle \bar{v} \bar{w} \rangle \), \( \langle \bar{u} \bar{T} \rangle \), \( \langle \bar{v} \bar{T} \rangle \), \( \langle \bar{u} \bar{T} \rangle \), and \( \langle \bar{T}^2 \rangle \) is obtained for each model. This system of equations is linear for the models KC and CA and nonlinear for the model RH. Despite the different structures of the systems of equations, they all result in the simple, well-known relations of the eddy viscosity and the eddy diffusivity principle:

\[
\langle \bar{u} \bar{v} \rangle = -c_{\mu} \frac{k^2}{E} \bar{u},
\]

\[
\langle \bar{v} \bar{w} \rangle = -c_{\mu} \frac{k^2}{E} \bar{v},
\]

\[
\langle \bar{u} \bar{T} \rangle = -c_{\mu} \frac{k^2}{E} \bar{u},
\]

\[
\langle \bar{v} \bar{T} \rangle = -c_{\mu} \frac{k^2}{E} \bar{v},
\]

with the eddy viscosity \( \nu \) and diffusivity \( \nu' \) respectively:

\[
\nu = c_{\mu} \frac{k^2}{E}, \quad \nu' = c_{\mu} \frac{k^2}{E}.
\]

This reflects the relation of Kolmogorov (1942) and Prandtl (1945), which assumes that eddy viscosity and diffusivity are proportional to a velocity scale and a length scale of turbulence. Here \( k/\varepsilon \) is the velocity scale and \( L = c_{\mu} k^{3/2} / \varepsilon \) a macrolength scale for energy containing eddies, calculated by means of the Taylor (1935) scaling. In (19) \( c_{\mu} \) is the value for \( c_{\mu} \) resulting from \( B = 0 \) and \( P = \varepsilon \). (See Table 1).

All the information on second-order correlators is now contained in the rather complex, nondimensional stability functions \( \alpha_{\mu} \) and \( \alpha_{\mu}' \). Despite their differences, these stability functions depend for all models on only two nondimensional parameters, the shear number and the buoyancy number, respectively:

\[
\alpha_{\mu} = \frac{k^2}{E^2} S^2, \quad \alpha_{\mu}' = \frac{k^2}{E^2} N^2.
\]

The different stability functions are given in section 3e. It should be noted that up to this point no assumption about the calculation of the turbulent dissipation rate \( \varepsilon \) has been made.

e. Nonequilibrium stability functions

Here the sets of stability functions are given for the models of KC (Kantha and Clayson 1994), HR (Rodi 1980; Hossain 1980; Burchard and Baumert 1995), and CA (Canuto et al. 2001). An alternative set of stability functions also proposed by Canuto et al. (2001) (from here on denoted by CB) is given as well. They are displayed as functions of \( \alpha_{\mu} \) and \( \alpha_{\mu}' \) in Figs. 1–4.

At this stage, the closure of the second-order moments is practically finished. It should be noted however that all these sets of stability functions should be limited by certain constraints in order to assure positivity of the eddy viscosity \( \nu \) and diffusivity \( \nu' \) and of the velocity variances \( \langle \bar{u}^2 \rangle \), \( \langle \bar{v}^2 \rangle \), and \( \langle \bar{w}^2 \rangle \); see Eqs. (A10–A12).
1) Model of Kantha and Clayson (1994)

In Kantha and Clayson (1994), only the quasi-equilibrium version of the stability functions is given. However, full versions can also be derived, which are then of the same form as the stability functions originally suggested by Mellor and Yamada (1982) with the exception that \( c_2 \) and \( c_3 \) are nonzero now.

In our notation (15)–(17), this set of stability functions may be formulated as

\[
\begin{align*}
\alpha c_\mu &= \frac{0.1682 + 0.03269 \alpha_N}{1 + 0.4679 \alpha_N + 0.07372 \alpha_M + 0.01761 \alpha_N \alpha_M + 0.03371 \alpha_N^2} \\
\alpha c'_\mu &= \frac{0.1783 + 0.01586 \alpha_N + 0.003173 \alpha_M}{1 + 0.4679 \alpha_N + 0.07372 \alpha_M + 0.01761 \alpha_N \alpha_M + 0.03371 \alpha_N^2}.
\end{align*}
\]

The exact form of (21) in terms of the empirical parameters (see Table 1) contained in Eqs. (5), (11), and (12) is given in section d of the appendix.

2) Model of Rodi (1980), Hossain (1980), and Burchard and Baumert (1995)

In contrast to the models of Kantha and Clayson (1994) and Canuto et al. (2001), the model of Rodi (1980) and Hossain (1980) in the version of Burchard and Baumert (1995) results in stability functions \( c_\mu \) and \( c'_\mu \), which not only depend on \( \alpha_M \) and \( \alpha_N \), but additionally depend on the nondimensional term \( (P + B) / \varepsilon \), that is, on the degree of deviation from local turbulence equilibrium. This is a consequence of the specific closure concept used in that model; see Eqs. (13) and (14). Traditionally, these stability functions have been solved in numerical models by using the value for \( (P + B) / \varepsilon - 1 \) on an old time level. In this form, the stability functions have been presented first by Rodi (1980) and Hossain (1980).

However, because of \( (P + B) / \varepsilon = c_\mu \alpha_M - c'_\mu \alpha_N \), these equations for \( c_\mu \) and \( c'_\mu \) can be expressed as implicit functions of \( \alpha_M \) and \( \alpha_N \). The evaluation procedure that has been suggested by Burchard and Baumert (1995) is first solving for \( (P + B) / \varepsilon - 1 \) and then inserting that value into the formulations for \( c_\mu \) and \( c'_\mu \). This procedure is discussed in detail in the section e of the appendix.

3) Model of Canuto et al. (2001)

The stability functions as they result from the closure assumptions carried out by Canuto et al. (2001) are as follows:

\[
\begin{align*}
\alpha c_\mu &= \frac{0.1070 + 0.01741 \alpha_N - 0.00012 \alpha_M}{1 + 0.2555 \alpha_N + 0.02872 \alpha_M + 0.008677 \alpha_N^2 + 0.005222 \alpha_N \alpha_M - 0.0000337 \alpha_M^2} \\
\alpha c'_\mu &= \frac{0.1120 + 0.004519 \alpha_N + 0.00088 \alpha_M}{1 + 0.2555 \alpha_N + 0.02872 \alpha_M + 0.008677 \alpha_N^2 + 0.005222 \alpha_N \alpha_M - 0.0000337 \alpha_M^2}.
\end{align*}
\]

Despite the higher complexity of the transport equations for Reynolds stresses and heat fluxes due to consideration of more terms for the pressure-strain correlators, these stability functions are structurally similar to those of Kantha and Clayson (1994).

