✓

25555 990

1286755

(5918675)

All rights reserved

INFORMATION TO ALL USERS

The quality of this reproduction is dependent upon the quality of the copy submitted.

In the unlikely event that the author did not send a complete manuscript and there are missing pages, these will be noted. Also, if material had to be removed, a note will indicate the deletion.

Published by ProQuest LLC (2017). Copyright of the Dissertation is held by the Author.

All rights reserved.

This work is protected against unauthorized copying under Title 17, United States Code
Microform Edition © ProQuest LLC.

ProQuest LLC.
789 East Eisenhower Parkway
P.O. Box 1346
Ann Arbor, MI 48106 – 1346

UNIVERSITY OF SURREY
Department of Mechanical Engineering

MODELLING TURBULENT SHEARED CONVECTION

by
A.R. Brown

A dissertation submitted for the degree of Doctor of Philosophy

1995

Summary

Large-eddy simulations of the atmospheric boundary layer have been performed over a range of stabilities between neutral and free convective conditions. The variation of various non-dimensionalized turbulence statistics over this stability range is presented and the results are compared with observations where possible. The robustness of the model results is also assessed by comparing those from high and low resolution simulations, and by reference to a number of additional sensitivity tests.

The simulation results for the variation with stability of the mean wind and temperature profiles and various similarity coefficients are presented. The large-eddy model datasets are then used to evaluate critically the performance of a number of simple closure schemes suitable for use in boundary layer parametrizations in large-scale weather forecasting and climate prediction models. The potential significance of the shortcomings of the simplest mixing length schemes is discussed, and an assessment is made of the types of closure most likely to give a significant improvement in performance without an excessive computational overhead.

Results are also presented from large-eddy simulations of the baroclinic boundary layer. The effects of the shear in the geostrophic wind on scaled turbulence statistics and the mean wind profiles are discussed. It is shown that this shear does not lead to significant degradation of the performance of two simple closure models, in either neutral or convective conditions.

Finally simulation results for the entrainment flux at the top of the boundary layer are presented. A parametrization of this flux is developed, based on the boundary layer root mean square vertical velocity.

Acknowledgements

First I must thank my supervisors, Prof. Ian Castro of the University of Surrey, and Prof. Paul Mason of the Meteorological Office. Their advice and enthusiasm has been much appreciated.

I would also like to thank friends and colleagues at the Meteorological Office who have helped in many ways. They include Mike Gray, Fiona Hower, Mike Hobson, Adrian Lock, Malcolm MacVean, Roderick Smith and Nigel Wood, and special thanks are due to Alan Grant whose patient help throughout has been much appreciated.

The large-eddy model used in this thesis has been developed in the Atmospheric Processes Research Branch of the Meteorological Office over a number of years. Although various diagnostics were added by the author for the present study, the coding of the basic model is not claimed as part of this dissertation.

Contents

1	Introduction	1
1.1	The atmospheric boundary layer	1
1.2	Observations of boundary layer structure	2
1.3	Theoretical models	8
1.4	Laboratory studies	11
1.5	Numerical modelling studies	12
1.6	Parametrization of the convective boundary layer	15
1.A	Annex to Chapter 1 : Ekman pumping	17
2	Large-eddy simulation of the convective boundary layer	20
2.1	The large-eddy model	20
2.2	Energy Transfers in LES	26
2.3	Simulations performed	31
2.3.1	Initial conditions and the inertial oscillation	32

2.3.2	Choice of domain	33
2.3.3	Lid runs	34
2.3.4	Inversion runs	35
2.A	Appendices to Chapter 2	38
2.A.1	New diffusion scheme	38
2.A.2	TVD advection scheme	40
3	Turbulent structure of the CBL	42
3.1	Preliminary simulations	42
3.1.1	Neutral simulations	43
3.1.2	Free convective simulations	50
3.1.3	Summary to Section 3.1	57
3.2	Simulations in the mixed shear and buoyancy regime	58
3.3	Flow fields	61
3.4	Turbulence statistics	67
3.4.1	Vertical velocity variance	68
3.4.2	Horizontal velocity variances	72
3.4.3	Temperature variance	75
3.4.4	Skewness	76

3.4.5	Dissipation length scale	78
3.4.6	Non-dimensional gradients	79
3.5	Summary	84
4	Mean structure of the CBL and its parametrization	85
4.1	Variation of mean wind profiles with stability	86
4.2	Variation of temperature profiles with stability	92
4.3	Comparison of LES and closure model results	95
4.4	CBL parametrization : mixing length models	98
4.4.1	Performance in neutral conditions	99
4.4.2	Performance in convective conditions	102
4.5	CBL parametrization : TKE models	107
4.6	CBL parametrization : Non-local models	110
4.6.1	Non-local TKE models	111
4.6.2	Specified viscosity profiles	116
4.6.3	Transilient turbulence models	121
4.7	Interaction of different parametrization schemes	122
4.7.1	Local boundary layer – convection scheme interaction	122
4.8	Summary	129

4.A	Appendices to Chapter 4	130
4.A.1	Sensitivity of surface stress to roughness length	130
4.A.2	Sensitivity of surface stress to boundary layer depth	132
5	The influence of baroclinicity on CBL turbulence	135
5.1	The thermal wind equations	136
5.2	Possible parametrization problems	137
5.3	LES of the baroclinic boundary layer	137
5.4	Mean fields	142
5.4.1	Neutral results	142
5.4.2	Convective results	145
5.4.3	Discussion	150
5.5	Turbulence statistics	151
5.6	Summary	156
6	Entrainment	157
6.1	Introduction	157
6.2	Mechanisms and models	158
6.3	LES of entrainment	159
6.3.1	Convective	160