These stability functions will be denoted by CA. The exact form can be found in section f of the appendix. In their paper, Canuto et al. (2001) give another set of stability functions derived on the ground of different assumptions. They will be denoted by CB and are of the following form:

\[
\begin{align*}
\alpha c_\mu &= \frac{0.1270 + 0.01526 \alpha_N - 0.00016 \alpha_M}{1 + 0.1977 \alpha_N + 0.03154 \alpha_M + 0.005832 \alpha_N^2 + 0.004127 \alpha_N \alpha_M - 0.000042 \alpha_M^2} \\
\alpha c'_\mu &= \frac{0.1190 + 0.00429 \alpha_N + 0.00066 \alpha_M}{1 + 0.1977 \alpha_N + 0.03154 \alpha_M + 0.005832 \alpha_N^2 + 0.004127 \alpha_N \alpha_M - 0.000042 \alpha_M^2}.
\end{align*}
\]
f. Quasi-equilibrium stability functions

Quasi-equilibrium is defined as the state where production and dissipation of turbulent kinetic energy are balanced; that is, $P + B = e$. This can be transformed to the relation

$$c_{\mu} \alpha_M - c'_{\mu} \alpha_N = 1. \quad (24)$$

This quasi-equilibrium state has often been used for simplifying stability functions depending on both $\alpha_M$ and $\alpha_N$. The most well-known example is the work of Galperin et al. (1988) where relation (24) has been used for improving the performance of the stability functions proposed by Mellor and Yamada (1982), which have been proven to be numerically unstable (see Deleersnijder and Luyten 1994). Galperin et al. (1988) found by applying the scale analysis introduced by Mellor and Yamada (1974) that it is not a model inconsistency to prescribe $P + B = e$ only for the stability functions but still retain the full dynamic TKE equation.

The bold lines in Figs. 1–4 indicate the quasi-equilibrium states for the four sets of stability functions discussed in this paper. The stability functions suggested by Galperin et al. (1988) are expressed as functions of $\alpha_N$. Relation (24) allows us also to express the stability functions depending on the gradient Richardson number $Ri = \alpha_N/\alpha_M$, which has often been done for further analyzing the stability functions as shown in Fig. 5 for the four sets of stability functions. The maximum value of $Ri$ that can be reached in quasi-equilibrium is called the “critical” Richardson number $Ri_{c}$. For the models discussed here, they have the values shown in Table 2. It can be seen that the model of Kantha and Clayson (1994) already suppresses turbulence for stratifications around $Ri = 0.2$, whereas the other models allow for mixing at Richardson numbers significantly higher.

For stable stratification, laboratory and LES data for the turbulent Prandtl number $Pr = c_{\mu}/c'_{\mu}$ are compared to the turbulent Prandtl number computed by the quasi-equilibrium stability functions (see Fig. 6). All the functions are within the uncertainty of the data. Only the KC quasi-equilibrium stability functions do not reach high turbulent Prandtl numbers due to their relatively small critical gradient Richardson number.

Another way of displaying the quasi-equilibrium stability functions is to transform them into the Monin–Obukhov similarity form. This has already been suggested by various authors (see Mellor and Yamada 1982; Kantha and Clayson 1994). Monin and Obukhov (1954) found for the atmospheric boundary layer the following relations between fluxes of momentum and heat and gradients of velocity and density, respectively.

$$u_{*} \sim \frac{B}{k \nu} \Phi_M' \left( \frac{z'}{L_M} \right), \quad b \sim -\frac{g \rho_0}{\rho_0} \Phi_H' \left( \frac{z'}{L_M} \right) \quad (25)$$

with the distance from the boundary $z'$ and buoyancy $b = -g(\rho - \rho_0)/\rho_0$.

With the friction velocity

$$u_{*} = c_{\mu} \kappa^2 \frac{k^2}{E} |\partial_z u|,$$

the buoyancy flux

$$B = -c_{\mu} \frac{k^2}{E} |\partial_z b|$$

and the macro length scale $L = k \kappa'$, the variables $\zeta = z'/L_M$, $\Phi_M$, and $\Phi_H$ can be expressed as
\[ \zeta = (c_\mu^{(0)})^{3/4} \frac{c_\mu^{(u)}}{c_\mu^{(0)}} \frac{\alpha_N}{\alpha_M^{1/4}}, \quad \Phi_M = (c_\mu^{(0)})^{3/4} \frac{\alpha_M^{1/4}}{c_\mu^{(0)}}, \]
\[ \Phi_H = (c_\mu^{(0)})^{3/4} \frac{c_\mu^{(u)}}{c_\mu^{(0)}} \frac{\alpha_M^{1/4}}{c_\mu^{(0)}}, \]

where \( \kappa = 0.4 \) is the von Kármán constant and \( \text{Pr} = \Phi_M/\Phi_H = c_\mu^{(u)} c_\mu^{(0)} \) the Prandtl number. Figure 7 shows the Monin–Obukhov similarity functions \( \Phi_M \) and \( \Phi_H \) as functions of \( \zeta \) in comparison to empirical curves by Businger et al. (1971). The stability functions by Kantha and Clayson (1994) are clearly the closest to the empirical curves, based on measurements in the atmospheric boundary layer. It should be noted that this is due to a tuning of the parameters \( c_2 \) and \( c_3 \). Mellor and Yamada (1982) achieved a good agreement with the Businger et al. (1971) data with their relatively simple closure by setting \( c_2 = c_3 = 0 \). It is difficult to explain why more complex parameterizations of the pressure–strain correlations cause worse agreement with the Monin–Obukhov theory. But it might be due to the fact that this theory is valid only close to boundaries where some of the closure assumptions could be wrong. Another reason could be that the Businger et al. (1971) measurements are taken at the atmosphere where in comparison to water different molecular viscosities and diffusivities are present. This could be particularly significant at strongly stable stratification with large positive values of \( \zeta \).

4. Two-equation models

In the second-moment closure presented here as formulations for the eddy viscosity and eddy diffusivity [see Eq. (18)], the turbulent kinetic energy \( k \) and its dissipation rate \( \varepsilon \) still occur as free parameters. They are contained in the stability functions as a ratio, defining a timescale \( \tau = k/\varepsilon \) and in the relations of Prandtl and Kolmogorov as ratio \( k^{2}/\varepsilon \). One straightforward solution of the remaining closure problem is therefore to construct prognostic equations for these two quantities. For both \( k \) and \( \varepsilon \), exact transport equations can be derived from the Navier–Stokes equations after applying ensemble averaging [see Eqs. (A37) and (A39) in the appendix].

The \( k \) equation has already been discussed, it can also be derived by taking the trace of the Reynolds stress equation (5):

\[ \partial_t k + \partial_j F(k) = P + B - \varepsilon. \]  

(27)

For closing the dissipation rate equation (A39), a number of closure assumptions are needed (see section g of the appendix):

\[ \partial_t \varepsilon + \partial_j F(\varepsilon) = \frac{\varepsilon}{k} (c_{14} P + c_{15} B - c_{16} \varepsilon). \]

(28)

with \( c_{14} = 1.44 \) and \( c_{16} = 1.92 \). It has been shown by Burchard and Baumert (1995) that \( c_{13} \) is not an independent parameter but depends on the definition of a steady Richardson number. Deviating from other authors, Burchard and Baumert (1995), Burchard et al. (1998), Burchard and Petersen (1999), and Baumert and Peters (2000) postulate that \( c_{13} \) should be a negative number. This is further discussed in section 5. However, for unstable stratification, \( c_{13} = 1 \) is used in order to provide a source term for the dissipation rate in shear-free convective regimes (see Rodi 1987).

The resulting expressions for the diffusive fluxes \( F(k) \) and \( F(\varepsilon) \) are third-order correlators for which closure assumptions have to be made as well. For simplicity, we adopt here the eddy viscosity principle, which leads to
where the diffusivities are chosen as \( \nu_t = \nu + \nu_s \) and \( \nu_s = \nu + \nu_s / \sigma \). Here, the logarithmic law for constant stress layers leads to the Schmidt number for dissipation:

\[
\sigma_k = \frac{\kappa^2}{(C_m^0)^{1/2}(c_{a2} - c_{a3})},
\]

which is of the order of unity and varies for different stability functions with \( C_m^0 \). It should be noted that non-local parameterizations for \( F(k) \) have been suggested in the literature, which should improve the model performance especially for convective regimes (see Canuto et al. 1994; D’Alessio et al. 1998). We did not use such models here since they are either very complex (Canuto et al. 1994) or based on bulk parameters such as the Deardorff convective velocity scale \( w_a \) (D’Alessio et al. 1998). This has the consequence that the turbulent transport of TKE under free convection is underestimated by approximately a factor of 2; see section 6b).

Boundary conditions for \( k \) and \( \varepsilon \) are based on the assumptions of a constant stress layer and local equilibrium (\( P = \varepsilon \)) near the boundaries and a macrolength scale of \( L = k(z + z_p) \) with the roughness length \( z_p \).

We use here flux boundary conditions as suggested by Burchard and Petersen (1999), which performed optimally in terms of numerical approximation and physical behavior (e.g., decrease of eddy viscosity near the stress-free surface).

It should be noted that the dissipation rate equation might be replaced by a transport equation for the product \( kL \) as suggested by Mellor and Yamada (1982). The dissipation rate would then have to be calculated by using Eq. (19). There is however an ongoing discussion whether or not the proportionality factor used in (19) should be a constant or depending on stratification (see Mellor 2001).

5. Stationary solutions in homogeneous shear layers

For some basic investigations of turbulence models it is instructive to consider idealized flows far away from boundaries with constant shear and stratification. This leads to the concept of homogeneous shear layers. Mathematically formulated, this concept leads to vanishing diffusion terms in all turbulence equations such that they become ordinary differential equations only depending on time \( t \). After denoting \( \dot{k} = \partial_t k \) and \( \dot{\varepsilon} = \partial_t \varepsilon \), the equations for \( k \) and \( \varepsilon \) may be written as

\[
\dot{k} = P + B - \varepsilon, \quad \dot{\varepsilon} = \frac{\varepsilon}{k}(c_{a1}P + c_{a3}B - c_{a2} \varepsilon). \tag{31}
\]

a. Steady-state Richardson number

If \( \dot{k} \) and \( \dot{\varepsilon} \) are zero, then the total equilibrium of the \( k-\varepsilon \) model is reached and the following relation, which is a precondition for the steady state, can be derived:

\[
\text{Ri} = \frac{\varepsilon}{k} = \frac{c_{a3} - c_{a1}}{c_{a2} - c_{a3}}. \tag{32}
\]

The steady-state Richardson number therefore depends on the empirical parameters \( c_{a1}, c_{a2}, \) and \( c_{a3} \) in the \( \varepsilon \) equation and on the actual stability function chosen. In contrast to \( c_{a1} \) and \( c_{a2} \), the buoyancy-flux-related parameter \( c_{a3} \) has never directly been determined by laboratory experiments. Figure 8 shows how \( c_{a1} \) and \( \text{Ri}_c \) are related to each other for the various stability functions. This figure may be compared to Fig. 3 by Burchard and Baumert (1995) where the flux Richardson number was considered instead. For steady-state Richardson numbers below 0.35, negative values for \( c_{a3} \) have to be used for all sets of stability functions. Suitable values for \( \text{Ri}_c \) will be calibrated in section 6 by means of an idealized wind mixing experiment.

An expression equivalent to (32) has recently been suggested by Burchard (2001) for the \( k-\varepsilon \) model by Mellor and Yamada (1982). The surprising result was that for reasonable values for the steady-state Richardson number of \( \text{Ri}_c = 0.2 \) the coefficient was far from the value suggested in the original paper. With this new calibration, a strict limitation of the length scale under stable stratification, which was needed for the old version, is no longer necessary.

b. Length scales

The so-called structural equilibrium of the system of Eq. (31) is reached when the timescale \( \tau = kL / \varepsilon \) is in steady state. It can be shown that—other than the total equilibrium discussed in section 5a—the solution for (31) tends to the structural equilibrium for all Richardson numbers. Baumert and Peters (2000) recently showed how a \( k-\varepsilon \) model equipped with an empirical closure for the stability functions could reproduce data found for ratios of relevant turbulent length scales. We repeat this for the four algebraic second-moment closures presented here.

The two length scales considered here are the Ozmidov scale

\[
L_o = \left( \frac{\varepsilon}{N^3} \right)^{1/2}, \tag{33}
\]

and the buoyancy scale

\[
L_b = \frac{k^{1/2}}{N}. \tag{34}
\]

Another important length scale is the Ellison scale, defined as \( L_e = -\bar{p} / \partial \bar{p} \) (with the density fluctuation \( \bar{p} \)), which is often set equal to the Thorpe scale and is related to the macrolength scale \( L \) [see Eq. (19)] as follows (see Baumert and Peters 2000):

\[
L_e = \frac{L}{2C(c_m^0)^3}. \tag{35}
\]
with $C = 1.4$. When assuming structural equilibrium for the $k-\varepsilon$ model in the homogeneous shear layer approximation, then the ratios $L_E/L_o$ and $L_E/L_b$ can be expressed as follows:

$$
\frac{L_E}{L_o} = \frac{1}{2C} \alpha_m^{3/4}, \quad \frac{L_E}{L_b} = \frac{1}{2C} \alpha_s^{1/2}.
$$

In order to calculate these ratios for the algebraic second-moment closures presented here, a relation between $\alpha_m$ and $\alpha_s$ is obtained after deriving a dynamic equation for $\tau$ and then setting $\dot{\tau} = 0$. This allows for displaying $L_E/L_o$ and $L_E/L_b$ as functions of the gradient Richardson number. For this calculation, the parameter $c_{\alpha,3}$ has to be prescribed, which we take for a steady-state gradient Richardson number of $Ri^* = 0.25$ (see Table 2). These have to be compared to empirical curves based on laboratory experiments; see Baumert and Peters (2000):

$$
\frac{L_E}{L_o} \approx 4.2Ri^{1/4}, \quad \frac{L_E}{L_b} \approx 1.6Ri^{1/2}.
$$

Figure 9 shows this functional relationship. It can be clearly seen that all curves except those resulting from the KC model are in fairly good agreement with the empirical curves.

6. Mixed layer studies

An idealized wind entrainment experiment and an idealized free convection experiment have been chosen here in order to test the $k-\varepsilon$ model together with the
stability functions of Kantha and Clayson (1994) (KC), Rodi (1980) and Hossain (1980) (RH), and Canuto et al. (2001) (CA, CB). Furthermore, the quasi-equilibrium version of the KC model and the full CA model are applied to the OWS Papa data and their results compared to temperature profile observations. It should be noted that the scope of this paper is to test mixed layer models to be implemented into three-dimensional ocean models. We therefore do not intend to compare here the model performance to measurements of turbulent quantities for which data are usually available only on short time-scales.

\textbf{a. Wind entrainment}

A wind entrainment experiment is used in order to test the assumptions on the stationary gradient Richardson number $Ri^*$. The wind entrainment experiment

\begin{table}[h]
\centering
\begin{tabular}{lcc}
\hline
Model & $Ri^*$ & $c_{e,0}$ \\
\hline
KC & 0.235 & -0.404 \\
RH & 0.615 & -0.444 \\
CA & 0.847 & -0.629 \\
CB & 1.02 & -0.566 \\
\hline
\end{tabular}
\caption{Critical Richardson number $Ri^*$ and $c_{e,0}$. The latter is based on a steady-state gradient Richardson number of $Ri^* = 0.25$, but for the model KC, $Ri^* = 0.225$ was used.}
\end{table}
carried out here is inspired by the laboratory experiment of Kato and Philipps (1969). In this experiment, a mixed layer induced by a constant surface stress penetrates into a stably stratified fluid with density increasing linearly downward from the surface. The water depth is assumed to be infinite. Price (1979) suggested a solution for the evolution of the mixed layer depth $D_m$ based on a constant Richardson number $R_i$

$$D_m(t) = 1.05 u'_s N_0^{-1/2} t^{1/2},$$

where $u'_s$ is the surface friction velocity and $N_0$ the constant initial Brunt–Väisälä frequency. Following several authors (see, e.g., Deleersnijder and Luyten 1994; Burchard et al. 1998) we transform this laboratory experiment to ocean dimensions with $u'_s = 10^{-2} \text{m s}^{-1}$ and $N_0 = 10^{-2} \text{s}^{-1}$.