6.3.2	Effects of shear	166
6.4	Parametrization in a large-scale model	170
6.5	Summary	175
7	Conclusions	177
	References	181

Notation

The notation used is hopefully fairly standard and in general will be introduced when it is first encountered. Cartesian ($x_1 = x$, $x_2 = y$, $x_3 = z$) coordinates are used, with the z direction normal to the surface (i.e. parallel to gravity). The x direction is variously aligned with the model x -axis, the geostrophic wind, the surface stress and the mean boundary layer wind, as described in the text. The velocity vector, $\mathbf{u}$, has components ($u_1 = u$, $u_2 = v$, $u_3 = w$). Angled brackets indicate an average (over the horizontal domain and time for the large-eddy model results), while primes denote perturbation quantities. The subscript zero is used to indicate a surface value.

Note that the stresses and energies considered are kinematic quantities i.e. units of m^2s^{-2} (no multiplication by density, $\rho \simeq 1.2 \text{ kgm}^{-3}$). Similarly the vertical flux of potential temperature ($\langle w'\theta' \rangle$) is referred to as the heat flux: the true flux of energy is equal to this quantity multiplied by (ρC_p) , where C_p ($\simeq 1005 \text{ Jkg}^{-1}\text{K}^{-1}$) is the heat capacity of air.

In the description of the model in Chapter 2, overbars are used to denote resolved quantities. All large-eddy model turbulence statistics presented (e.g. variances and fluxes) are total quantities (i.e. resolved plus subgrid estimate), unless otherwise stated.

The abbreviations CBL, LES, NWP and TKE stand for convective boundary layer, large-eddy simulation, numerical weather prediction and turbulent kinetic energy respectively. Note that CBL will often be used loosely to cover all boundary layers between neutral and free convective conditions.

Chapter 1

Introduction

1.1 The atmospheric boundary layer

The atmospheric boundary layer can be loosely defined as that part of the atmosphere which is directly influenced by the Earth's surface. Its depth might be only a few tens of metres in the stable nocturnal boundary layer, but can be a kilometre or more in convective conditions on a summer's day. Turbulence in the boundary layer transports momentum, heat and moisture and an understanding of the relevant processes is crucial, both for local forecasting and in devising a parametrization which can represent these processes which cannot be resolved in a large-scale weather or climate prediction model.

This work will concentrate on the unstable boundary layer in which the surface heat flux is upwards, and will look at changes in the flow structures and turbulence statistics as the stability of the boundary layer is changed. On the one hand there is free convection, conditions which are often approached over land, in which the boundary layer is exclusively driven by buoyancy. At the other end of the scale there are near neutral conditions, most commonly observed in strong-wind conditions over the sea, when the input to turbulent kinetic energy through buoyancy is small compared to that generated through shear production. Significant changes in eddy structure are observed across the

CHAPTER 1: INTRODUCTION

intermediate regime where both buoyancy and shear production are important. In particular, there is a tendency for the convection to become organized into bands, often leading to the formation of cloud streets which are visible on satellite imagery and may extend for hundreds of kilometres.

This is primarily a modelling study, using large-eddy simulation to obtain turbulence datasets for analysis. This method is relatively cheap and convenient, but the use of model rather than actual field data needs to be justified. In this chapter various field studies are reviewed, highlighting common features and deficiencies of the results. Earlier numerical modelling studies are also considered, along with two other possible sources of data, namely laboratory experiments and theoretical models. It is stressed that these different methods of acquiring data are complementary and efforts will be made to compare model results with published data wherever possible.

1.2 Observations of boundary layer structure

Woodcock (1940) and Priestley (1957) studied the flight characteristics of herring gulls, as a function of wind speed and sea-air temperature difference. In this way, the behaviour of the gulls was shown to depend on the atmospheric stability, and was related to the subcloud-layer eddy structure. In near neutral conditions (high wind speed and/or small sea-air temperature difference) soaring was not observed, whilst soaring was observed in more unstable conditions (reduced wind speed and/or increased sea-air temperature difference). Within the 'soaring regime', linear soaring was observed in cases only moderately unstable, and circular soaring in the more unstable cases. In some cases linear and circular soaring were observed simultaneously, suggesting that the eddy structures responsible could coexist in certain conditions. Note that the existence of eddy types favouring different types of soaring is also well known to glider pilots.

Priestley measured stability through a bulk Richardson number between the surface

CHAPTER 1: INTRODUCTION

and 6.5m

$$Ri = \frac{\left(\frac{g}{\langle\theta\rangle}\right) \frac{\partial\langle\theta\rangle}{\partial z}}{\left|\frac{\partial\langle\mathbf{u}\rangle}{\partial z}\right|^2} \quad (1.1)$$

Here θ is the potential temperature, and $\mathbf{u}$ is the wind vector. It was shown that contours of constant stability, as measured by Ri , divided the regimes reasonably satisfactorily, with no soaring for $Ri \gtrsim -0.01$, circular soaring for $Ri \lesssim -0.035$ and linear and mixed soaring for intermediate Ri . Deardorff (1976) recast the results in terms of the Monin-Obukhov length, L , defined through

$$L = \frac{-u_*^3}{\kappa (g/\langle\theta\rangle) \langle w'\theta' \rangle_0} \quad (1.2)$$

where u_*^2 is the surface stress, $\langle w'\theta' \rangle_0$ is the surface heat flux and κ is the von Karman constant. Above $z = -0.6L$ it was assumed that the thermals were essentially buoyancy driven and strong and long-lived enough for soaring to occur. Soaring was therefore expected when this height was below some maximum height to which gulls are willing to ascend in flapping height in order to seek out thermals.