First of all, the concept of the steady-state gradient Richardson number $R_{ist}$ can be validated by means of this entrainment experiment. The stability functions CA and CB are applied with values for $R_{ist}$ ranging from 0.2 to 0.8. Figure 10 shows the evolution of the en-
The ratios $L_E/L_o$ and $L_E/L_b$ as functions of the gradient Richardson number $Ri$, where $L_E$ is the Ellison, $L_o$ the Ozmidov, and $L_b$ the buoyancy scale. Shown are curves resulting from the Kantha and Clayson (1995) (KC), the Rodi (1980) and Hossain (1980) (RH), the Canuto et al. (2001) (CA, CB) second-moment closures. These are compared to the empirical estimates from Eq. (37).

**Table 3.** Entrainment depth for various mixed layer models after 3 days of constant cooling with 100 W m$^{-2}$, with an initially stable temperature gradient of 0.1°C m$^{-1}$ and a constant salinity of 35 psu.

<table>
<thead>
<tr>
<th>Model</th>
<th>Entrainment depth (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$-$\varepsilon$ model, KC</td>
<td>12.5</td>
</tr>
<tr>
<td>$k$-$\varepsilon$ model, RH</td>
<td>11.9</td>
</tr>
<tr>
<td>$k$-$\varepsilon$ model, CA</td>
<td>12.2</td>
</tr>
<tr>
<td>$k$-$\varepsilon$ model, CB</td>
<td>12.4</td>
</tr>
<tr>
<td>KPP</td>
<td>13.0</td>
</tr>
<tr>
<td>Convective adjustment</td>
<td>11.2</td>
</tr>
</tbody>
</table>

**Fig. 9.** The ratios $L_E/L_o$ and $L_E/L_b$ as functions of the gradient Richardson number $Ri$. For low values of $Ri^\nu$, a situation with $Ri > Ri^\nu$ is reached earlier with the consequence that turbulence is decaying and the entrainment is reduced. For high values of $Ri^\nu$, $Ri < Ri^\nu$ holds over nearly the entire mixed layer and therefore mixing and entrainment is enhanced. It can be seen from this experiment that $Ri^\nu = 0.25$ seems to be a reasonable value for the steady-state Richardson number. With this choice, we can now fix $c_{\alpha}$ for each set of stability functions (see Table 2). The value of $Ri^\nu = 0.25$ cannot be reached by the model of Kantha and Clayson (1994). We therefore use $Ri^\nu = 0.225$ for their model, which corresponds to the value for $c_{\alpha}$ given in Table 2. Figures 11 and 12 show results for the mixed layer depth evolution and profiles of eddy viscosity and diffusivity and turbulent kinetic energy at 30 hours after the onset of surface stress. Eight different sets of stability functions have been used for these simulations, namely the models KC, RH, CA, CB and their quasi-equilibrium versions. For all simulations, the dissipation

**Fig. 10.** Development of the mixed layer depth (deepest point with $k > 10^{-5}$ J kg$^{-1}$) for the simulation of the Kato–Phillips experiment. Model results for the complete versions of the models A (left) and B (right) of Canuto et al. (2001) for various values of $Ri^\nu$. 
rate equation (28) has been used with the values for $c_{e_3}$ from Table 3. It can be seen from Fig. 11 that the non-equilibrium version of the KC model [it should be noted that it is the quasi-equilibrium version suggested by Kantha and Clayson (1994)] tends to strong oscillations and therefore produces useless results. This has already been reported by Deleersnijder and Luyten (1994) for the similar model of Mellor and Yamada (1982). In contrast to this, the quasi-equilibrium version of the KC model performs well; the empirical and simulated mixed
layer depth are very close to each other (see Fig. 12). It is however strange that the profile of turbulent kinetic energy shows a maximum in the lower part of the mixed layer. This effect has already been demonstrated by Burchard et al. (1998). Turbulence measurements for this mixed layer experiment do unfortunately not exist. However, in a large eddy simulation study of a similar experimental setup (but with consideration of rotation) carried out by Moeng and Sullivan (1994) such a local maximum of $k$ is not visible.
The other sets of stability functions at show (i) a perfect fit with the empirical curve of Price (1979), (ii) the expected monotone decrease of turbulent kinetic energy down from the surface, and (iii) a numerically stable performance.

b. Free convection

Although strong convective events occur in the ocean in only a few areas, they are important for the ocean circulation and it is therefore desirable that they are sufficiently reproduced by turbulence closure models. A free convection simulation similar to the laboratory experiment carried out by Willis and Deardorff (1974) will be presented here. The scenario simulated here is the same as that used by Large et al. (1994). By means of a constant negative surface heat flux of 100 W m$^{-2}$, a convective boundary layer is entrained into a stably stratified ocean with a surface temperature of 22°C and a temperature gradient of 1°C per 10 m. Shear and rotation are not present. For this free convection simulation recent LES data are available (see Mironov et al. 2000).

In Table 3, the entrainment depth (position of minimum normalized turbulent heat flux) for all experiments after 3 days of cooling is given. Comparison is made to a simple scheme with convective adjustment [see Bryan (1969), the depth is here the height of the homogenized layer] and the KPP model [see Large et al. (1994), the value has been estimated from their Fig. 1]. As expected, all depths for the models presented here are between the latter two depths. The least deepening (11.2 m) is provided by the convective adjustment scheme, which does not perform any active entrainment in terms of steepening the buoyancy gradient below the convective boundary layer. The models presented here mix deeper (11.9±12.5 m) due to their capability of reproducing active entrainment. The fully empirical, nonlocal KPP model provides further deepening (13.0 m) of the convective boundary layer.

Furthermore, after 3 days of cooling profiles of various quantities are shown, normalized by the Deardorff convective velocity scale $w_\ast = (B_0 H)^{1/3}$, the temperature scale $T_\ast = (\nu \partial_z T)_{z_H=0}/w_\ast$, and the surface buoyancy flux $B_0$ versus $z/H$. Here $H$ is the depth of the entrainment layer the base of which is defined as the height with the minimum heat flux. The results for mean temperature, heat flux, dissipation rate, and the variances $\langle \tilde{u}^2 \rangle$, $\langle \tilde{w}^2 \rangle$, and $\langle T^2 \rangle$ [see Eqs. (A10)–(A12)] are shown in Fig. 13. Three shortcomings of the model are obvious:

1) Countergradient fluxes occur over a large portion (roughly $-0.8 \leq z/H \leq -0.4$) of the convective

---

**Fig. 13.** Free convection experiment of Willis and Deardorff (1974). Profiles of the normalized temperature profile $(T - T_{\text{max}})/T_{\ast}$, normalized temperature flux $(\tilde{w}T)/w_\ast T_{\ast}$, and the normalized autocorrelations $\langle \tilde{u}^2 \rangle / \langle \tilde{w}^2 \rangle$, and $\langle T^2 \rangle / \langle T_{\ast}^2 \rangle$ and dissipation rate $\epsilon/B_0$ calculated by using different models for the stability functions: Kantha and Clayson (1994) (KC), Rodi (1980) and Hossain (1980) (RH), Canuto et al. (2001) version A (CA), and Canuto et al. (2001) version B (CB). The model simulations are compared to LES simulations by Mironov et al. (1999).
boundary layer, which is not included in the model because of its inherent downgradient approximation. Therefore, temperature profiles of LES and turbulence closures are principally different. This suggests that nonlocal processes are important here.

2) The height of the active entrainment layer is underestimated by the turbulence closure models. This can best be seen in the profiles of \( \langle \vec{w}T \rangle \) and \( \langle T^2 \rangle \). Potential reasons could here be the downgradient approximation for the TKE flux and the fact that turbulent transport of \( \langle \vec{w}T \rangle \) and \( \langle T^2 \rangle \) is neglected. It can be seen from Fig. 14 that the TKE-diffusion term is qualitatively reproduced by the model (here CA), but underestimated by a factor of approximately 2.

3) The profile of \( \langle \vec{u}^2 \rangle \) near the surface suggests that the turbulent transport of this quantity should not be neglected here.

It should be noted that Canuto et al. (1994) obtained good agreement between LES data and simulation results for a free convection experiment with a full Reynolds closure model using dynamic transport equations for \( \langle \vec{w}T \rangle \), \( \langle T^2 \rangle \), \( \langle \vec{u}^2 \rangle \), \( \langle \vec{v}^2 \rangle \), and \( \langle \vec{w}^2 \rangle \), and \( \varepsilon \) including complex algebraic closure schemes for all relevant third-order moments. It should be the aim of future work to find a reasonable compromise between this complex model by Canuto et al. (1994) and the two-equation models presented here, in terms of both efficiency and predictability.

c. Wind and convective mixing in the open sea

For the northern Pacific, long-term observations of meteorological parameters and temperature profiles are available. OWS Papa at 50°N, 145°W has the advantage that it is situated in a region where the horizontal advection of heat and salt is assumed to be small. Various authors used these data for validating turbulence closure schemes (Denman 1973; Martin 1985; Large et al. 1994; Kantha and Clayson 1994; D’Alessio et al. 1998). As for any realistic oceanic test case, other factors than the choice of the mixed layer model also play an important role for the agreement between the model results and the measurements. First of all, the momentum and heat fluxes at the sea surface are never available as direct observations but are calculated using bulk formulae. Measurements such as fractional cloud cover are never exact. Furthermore, horizontal advection of heat and salt, neglected in one-dimensional water column models, can strongly influence the measured profiles of temperature and salinity. Maybe most important, the bulk formulae for the parameterization of cross-surface fluxes of momentum, heat, and freshwater are strictly empirical.

How the bulk formulae for surface heat and momentum fluxes have been used here is discussed in detail in Burchard et al. (1999). The relative heat content of the upper 250 m of the water column from temperature profiles and surface heat fluxes between March 1961 and March 1962 is shown in Fig. 15. Until the beginning of November 1961 (around day 310), the agreement between the curves is sufficient enough for allowing for one-dimensional simulation. Afterward, cold water is horizontally advected, a process described in detail by Large et al. (1994). For mixing below the thermocline, an internal wave and shear instability parameterization as suggested by Large et al. (1994) has been used.

Figure 17 shows results of the model simulations with the stability functions of Canuto et al. (2001) in comparison to measured temperature profiles (Fig. 16). The overall temperature evolution is well simulated by this model. A more detailed comparison between measurements and two different model simulations of temperature profiles is shown in Fig. 18. Besides the aforementioned Canuto et al. (2001) model (CA) the simulations are carried out here additionally with the quasiequilibrium version of Kantha and Clayson (1994) (KC). Until day 210, the agreement between both simulations and the observations is fairly good. Then, around day 240, the models predict a too shallow mixed layer, obviously due to erroneous surface fluxes or
strong advective events such as downwelling (see Fig. 15), where a mismatch between the heat content of the water column and the accumulated surface heat fluxes is evident around day 240. It can be seen as well that the KC model predicts a slightly shallower mixed layer than the CA model. This has the consequence that the KC model overpredicts the SST during summer (days 210–280 see Fig. 19). Until day 280, the rms error for SST between both simulations and the observations is rather small, 0.36°C for the Canuto et al. (2001) and 0.33°C for the Kantha and Clayson (1994) model. However, the SST evolution strongly depends on the internal wave parameterization, and thus these rms errors are not discriminative of the quality of the turbulence models. It should be noted that we have used exactly the parameters of Large et al. (1994) for this, other than Kantha and Clayson (1994), who had (while applying a $kL$ instead of an $e$ equation) to use a background diffusivity five times higher in order to predict the SST realistically. This leads however to a thermocline too diffusive compared to measured temperature profiles (see Burchard et al. (1999)).

7. Discussion and conclusions

The concept of the steady-state gradient Richardson number $Ri^{st}$ is applied here for adjusting mixed layer models such that they realistically predict the mixed layer depth and consequently the sea surface temperature in the ocean. The simulations of the wind entrainment experiment suggest a value of $Ri^{st} = 0.25$. Although the empirical relation for the mixed layer sug-

![Fig. 16. Temperature evolution for OWS Papa in the northern Pacific Ocean from Mar 1961 to Mar 1962 from CTD measurements.](image)

![Fig. 17. Temperature evolution for OWS Papa in the northern Pacific Ocean from Mar 1961 to Mar 1962. Results of the simulation with the version A of the Canuto et al. (2001) model with the stationary gradient Richardson number set to $Ri^{st} = 0.25$.](image)
gested by Price (1979), Eq. (38), cannot be used for calibrating $R_i^\sigma$ in a strict way, it can be concluded from Fig. 10 that it should be between 0.2 and 0.3. According to Schumann and Gerz (1995), $R_i^\sigma < 0.25$ should hold. By analyzing laboratory data from Rohr (1985) obtained from homogeneously shear-layered saltwater flow, they conclude that $R_i^\sigma = 0.16 \pm 0.06$, a value significantly smaller than the value we suggest. The discrepancy could be explained by the argument that mixed layer dynamics are quantitatively different than homogeneous shear layers due to the nonnegligible vertical fluxes of turbulent quantities. More efficient parameterizations for turbulent transport of TKE than the downgradient approach used here could assumedly result in more realistic estimates for $R_i^\sigma$.

Eight different sets of stability functions are tested here, namely the full and the quasi-equilibrium versions of Kantha and Clayson (1994) (KC), Rodi (1980) and Hossain (1980) [version of Burchard and Baumert (1995), RH], and versions A and B of Canuto et al. (2001) (CA, CB). The analysis of the quasi-equilibrium versions of the stability functions shows that the model of Kantha and Clayson (1994) cannot reach $R_i^\sigma = 0.25$ because of its critical gradient Richardson number of $R_i^c = 0.235$. We therefore used $R_i^\sigma = 0.225$ only for this model, and the predicted mixed layer depth is in good agreement with the curve of Price (1979). It should be noted again, that the KC model is a slight improvement of the models of Mellor and Yamada (1982) and Galperin et al. (1988), which compute $R_i^\sigma = 0.19$. The wind entrainment experiment shows that the stability functions of Kantha and Clayson (1994) do not perform well. This is due to inherent numerical instabilities (full version) and an unrealistic local maximum of turbulent kinetic energy right above the pycnocline (quasi-equilibrium version). A further weakness of the KC model became apparent when the ratios of Ellison to Ozmidov length scale and Ellison to buoyancy length scale had been compared to empirical curves for structural equilibrium turbulence. These ratios were far larger than those for the other models, which all performed sufficiently well. For the case of free convection, all models predict significant deviations from recent LES data. The major deficiencies are possibly due to the neglect of turbulent fluxes of second moments, which can in principle be added to the models presented here.
Two models are finally used for simulations of ocean mixed layer dynamics: the quasi-equilibrium version of the KC model and the full version of the CA model. The result is that the CA model mixes slightly deeper than the KC model, maybe due to the smaller steady-state gradient Richardson number chosen for the latter model. Too shallow mixed layers computed by so-called differential mixed layer models (defined in contrast to bulk models that average over the entire mixed layer) have been reported by Martin (1985), who used, among others, the OWS Papa data for comparing various models. He explained this phenomenon by a too small critical Richardson number and could obtain acceptable model results at OWS Papa by increasing the critical Richardson number to $R_i^c = 0.3$.