Note however that both Ri and L are surface layer parameters, and therefore might not be the best measures of the stability of the boundary layer as a whole. Bulk Richardson numbers can be calculated over the entire boundary layer depth, z_i , or some fraction thereof (e.g. Brown, 1980), but z_i/L is the most commonly used stability parameter in the literature, and is adopted here.

Other early studies also noted the tendency of convection to have a banded structure in certain conditions. Information about subcloud eddy structure has often been inferred from the cloud pattern, hypothesizing that cloudy areas are associated with regions of ascending air in the subcloud layer. For example, Kuettner (1959) looked at the tendency of clouds to form in a banded rather than an irregular structure, and found that this occurred in 'convective layers with higher than normal winds...'. Saunders (1964) investigated the formation of fogs resulting from the advection of cold air over relatively warm water. Although primarily interested in the conditions necessary for fog formation, the author noted that 'in moderate winds sea smoke commonly has a banded structure with the bands approximately along the wind'.

CHAPTER 1: INTRODUCTION

Many experiments have since been carried out specifically to study the eddy structures in the convective boundary layer. Satellite cloud pictures have often been used to infer information about boundary layer motions, and direct measurements have been made using instrumented aircraft and towers, and radars. The results of some of these studies are now reviewed, emphasizing the common features of the results and also looking at some of the difficulties and uncertainties involved.

The Barbados Oceanographic and Meteorological Experiment (BOMEX) was held in the summer of 1969 in the northeast trade wind region east of the island of Barbados. A dominant ridge of high pressure to the north of the measurement area resulted in suppressed convective activity with easterly winds. The boundary layers were typically 600m in depth, and the most common cloud form was cumulus humilis. Wind measurements were made at 18m, 46m and 152m from a DC-6 aircraft fitted with a fixed-vane gust probe referenced to an inertial platform. Grossman (1982) used vertical velocity as an indicator of organized motions in the lower subcloud layer and analysed spectra obtained in along- and cross-wind runs. Individual spectra obtained from runs at similar stabilities were composited to increase confidence in the spectral signatures. In the most unstable conditions, similar spectra were found in the two directions. They showed double peaks, one at wavelengths of order a few hundred metres, and one of order 1-2 km. The kilometre scale peaks were associated with convective cells, randomly orientated with respect to the mean wind. In contrast, composite spectra from runs in near neutral conditions showed the double peak in cross-wind runs while the kilometre scale peak was absent in along-wind runs. This is consistent with the elongation of the convective eddies along the wind, forming large roll vortices (also known as horizontal convective rolls) with spacing $2-3z_i$. The transition from the regime favouring cellular convection to that favouring large nearly two-dimensional rolls was not found to be clear cut, with evidence for both structures at some intermediate stabilities. This is consistent with Woodcock's (1940) observation of mixed circular and linear soaring. Grossman categorized the structures observed in BOMEX as shown in Table 1.1. Whilst the transition between different eddy structures has clearly been observed, some reservations must be expressed about the val-

CHAPTER 1: INTRODUCTION

Category	Stability	
1	$-z_i/L < 5.0$	Only roll vortex motion
2	$5.0 < -z_i/L < 7.3$	Rolls coexist with convective cells and are necessary for their maintenance; rolls dominate.
3	$7.3 < -z_i/L < 21.4$	Rolls coexist with random cells but are not necessary for their maintenance; random cells dominate.
4	$21.4 < -z_i/L < 30$	Random cells only but shear important to cell structure and morphology.
5	$-z_i/L > 30$	Random cells only; shear unimportant to cell structure and morphology.

Table 1.1: Categories of dominant eddy structure taken from BOMEX data. 1-4 were observed in BOMEX data, and the condition for category 5 was estimated using the Richardson number criterion of Priestley (1957). After Grossman (1982)

ues of z_i/L quoted. Lateral gusts were not measured, and the surface stress had to be estimated by combining data from along- and cross-wind runs. The errors which might have been introduced due to a consistent turning of the wind with height were estimated to be small, but it was suspected that the measured values of $\langle u'w' \rangle$ contained a significant heading-independent error. This conclusion was based on the high value of u_* calculated compared to that found in other experiments in the near neutral trade wind boundary layer (e.g. Pennell and LeMone, 1974). Accordingly, measured u_* values were assumed to be 80% too large, leading to a reduction in L by a factor of almost six. This does not invalidate the results, and in fact the table was shown as being broadly consistent with the results of a number of other studies. However, the need to make such corrections does give some idea of the difficulties involved in making field measurements.

The most widely studied conditions have been those in which the production of energy

CHAPTER 1: INTRODUCTION

Figure 1.1: Schematic diagram of boundary layer rolls (after Brown, 1980). h is the boundary layer depth, and λ is the wavelength.

is dominated by buoyancy. Experiments carried out in these conditions include Minnesota (Kaimal *et al.*, 1976), Ashchurch (Caughey and Palmer, 1979), AMTEX (Lenschow *et al.*, 1980) and Phoenix 78 (Young, 1988). Young found that the forms of turbulence profiles from these (and other) experiments generally showed little variation, although some differences were ascribed to different cross inversion entrainment fluxes. However, the author noted that very little observational work had been reported on the effect of the size of this downward buoyancy flux at the inversion on other turbulence statistics.

A large number of studies have also been made of boundary layer rolls, which are shown schematically in Figure 1.1. LeMone (1973) used data both from a 444m tower in Oklahoma, and from aircraft measurements over Colorado, Lake Michigan and one BOMEX flight. Observations from a fixed point can only show variations in the along-wind direction as turbulent eddies are advected past by the mean wind. Roll vortices are approximately aligned with the mean wind and LeMone noted that it could take up to an hour to sample a single wavelength. Uncertainty in the tower data was therefore primarily due to small sample size, although instrumental errors were again thought to be significant in the stability calculations. Horizontal convective rolls were identified on eight separate

CHAPTER 1: INTRODUCTION

occasions. Their aspect ratios (ratio of wavelength to layer depth) were between 2.2 and 6.5, and they were oriented between 15° left and 5° right of the inversion level geostrophic wind ¹. Values of $-z_i/L$ when rolls were observed varied between 3 and 10. These results are broadly consistent with the BOMEX results of Grossman (1982), although $-z_i/L = 10$ is in the category where random cells are expected to be the dominant structure. The variation in observed aspect ratio is indicative of the uncertainties involved, although all cases bar one had aspect ratios between 2 and 4.

Kuettner (1971) studied pictures of cloud streets taken from aircraft, satellites and spacecraft over Wisconsin, Florida, Georgia, the Gulf of St. Lawrence and the BOMEX area. He found spacings between the streets of between 2 and 8km which, using layer depths estimated from radiosonde ascents, correspond to aspect ratios of between 2 and 4. Typical conditions were almost uni-directional wind in the boundary layer, and the rolls were observed to lie within 10° of this direction. In a similar study using satellite and radiosonde data, Weston (1980) looked at 21 occurrences of cloud streets over the British Isles, and found roll aspect ratios between 2.3 and 4.7 with an average of 3.2. In 75% of the individual cases the streets were aligned within 10° of the mean wind of the convective layer. Thus the results of these studies are consistent with those mentioned earlier, although the lack of turbulent flux data prevents calculation of stability as measured by z_i/L . Walter and Overland (1984) looked at Arctic sea smoke formed over leads in the ice-covered Bering sea using satellite pictures and identified several predominant scales of motion. The use of a NOAA-P3 research aircraft enabled them to obtain some flux data and they identified rolls with aspect ratios between 2.0 and 2.6 at $-z_i/L = 1.2$. Kelly (1984) also used aircraft data, but is mentioned here as an example of a study which used Doppler radar data. Rolls of widely varying aspect ratios were observed, aligned approximately with the geostrophic wind. Kelly noted that the inability of the radars to sample the lowest third of the boundary layer due to ground obstructions was probably a significant problem, as was the fact that no allowance could be made for changes in the mean wind direction at different ranges.

¹The geostrophic wind is that required for the Coriolis force to exactly balance the large-scale pressure gradient, and is directed 90° to the left of the pressure gradient in the northern hemisphere. See Chapter 2.

CHAPTER 1: INTRODUCTION

A selection of studies which have looked at horizontal convective rolls has been discussed. More exhaustive lists of such studies can be found in Kelly (1984) and Christian and Wakimoto (1989). However, many have concentrated very much on the flow structures present, and relatively little has been published on the variation of turbulence statistics with stability. Pennell and LeMone (1974) presented some variance data from aircraft measurements in the trade-wind boundary layer at $z_i/L \simeq -1.5$, but stressed how few earlier studies had measured both mean and turbulence quantities to sufficient accuracy and vertical resolution to determine the budgets of turbulent kinetic energy and momentum. Nicholls and Readings (1979) also presented statistics measured by aircraft over the convective maritime boundary layer. They divided their runs into two classes, class A for $z_i/L < -1.5$ (average -3.9) and class B for $z_i/L > -1.5$ (average -0.9). This grouping was made due to the scatter in individual data points and enabled the authors to look at the variation in vertical profiles of mean winds and turbulent variances and fluxes with z_i/L . Data obtained by aircraft in near neutral conditions over the sea during the KONTUR experiment can be found in Grant (1986). Three flights for which $-z_i/L \leq 1$ were analyzed, and in addition, profiles were presented for one flight in more convective conditions when $-z/L \simeq 6$. Changes in the variance profiles between the near neutral cases and the more convective case were associated with the formation of boundary layer rolls in the more unstable conditions.

1.3 Theoretical models

Many authors have attempted to explain the observed boundary layer flow structures through theoretical models. These studies are generally carried out by subjecting the mean flow to a normal mode perturbation analysis. The predicted wavelength and orientation of the instability mode can then be compared to observed values. Critical mean flow parameters such as the Rayleigh number for the onset of convection can also be estimated and compared with experiment.

CHAPTER 1: INTRODUCTION

The free convective boundary layer was first modelled by Rayleigh (1916). His linearized analysis for a non-rotating fluid led to the parameter now named after him and governing the onset of convection. The three-dimensional Benard cells result from the superposition of three evenly partitioned perturbation wave trains. Later authors have refined the criterion by including more realistic boundary conditions, the effects of rotation and time dependency. See for example Krishnamurti (1975).

The neutral boundary layer has also been extensively studied. Lilly (1966) calculated the normal mode instability of the Ekman solution and identified two types of instability, consistent with the laboratory experiments with rotating fluids of Faller (1963). One was the parallel instability in which energy from the mean flow is fed into rolls via Coriolis turning. LeMone (1973) noted that the Coriolis accelerations are too small for this mode to be significant in the convective boundary layer. The other was the well known instability which results from the presence of an inflection point in one of the components of the mean wind.