It should however be noted that it is mainly the steady-state Richardson number that determines the growth or decay of turbulence rather than the critical Richardson number, which just sets an upper limit to the gradient Richardson number.

Coming back to the five paradigms for good turbulence closure mentioned in the introduction—(i) derivation from second-moment transport equations, (ii) physical soundness, (iii) high predictability, (iv) computational economy, and (v) numerical robustness—the Canuto et al. (2001) stability functions are those that best fulfill these requirements. (i) They consider more terms for the pressure–strain relations than all other models. (ii) They are physically sound since they allow for vertical mixing even at high Richardson numbers. (iii) They proved in this investigation a high predictability since they produced good results for OWS Papa without tuning them to these scenarios. (iv) They are rather economical with only two additional equations for turbulent quantities plus evaluating the ratio of two polynomials. (v) They were numerically robust since the time step was $\Delta t = 300$ s with a vertical resolution of $\Delta z = 1$ m for OWS Papa and no numerical instabilities could be seen. The ability of $k$–$\epsilon$ models to produce high-order approximations also for coarse vertical resolutions has already been shown by Burchard and Petersen (1999). In order to achieve this, a special numerical treatment of the dissipation rate near the surface is needed (see Burchard and Petersen 1999). Ocean general circulation models have already been coupled to two-equation turbulence models a decade ago [see Rosati and Miyakoda (1988), who applied the Mellor and Yamada (1982) $k$–$\epsilon$ model for a World Ocean circulation study]. Applications of $k$–$\epsilon$ models in OGCMs have to the knowledge of the authors not been made yet. With the ongoing growth of computer resources, the extensive use of more complex turbulence closure schemes will be more feasible.

In contrast to the properties (i)–(v) of the stability functions by Canuto et al. (2001), those of Rodi (1980) and Hossain (1980) [version of Burchard and Baumert (1995)] definitely do not fulfil (iv), computational economy, due to their implicit formulation. As already mentioned above, the quasi-equilibrium version of the Kantha and Clayson (1994) stability functions do not fulfil (ii), physical soundness, due to the local TKE maximum in the entrainment experiment, and predict ratios of relevant turbulent length scales for structural-equilibrium turbulence that are far from observations. The full version of the Kantha and Clayson (1994) as well as the Mellor and Yamada (1982) stability functions did not even allow for a numerically stable computation.

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**Mathematical Details**

*a. Notation*

Different notations have always been a major threshold for comparing different turbulence parameterizations. For calculating the eddy viscosity \( \nu \), and eddy diffusivity \( \nu' \), we use the following form (see section 3d):

\[
\nu = c_m \frac{k^2}{\varepsilon}, \quad \nu' = c'_m \frac{k^2}{\varepsilon}, \quad (A1)
\]

which automatically results from the algebraic Reynolds stress closure. In other models such as Mellor and Yamada (1974, 1982), an alternative formulation is used:

\[
K_m = S_m q_L, \quad K_n = S_n q_L \quad (A2)
\]

with \( q^2 = 2k \) and \( K_m \) and \( K_n \) being other notations for the eddy viscosity and diffusivity \( \nu \) and \( \nu' \), respectively; \( S_m \) and \( S_n \) correspond to the stability functions \( c_m \) and \( c'_n \), with the conversion

\[
S_m = \frac{c_m}{\sqrt{2c_L}}, \quad S_n = \frac{c'_n}{\sqrt{2c_L}} \quad (A3)
\]

with \( c_L \) from (19).

The nondimensional shear and buoyancy numbers on which the stability functions depend are here consequently expressed as

\[
\alpha_M = \frac{k^2}{\varepsilon} S^2, \quad \alpha_N = \frac{k^2}{\varepsilon} N^2. \quad (A4)
\]

With the Mellor and Yamada (1974, 1982) notation for these nondimensional parameters,

\[
g_m = \frac{L^2}{q^2} S^2, \quad g_b = \frac{L^2}{q^2} N^2, \quad (A5)
\]

the conversion between \( \alpha_M, \alpha_N, \) and \( g_m, g_b \) is of the following form:

\[
g_m = \frac{c_m^2}{2} \alpha_M, \quad g_b = \frac{c_m^2}{2} \alpha_N. \quad (A6)
\]

By means of (A3) and (A6), the sets of stability functions presented in sections 3e(1)–(3) may be transformed to the other notation.

It should be noted that further definitions of stability functions are often used such as \( \nu = c_m \sqrt{kL} \) (see Burchard et al. 1998) and \( \nu = 2c_m k^2/\varepsilon \) (see Canuto et al. (2001)). Another reason for confusion is often the different use of the parameter \( c_{e3} \) in the dissipation rate equation (28). In this paper, the right-hand side of that equation reads as \( (\varepsilon k) c_{e3} P + c_{e2} B - c_{e2} e \), but often the form \( (\varepsilon k) [c_{e1}(P + c_{e2} B) - c_{e2} e] \) (Rodi 1980; Burchard and Baumert 1995) is used. This, of course will lead to different values for \( c_{e3} \).

*b. Production, shear, and vorticity after boundary layer approximation*

Here, the matrices \( P_{ij}, B_{ij}, S_{ij}, \) and \( V_{ij} \) resulting from the boundary layer approximation (see section 3d) are given:

\[
P_{ij} = \begin{pmatrix}
-2\partial_x \Pi (\tilde{w}\tilde{v}) & -\partial_x \Pi (\tilde{\psi}\tilde{v}) - \partial_y \Pi (\tilde{w}\tilde{v}) - \partial_y \Pi (\tilde{\psi}\tilde{v}) - \partial_y \Pi (\tilde{w}^2) \\
-\partial_x \Pi (\tilde{\psi}\tilde{v}) & -2\partial_y \Pi (\tilde{w}\tilde{v}) - \partial_y \Pi (\tilde{w}^2) \\
-\partial_y \Pi (\tilde{w}^2) & -\partial_y \Pi (\tilde{w}^2) & 0
\end{pmatrix}, \quad (A7)
\]

\[
B_{ij} = \begin{pmatrix}
\beta (\tilde{w}\tilde{T}) \\
\beta (\tilde{w}\tilde{T}) & \beta (\tilde{v}\tilde{T}) & 2\beta (\tilde{v}\tilde{T})
\end{pmatrix}, \quad (A8)
\]

\[
S_{ij} = \frac{1}{2} \begin{pmatrix}
0 & 0 & \partial_x \Pi \\
0 & 0 & \partial_y \Pi \\
\partial_x \Pi & \partial_y \Pi & 0
\end{pmatrix}, \quad V_{ij} = \frac{1}{2} \begin{pmatrix}
0 & 0 & \partial_x \Pi \\
0 & 0 & \partial_y \Pi \\
-\partial_x \Pi & -\partial_y \Pi & 0
\end{pmatrix}. \quad (A9)
\]

*c. Autocorrelations*

Although not needed for closure of the turbulent transport terms for momentum and heat, it is possible to compute the autocorrelations (or variances) of velocity and temperature. They can be used for model validation (see section 6b). The autocorrelation terms are often measured in the field or obtained in idealistic situations by large eddy simulations or direct numerical simulations. For three closure procedures, these autocorrelators can be written as
where the empirical parameters $E_1, \ldots, E_4$ are given in Table A1. Exact expressions for these parameters are given in the appendix sections d–f.

It can be easily seen that (A10–A12) are consistent with the definition of turbulent kinetic energy $k$ [see Eq. (21)]. This allows us to change parameterizations and carry out sensitivity studies with these formulas:

$$c_{\mu} = \frac{s_0 + s_1 \alpha_{\mu} + s_2 \alpha_{\mu} + s_3 \alpha_{\mu} + t_0 \alpha_{\mu}}{1 + t_1 \alpha_{\mu} + t_2 \alpha_{\mu} + t_3 \alpha_{\mu} + t_4 \alpha_{\mu}}$$

$$c_{\mu}' = \frac{s_0' + s_1' \alpha_{\mu} + s_2' \alpha_{\mu} + s_3' \alpha_{\mu} + t_0' \alpha_{\mu}}{1 + t_1' \alpha_{\mu} + t_2' \alpha_{\mu} + t_3' \alpha_{\mu} + t_4' \alpha_{\mu}}$$

Here the parameters are defined as follows:

**Table A1. Parameters for calculating the variances $\langle \tilde{u}^2 \rangle$, $\langle \tilde{v}^2 \rangle$, $\langle \tilde{w}^2 \rangle$, and $\langle \tilde{T}^2 \rangle$.**

<table>
<thead>
<tr>
<th>Model</th>
<th>$E_1$</th>
<th>$E_2$</th>
<th>$E_3$</th>
<th>$E_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>KC</td>
<td>0.224</td>
<td>2.0</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>RH</td>
<td>0.185</td>
<td>1.6</td>
<td>0.8</td>
<td>0.556</td>
</tr>
<tr>
<td>CA</td>
<td>0.160</td>
<td>1.093</td>
<td>0.027</td>
<td>0.0</td>
</tr>
<tr>
<td>CB</td>
<td>0.135</td>
<td>1.362</td>
<td>0.033</td>
<td>0.0</td>
</tr>
</tbody>
</table>

\[
\left\langle \tilde{u}^2 \right\rangle = \frac{2}{3} k + E_1 \left( \frac{k E_2 v_1 (\partial u / \partial x)^2}{1 + E_3 \left( \frac{P}{e} + \frac{B}{e} - 1 \right)} - E_1 v_1 (\partial u / \partial x)^2 - B \right)
\]

\[
\left\langle \tilde{v}^2 \right\rangle = \frac{2}{3} k + E_1 \left( \frac{k - E_1 v_1 (\partial u / \partial x)^2 + E_2 v_1 (\partial u / \partial x)^2 - B}{1 + E_3 \left( \frac{P}{e} + \frac{B}{e} - 1 \right)} \right)
\]

\[
\left\langle \tilde{w}^2 \right\rangle = \frac{2}{3} k - E_1 \left( \frac{k (E_2 - E_1) v_1 (\partial u / \partial x)^2 + (E_2 - E_1) v_1 (\partial u / \partial x)^2 - 2B}{1 + E_3 \left( \frac{P}{e} + \frac{B}{e} - 1 \right)} \right)
\]

\[
\left\langle \tilde{T}^2 \right\rangle = \frac{k}{e} v_1^2 \left( \frac{\partial T}{\partial \bar{T}} \right)^2
\]

It can be easily seen that (A10–A12) are consistent with the definition of turbulent kinetic energy $k$ [see Eq. (21)]. This allows us to change parameterizations and carry out sensitivity studies with these formulas:

\[
s_0 = \frac{4 A_1}{B_1} (1 - 3 C_1)
\]

\[
s_1 = 16 \frac{A_1 A_2}{B_1^3} \left[ (1 - 3 C_1) [3 B_2 (1 - C_3) + 12 A_1] - 3 [4 A_1 + 3 A_2 (1 - C_3)] \right]
\]

\[
t_0 = \frac{A_0}{B_1}
\]

\[
t_1 = 12 \frac{A_2}{B_1} [B_2 (1 - C_3) + 7 A_1]
\]

\[
t_2 = 24 \frac{A_2}{B_1^2}
\]

\[
t_3 = 288 \frac{A_1 A_3}{B_1^4} [-3 A_2 (1 - C_2) + B_2 (1 - C_3)]
\]

\[
t_4 = 432 \frac{A_1 A_2^2}{B_1^4} [B_2 (1 - C_3) + 4 A_1]
\]

The parameters $A_1, A_2, B_1, B_2, C_1, C_2$, and $C_3$, are taken from Kantha and Clayson (1994) and relate to the parameters given in Table 1 as follows:

\[
A_1 = \frac{B_1}{6 c_1} = 0.92, \quad A_2 = \frac{B_1}{6 c_{1T}} = 0.74,
\]

\[
B_1 = 16.6, \quad B_2 = 0.5 B_{c_e}, c_e = 10.1,
\]

\[
C_1 = \frac{1}{3} \left( 1 - \frac{1}{B_1^3} A_1 - \frac{6 A_2}{B_1} \right) \approx 0.008,
\]

\[
C_2 = c_{2T}, \quad C_3 = c_{3T}.
\]
e. Exact form of the Rodi (1980) and Hossain (1980) stability functions

As already mentioned, the stability functions of Rodi (1980) and Hossain (1980) in the version of Burchard and Baumert (1995) are implicit and therefore require numerical methods for solution. First of all, the largest solution of the following fifth-order equation has to be found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need numerical methods for solution. First of all, the largest solution of the following fifth-order equation has to be found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found. We apply a simple Newton iteration, and need less than ten iterations in order to receive the solution found.

\[

\left( \frac{P + B}{e} \right)^5 + k_1 \left( \frac{P + B}{e} \right)^4 + k_2 \left( \frac{P + B}{e} \right)^3 + k_3 \left( \frac{P + B}{e} \right)^2 + k_4 \left( \frac{P + B}{e} \right) + k_5 = 0 \tag{A19}

\]

with the coefficients

\[
k_1 = 2a_i + 2(2a_i + a_{10} \alpha_N),
\]

\[
k_2 = 4a_i(a_i + a_{10} \alpha_N) + 4a_i(2a_i + a_{10} \alpha_N) + a_i^2 + \frac{8}{3} a_i(1 - a_i) + \frac{2}{3} (1 - a_i) a_i \alpha_M,
\]

\[
k_3 = \frac{16}{3} a_i(1 - a_i) + a_i \alpha_N + 4a_i(2a_i + a_{10} \alpha_N) \alpha_N - \frac{4}{3} a_i(1 - a_i) + a_i \alpha_M
\]

\[
+ 8a_i a_i(2a_i + a_{10} \alpha_N) + 2a_i^2(2a_i + a_{10} \alpha_N),
\]

\[
k_4 = \frac{16}{3} a_i a_i(1 - a_i) + a_i \alpha_N + 4a_i a_i(2a_i + a_{10} \alpha_N) \alpha_N
\]

\[
- \frac{8}{3} a_i(1 - a_i) + a_i \alpha_N + 4a_i(2a_i + a_{10} \alpha_N)
\]

\[
+ \frac{8}{3} a_i a_i a_i \alpha_N + 4a_i^2(2a_i + a_{10} \alpha_N)
\]

\[
- \frac{8}{3} (c_1 - 1) \left( \frac{1}{4} \alpha_M(1 - a_i) - \frac{1}{2} \alpha_N \right)
\]

\[
\]
Finally, these parameters can be used for calculating the stability functions $c_\mu$ and $c'_\mu$:

$$c_\mu = \frac{1 - c_2}{c_1 + \left\{ \frac{P}{\epsilon} + \frac{G}{\epsilon} - 1 \right\}} \frac{A}{D} \langle \tilde{\omega}^2 \rangle,$$

$$c'_\mu = \frac{A}{c_{17} + \left\{ \frac{P}{\epsilon} + \frac{G}{\epsilon} - 1 \right\}} \langle \tilde{\omega}^2 \rangle.$$