The structure of the intermediate boundary layer, driven by both buoyancy and shear, is less well understood. In particular, there are two schools of thought on the mechanism responsible for the production of the horizontal convective rolls which are observed in the atmosphere. The first assumes that they result from the dynamic inflection point instability with some modification due to buoyancy, the second that they are essentially buoyancy driven and organized by wind shear.

A good summary of dynamical instability models can be found in Brown (1980). LeMone (1973) and Brummer (1985) compared their roll observations with the model of Brown (1970) and found reasonable agreement, although the model slightly underestimated roll aspect ratio and observed rolls had magnitudes around 40% greater than predicted. LeMone concluded that energy input from buoyancy was significant, and Brummer that only two of his three roll events could be explained through dynamical instability. There is a tendency in these studies to regard rolls as a distinct feature, quite separate from boundary layer turbulence. LeMone and Brummer amongst others actu-

CHAPTER 1: INTRODUCTION

ally used filtering operations to separate the 'roll scale motions' from the 'turbulence scale motions', although Brummer recognized that 'a clear gap between the turbulence scale and the roll scale is not present'.

The second mechanism assumes that the roll motions are driven by buoyancy and organized by wind shear. Kuo (1963) studied the unstable modes of parallel flow with linear shear (Couette flow), and found that longitudinal bands were the dominant form of convection for small negative values of Richardson number, while transverse waves were also excited in more unstable conditions. Kuettner (1971) considered the effects of curvature of the shear profile. This leads to a restoring force on any fluid element displaced upwards by buoyancy (in the absence of an inflection point in the wind profile) unless all elements along a horizontal line in the direction of the mean flow move upwards simultaneously. In this case no differential vorticities will result and the convection is uninhibited by restoring forces. As shear becomes progressively more important, the restoring forces will become larger and so roll vortices become increasingly dominant over convective cells. An attraction of these methods is that they explain the transition from a cellular to roll pattern, rolls being seen simply as an organized form of convection rather than as a separate phenomenon. Roll aspect ratios and orientations are also successfully predicted.

The true picture must incorporate both the dynamic and thermal instabilities to some extent. However, in the last decade, work has been performed which led Etling and Brown (1993) to comment in a comprehensive review that 'under most circumstances large roll vortices in the planetary boundary layer are driven by thermal instabilities'. The studies which led to this conclusion include theoretical work on the suppression of inflection point instability by a capping inversion (e.g. Etling and Raasch, 1987), and modelling studies of the neutral boundary layer which failed to show evidence of roll vortex motion (e.g. Mason and Thomson, 1987).

Overall, the linear models are generally successful in explaining the types of structure observed in the convective boundary layer. The insight gained into the relevant physical

CHAPTER 1: INTRODUCTION

processes is useful but, whilst the agreement with observations is reasonable, the results are insufficiently reliable to be used as the basis of a boundary layer parametrization.

1.4 Laboratory studies

Surrogate observations of boundary layer turbulence can be obtained in the laboratory, either in wind tunnel or tank experiments. Such studies are much cheaper to perform than field experiments and can be carried out in a much more controlled environment. However, generalizations of the results to atmospheric flows must be made with care as laboratory studies suffer from the problem of obtaining Reynolds' number similarity (Teunissen *et al.*, 1987). The length scales in the laboratory must be much smaller than those in the atmosphere so, given the similar values of molecular viscosity, the Reynolds' number must be much smaller and the effects of molecular viscosity relatively more important.

In spite of these reservations, results have been obtained in the laboratory which are in good agreement with those found in the atmosphere. Teunissen *et al.* (1987) showed good consistency between wind tunnel simulations of flow over an isolated low hill and field measurements on Askervein Hill in the Outer Hebrides of Scotland. Deardorff and Willis (1985) discussed how, as the laboratory model is made larger, the Reynolds' number becomes 'large' and its exact value becomes progressively less relevant. The results for scaled turbulence statistics should not then be heavily dependent on molecular properties, which is particularly desirable when, as in their case, the tank utilizes water rather than air. In fact, the results from Deardorff and Willis and the earlier study of Willis and Deardorff (1974) are consistent with atmospheric observations (Young, 1988). The tank results of Adrian *et al.* (1986) differ in some respects as they studied non-penetrative convection between fixed plates.

Laboratory studies of turbulence in shear driven mixed layers have also been used by atmospheric modellers as a surrogate for field measurements. For example, Zeman and Tennekes (1977) used results of the annular tank experiments of Kato and Phillips

CHAPTER 1: INTRODUCTION

(1969) to calibrate a parametrization of the energy budget at the inversion. However, the present author is not aware of any attempts in the laboratory to systematically study the variation of turbulence statistics with stability in conditions where both shear and buoyancy forcing are significant.

1.5 Numerical modelling studies

Numerical models can also be used to simulate the turbulent atmospheric boundary layer. Direct numerical simulation (DNS) aims to provide solutions to the full Navier-Stokes equations without a turbulence closure, but is currently restricted to relatively low Reynolds' number flows due to computer limitations. All other numerical simulation results are subject to uncertainties due to the turbulence closure problem. However there has been some success in demonstrating that the results of some of the more complex models (e.g. large-eddy and second order closure) are not unduly sensitive to the parametrization used. In many cases the results of fairly idealized studies have also been shown to be encouragingly consistent with those found in the atmosphere and in the laboratory.

The pioneering study using large-eddy simulation (LES) was carried out by Deardorff (1972a). In this technique the 'large eddies' are resolved explicitly on a numerical grid, and the effects of the smaller eddies are parametrized through a subgrid model. More details on the technique can be found in the next chapter. Deardorff's model considered a dry boundary layer driven by an imposed mean pressure gradient and surface buoyancy flux, and capped by a stress-free rigid lid which acted as an infinite strength inversion at height $z = z_i$. Periodic boundary conditions were imposed in the horizontal directions in domains of length $4z_i$ in the streamwise direction, and either $4z_i$ or $2z_i$ in the cross-stream direction. In spite of these idealizations and the low resolution of the numerical mesh (maximum $40 \times 40 \times 20$ mesh-points), simulations were successfully performed at values of $-z_i/L=0, 1.5, 4.5$ and 45 . The expected changes in flow structure were observed,

CHAPTER 1: INTRODUCTION

and various flow statistics were presented. Nicholls and Readings (1979) compared their measured flux and variance profiles with those of Deardorff and found good agreement. The results of the second order closure model of Wyngaard *et al.* (1974) were also shown to be in good agreement with their measurements.

The convective boundary layer has been shown to be particularly amenable to large-eddy simulation, due to the dominance of large thermals. Detailed studies have been carried out by Moeng (1984), Mason (1989) and Schmidt and Schumann (1989). An intercomparison study by Nieuwstadt *et al.* (1991), considered a dry inversion-capped boundary layer driven by surface heating and found that the results of four different codes were in good agreement with each other, and with the atmospheric data of Lenschow *et al.* (1980) and the laboratory data of Willis and Deardorff (1974) and Deardorff and Willis (1985).

The dry shear-driven boundary layer has also been extensively studied using LES by, amongst others, Mason and Thomson (1987, 1992), Andrn and Moeng (1993), Andrn *et al.* (1994), and Mason and Brown (1994). The Andrn *et al.* intercomparison study again showed an encouraging degree of consistency between the results of four different codes, and Mason and Brown showed that the results of a similar run were in reasonable agreement with the KONTUR data of Grant (1986). The absence of roll vortices in the neutral LES of Mason and Thomson (1987) and in the highest Reynolds' number DNS of Coleman *et al.* (1990) was cited by Etling and Brown (1993) as evidence for the importance of thermal instabilities in producing such structures in the atmosphere.

Other studies have looked at changes in boundary layer turbulence due to the combined effects of shear and buoyancy. Many have noted the observed two-dimensionality of roll vortices and have used two-dimensional models. For example, Mason and Sykes (1980, 1982) performed studies of the dry boundary layer. The first of these considered the neutral boundary layer, and the second extended the model to include a surface buoyancy flux and capping inversion. The roll structures observed in the second study were found to be in better agreement with observation, and the authors stated that observed rolls 'are

CHAPTER 1: INTRODUCTION

driven mainly by buoyancy effects and are not really related to shear instabilities of the Ekman boundary layer'. Mason (1985) considered the moist boundary layer, and modelled the formation of cloud streets. Turbulent energy and dissipation were found to be similar to those in the dry boundary layer (except close to the cloud top) and it was concluded that latent heat release has no marked influence on vortex roll development. Sykes *et al.* (1988) also used a two-dimensional model and found rather more marked effects (e.g. an increase in roll aspect ratio) due to the effects of latent heating and entrainment of warm dry air from above the cloud top.

In two-dimensional studies a certain amount of empirical tuning is required in order to find the most appropriate values for the turbulence length scale and the angle between the geostrophic wind and the computational domain. Also thermal convection is forced to have a roll-like structure, whether or not this is the preferred mode in the atmosphere. Therefore the results of some three-dimensional large-eddy simulations are now discussed.

Sykes and Henn (1989) performed three-dimensional large-eddy simulations of convection between fixed plates, and showed reasonable agreement between their results and those found in the laboratory by Adrian *et al.* (1986). The investigation was extended by moving the plates relative to one another to give a convective plane Couette flow. The authors concentrated mainly on the existence of roll structures which were observed for $-z_i/L < 9$, but also considered the variation of the variance profiles with stability. Tests were also carried out which revealed that it was possible to produce reasonable results for velocity variances and aspect ratio in the roll regime, using a two-dimensional model with appropriately chosen length-scale and domain orientation. However, it was also possible to produce misleading results and, computational resources permitting, the use of three-dimensional models is to be preferred.

Chlond (1992) used a model which included cloud physics, radiative cloud cooling and the effects of large-scale subsidence. The model was applied to conditions in which cloud street formation was observed off Greenland, and encouraging consistency with the observed cloud pattern was found.

CHAPTER 1: INTRODUCTION

Others authors have used simpler models to perform series of runs in different conditions (e.g. the dry LES studies of Mason (1992), and Moeng and Sullivan (1994)). Moeng and Sullivan (1994) described high resolution studies of inversion capped boundary layers in neutral conditions ($-z_i/L = 0$), in highly convective conditions ($-z_i/L = 18$) and in the intermediate regime where both buoyancy and shear are important ($-z_i/L = 1.4$ and 1.6). Various turbulence statistics including the turbulent kinetic energy budget were considered. Interestingly, the runs in the intermediate regime showed similar turbulence statistics although one showed an organized roll structure while the other did not. This is consistent with the rolls being simply an organized form of convection rather than separate additional features.