(A27) (A28)

The coefficients for calculating the autocorrelators in Eqs. (A10)–(A12) are given as

$$E_1 = \frac{2}{3} \left( 1 - c_2 \right), \quad E_2 = \frac{2}{3} \left( 1 - c_2 \right),$$

$$E_3 = \frac{1 - c_2}{1 - c_3}, \quad E_4 = \frac{1}{c_1}.$$

(A29)

f. Exact form of the Canuto et al. (2001) stability functions

Only for version A of the Canuto et al. (2001) stability functions, the exact form is given here:

$$c_\mu = \frac{s_0 + s_1 \alpha_\omega + s_2 \alpha_M}{1 + t_1 \alpha_\omega + t_2 \alpha_M + t_3 \alpha_\omega^2 + t_4 \alpha_M^2 + t_5 \alpha_{\omega M}^2},$$

$$c'_\mu = \frac{s_0 + s_1 \alpha_\omega + s_2 \alpha_M}{1 + t_1 \alpha_\omega + t_2 \alpha_M + t_3 \alpha_\omega^2 + t_4 \alpha_M^2 + t_5 \alpha_{\omega M}^2},$$

(A30) (A31)

where

$$s_0 = 1.5L_1L_3^2 \frac{L_2}{t_0},$$

$$s_1 = \left[ -L_4(l_6 + l_7) + 2L_4l_5 \left( L_1 - \frac{1}{3} L_2 - L_3 \right) \right. \left. + 1.5L_1L_4 \right] \frac{8}{t_0},$$

$$s_2 = 2L_2 \frac{2}{t_0}, \quad s_4 = 2L_2 \frac{2}{t_0}, \quad s_5 = 2L_4 \frac{8}{t_0},$$

$$s_6 = \left[ \frac{2}{3} L_5(3L_3^2 - L_2^2) - 0.5L_5 L_1(3L_3 - L_2) \right. \left. + 0.75L_1(L_6 - L_5) \right] \frac{8}{t_0}.$$

(A32)

$$t_0 = 3L_3^5, \quad t_1 = L_4(7L_4 + 3L_6) \frac{4}{t_0},$$

$$t_2 = [L_4(3L_3^2 - L_2^2) - 0.75(L_5^2 - L_3^2)] \frac{4}{t_0},$$

$$t_3 = L_4(4L_4 + 3L_6) \frac{16}{t_0},$$

$$t_4 = [L_4(L_5^2 + 3L_5L_7 - L_7(L_2^2 - L_3^2)) + L_5L_6(3L_3^2 - L_2^2)] \frac{16}{t_0},$$

$$t_5 = 0.25(L_2^2 - 3L_3)(L_6^2 - L_3) \frac{16}{t_0}.$$

(A33)

with

$$L_1 = \frac{4}{15} c_1, \quad L_2 = \frac{1 - c_2}{2c_1}, \quad L_3 = \frac{1 - c_2 + c_3}{2c_1},$$

$$L_4 = \frac{c_3 - 1}{2c_1}, \quad L_5 = 2c_{17}, \quad L_6 = 1 - c_{27},$$

$$L_7 = 1 - \frac{5}{3} c_{27}, \quad L_8 = \frac{1}{3} c_{17}.$$

(A34)

It should be noted that $c_{17} = \frac{9}{5} c_{27}$.

The coefficients for calculating the autocorrelators in equations (A10)–(A12) are given as

$$E_1 = \frac{4}{3} L_4, \quad E_2 = \frac{1}{2} \frac{L_2 + 3L_4}{L_4}, \quad E_3 = \frac{L_2}{L_4},$$

$$E_4 = 0.$$

(A35)

g. Exact equations for $k$ and $\varepsilon$

The turbulent kinetic energy $k$, defined as the kinetic energy per unit mass of the velocity fluctuations is defined as

$$k = \frac{1}{2} \langle \tilde{\omega}^2 \rangle,$$

(A36)

(the unit is usually J kg$^{-1}$). A transport equation for $k$ can be derived directly from the exact transport equation for the Reynolds stresses (see, e.g., Sander 1998):

$$\partial_t \tilde{\omega} + \tilde{\nabla}_\omega \left( \tilde{\nabla} \tilde{\omega} + \left\{ \frac{1}{2} \tilde{\nabla}_\tilde{\omega} \right\} - \tilde{\nabla}_\tilde{\omega} \right) + \frac{1}{\rho_0} \left( \frac{\tilde{\omega}}{\rho_0} \right)$$

$$= -\langle \tilde{\nabla}_\omega \tilde{\nabla} \rangle \tilde{\nabla} - \frac{g}{\rho_0} \langle \tilde{\nabla}_\omega \tilde{\rho} \rangle - \nu (\tilde{\nabla} \tilde{\omega})^2.$$

(A37)

For the dissipation rate,

$$\varepsilon = \nu (\tilde{\nabla} \tilde{\omega})^2$$

(A38)
(the unit is usually $\text{W kg}^{-1}$), which appears as a sink on the left-hand side of the $k$ equation, an exact equation can be derived as well:

$$
\partial_t e + \partial_i \left( \bar{u}_i e + \langle \bar{u}_i \partial_j (\bar{u}_j) \rangle^2 \right) - \nu \partial_i \partial_j e + 2 \nu \frac{g}{\rho_0} \langle \partial_i \bar{u}_j \partial_j \bar{u}_i \rangle
$$

$P_t$ $B_i$ $e_i$ $e$

$$
= -2 \nu \partial_i \left( \langle \partial_j \bar{u}_i \partial_j \bar{u}_i \rangle \right) - 2 \nu \frac{g}{\rho_0} \langle \partial_i \bar{u}_j \partial_j \bar{u}_i \rangle
$$

It is evident that both equations (A37) and (A39), are not affected by Coriolis rotation and that pressure fluctuations do not act as sources or sinks for $k$ and $e$, but only transport these quantities as advective or diffusive transports. The right-hand side of the transport equation for $k$ can be left unchanged; however, the right-hand side of the $e$ equation needs some drastic empirical assumptions to be closed. In principle, it is assumed that the sources and sinks of $e$ (after scaling them with the turbulent timescale $\kappa e$) are proportional to those in the $k$ equation [see Eq. (28)]. The empirical coefficients $c_{e1}$, $c_{e2}$, and $c_{e3}$ are then derived from laboratory experiments (freely decaying grid turbulence for $c_{e2}$) and the log-law ($c_{e3}$, see Rodi 1980). The meaning of $c_{e3}$ has first been discussed in detail by Burchard and Baumert (1995) and is further investigated in this paper (see section 5).

### REFERENCES