1.6 Parametrization of the convective boundary layer

Large-scale numerical weather prediction (NWP) and climate prediction models typically have horizontal mesh-spacings of order tens or hundreds of kilometres, and vertical spacings of order a hundred metres. They are therefore quite incapable of resolving the boundary layer turbulence, the effects of which must be parametrized.

As discussed by Beljaars and Betts (1992), a realistic representation of the boundary layer is important for a number of reasons. First of all, the surface fluxes affect the large-scale atmospheric budgets on a time scale of a few days. For example, in Annex 1.A at the end of this chapter, it is shown that the time scale for the filling of a low pressure system through Ekman pumping is inversely proportional to u_*^2 . Secondly, the boundary layer scheme interacts with other parts of a large-scale model. For example, incorrect prediction of boundary layer clouds will lead to errors in the fluxes predicted by the radiation scheme. Thirdly, many of the boundary layer variables are important forecast products. This is clearly the case for the 10 m wind and screen level temperature, but profiles from the entire boundary layer and values of z_i and z_i/L may also be used for other applications (e.g. dispersion modelling).

21 p 19

CHAPTER 1: INTRODUCTION

A parametrization of the convective boundary layer must adequately represent the effects of the turbulence on the mean fields across the entire stability range from conditions of free convection to pure shear flow. It has been shown that major changes in flow structure occur across this stability range, notably with the appearance of horizontal convective rolls when both shear and buoyancy forcing are important. These conditions are particularly common over the sea and as oceans cover roughly 70% of the Earth's surface, a good parametrization of the sheared convective boundary layer is obviously important. In their review article, Etling and Brown (1993) suggested that the effects of large-scale structures such as rolls cannot be adequately modelled with the simple diffusion coefficient closures which are often used in large-scale models and advocated a separate parametrization of these features. However, if rolls are believed to be no more than an organized form of convection, then it is not clear that their existence should have a major effect on turbulence statistics. This would suggest that the performance of diffusion coefficient models, although potentially poor in all convective conditions, is unlikely to be significantly worsened by the presence of rolls.

In order to evaluate critically the performance of turbulence parametrizations, high quality turbulence data is required across the whole range of boundary layer stability. As noted in Section 1.2, field data from the very unstable boundary layer is readily available, although even here considerable uncertainties remain over the effects of cross-inversion entrainment (Young, 1988). Additional data from laboratory and modelling studies is also available.

Although many field studies have looked at horizontal convective rolls, detailed measurements showing the changes in the turbulence statistics with stability are in short supply. The studies of Pennell and LeMone (1974), Nicholls and Readings (1979) and Grant (1986) are useful in this respect, but more data is needed. Data on the variation of geostrophic drag coefficients with stability is also available (e.g. from the Wangara experiment described in Clarke *et al.*, 1971), but the results tend to be very scattered (see e.g. Arya, 1975). Etling and Brown (1993) noted that relatively few three-dimensional modelling studies of the sheared convective boundary layer have been carried out, and

CHAPTER 1: INTRODUCTION

advocated the use of large-eddy models to produce turbulence datasets. The model data could then be used, in conjunction with such field observations as are available, to evaluate boundary layer parametrization schemes.

This is the approach taken in the present study. Although large-eddy models have to use a turbulence closure ('the subgrid model'), the results from a number of previously published studies have been shown to be in good agreement with observations. They can provide spatial and temporal resolution far greater than any experiment and provide a self-consistent set across the whole stability range. The simulations are almost invariably idealized (those in this study, for example, will be dry), but this can be of use in isolating the effects of different physical processes such as entrainment. Also there is no danger of contamination due to unknown external influences such as mesoscale and orographic forcing which may be important in the field. A discussion of the large-eddy model used in this study can be found in the next chapter.

It should be noted that the use of model rather than field data to assess the value of various parametrizations is not new. For example, Moeng and Wyngaard (1986) used LES to obtain data on pressure-scalar covariances which are almost impossible to measure in the field. Similarly, Andrn and Moeng (1993) used LES simulations of the neutral boundary layer to evaluate some commonly used closures schemes for the dissipation and pressure redistribution terms appearing in second-order single-point closure formulations.

1.A Annex to Chapter 1 : Ekman pumping

This annex considers a boundary layer which is driven by a large-scale pressure gradient which is constant with height. The pressure gradient can be related to a geostrophic wind (speed G) which is the wind for which the Coriolis force would exactly balance the pressure gradient force (see Chapter 2). The average boundary layer flow is backed (rotated anticlockwise) relative to the geostrophic wind due to the turbulent stresses. By taking a coordinate system with the x -axis aligned with the geostrophic wind and integrating

CHAPTER 1: INTRODUCTION

the equations of motion neglecting the advection terms and assuming stationarity and no fluxes at z_i , an expression can be obtained for v_m , the boundary layer average cross-isobar wind speed

$$v_m = \left(\frac{u_*^2}{f z_i} \right) \cos \alpha_0 \quad (1.3)$$

Here f is the Coriolis parameter and α_0 is the surface ageostrophic angle. Using this result and the continuity equation for an incompressible fluid (neglecting variations in the x -direction), the following estimate of the mean vertical velocity at the top of the boundary layer can be obtained

$$w_i = - \int_0^{z_i} \left(\frac{\partial v}{\partial y} \right) dz = - \frac{\partial}{\partial y} \int_0^{z_i} v dz = - \frac{\partial}{\partial y} \left(\frac{u_*^2 \cos \alpha_0}{f} \right) \quad (1.4)$$

For a low pressure region there will be near surface convergence and ascent which will tend to fill the depression (in the absence of large-scale divergence aloft). The ‘spin-down time’ can be estimated using the vorticity equation which, for synoptic scale motions, can be written approximately as

$$\frac{d\zeta}{dt} = f \frac{\partial w}{\partial z} \quad (1.5)$$

where ζ is the vorticity, or strictly its vertical component (Holton, 1979). Integrating from the top of the boundary layer ($z = z_i$) to the tropopause ($z = H$), assuming that $w = 0$ at $z = H$, $H \gg z_i$ and $\zeta \simeq \zeta_g$ (where ζ_g is the geostrophic vorticity), and substituting for w ; from (1.4) leads to

$$\frac{d\zeta_g}{dt} = \frac{1}{H} \frac{\partial (u_*^2 \cos \alpha)}{\partial y} \quad (1.6)$$

To relate the surface stress and ageostrophic angle to the geostrophic wind requires a knowledge of the Rossby similarity coefficients, A and B . However, it is possible to proceed further by noting that observed values of α_0 in mid-latitudes are rarely outside the range $0^\circ - 40^\circ$, and that a variation in angle between these limits leads to only a 25% change in $\cos \alpha_0$. In contrast, values of u_*^2 are observed to vary much more markedly and so, to a first approximation, $\cos \alpha_0$ can be treated as a constant. Substituting $u_* = C_g G$ and assuming that C_g , the geostrophic drag coefficient, is constant leads to

$\frac{d\zeta_g}{dt} = \frac{\partial}{\partial x} \left(\frac{GC_g^2 \cos \alpha_0}{H} \right) = -\zeta_g \left(\frac{GC_g^2 \cos \alpha_0}{H} \right)$

CHAPTER 1: INTRODUCTION

discrepancy
 $t_s \propto \frac{1}{u_a}$
inversely proportional to $1/u_a$!!

i.e. t_{sd} , the spin-down time scale is given by

$$t_{sd} = \left(\frac{H}{G C_g^2 \cos \alpha_0} \right) = \frac{HG}{u_*^2 \cos \alpha} \quad (1.8)$$

Using realistic values of $H = 10000$ m, $G = 10 \text{ ms}^{-1}$, $C_g^2 = 0.002$ and $\alpha_0 = 25^\circ$, gives a time scale of around 6 days which is of the correct order of magnitude. Note that for given geostrophic wind, the time scale is proportional to $1/(u_*^2 \cos \alpha_0)$. Hence accurate prediction of the surface stress by the boundary layer scheme is important for large-scale development.

?

Chapter 2

Large-eddy simulation of the convective boundary layer

This chapter gives details of the large-eddy model which has been used to simulate the dry convective boundary layer in this study. A broad outline is given of the types of simulation performed, and various modelling issues such as the choice of the most suitable domain size, are discussed. Detailed descriptions of some of the simulations, the results of which are used repeatedly throughout the remainder of this thesis, are given in Sections 2.3.3 and 2.3.4.

2.1 The large-eddy model

The spectra of atmospheric turbulence can span several decades in wavenumber space. Large eddies in a convective boundary layer scale on the boundary layer depth and are typically of size $O(1 \text{ km})$. However the smallest turbulence scale, the Kolmogorov microscale $\eta = (\nu_{mol}^3/\epsilon)^{1/4}$ (where ν_{mol} is the molecular viscosity of air and ϵ is the dissipation rate) is of $O(1 \text{ mm})$ in the atmosphere. Direct simulation of all scales simultaneously is thus impossible and likely to remain so for the foreseeable future. However, as the length

CHAPTER 2: LES OF THE CBL

scales for production (l_{prod}) and molecular dissipation ($l_{dis} \simeq \eta$) differ by several orders of magnitude, there is an inertial subrange for $l_{prod} \gg l \gg l_{dis}$ which is characterized only by l and ϵ . In large-eddy simulation (LES) a filter is applied, separating those motions which are going to be resolved from those which will have to be parametrized. Ideally this filter lies in the inertial subrange, in which case the subgrid parametrization is fairly simple and rationally based. In practice the model may not resolve into the inertial subrange but, as the resolved large eddies carry most of the turbulence energy and fluxes, the technique remains useful.

Accordingly a filter operation is applied to the Navier-Stokes equations and a solution is sought to the following continuous equations for the resolved velocity, $(\bar{u}_1, \bar{u}_2, \bar{u}_3) = (\bar{u}, \bar{v}, \bar{w})$, and potential temperature, $\bar{\theta}$, in a Boussinesq fluid with reference temperature θ_r and density ρ_r . Einstein summation notation is used, and the overbars denote resolved quantities.

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho_r} \frac{\partial p}{\partial x_i} - \frac{1}{\rho_r} \frac{\partial P_0}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) (\bar{\theta} - \theta_r) - \frac{\partial \tau_{ij}}{\partial x_j} - 2\epsilon_{ijk} \Omega_j \bar{u}_k \quad (2.1)$$

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (2.2)$$

$$\frac{\partial \bar{\theta}}{\partial t} + \frac{\partial (\bar{u}_i \bar{\theta})}{\partial x_i} = -\frac{\partial H_i}{\partial x_i} \quad (2.3)$$

Note that effects of molecular viscosity on the resolved fields are neglected. This infinite Reynolds' number approximation is valid because of the scale separation which exists between the filter scale and l_{dis} . The last term in Equation (2.1) is the Coriolis term. p is the pressure and $\partial P_0 / \partial x_i$ is an imposed pressure gradient. This can be related to an imposed geostrophic wind, $\mathbf{G}$, which is the wind for which the Coriolis force would exactly balance the pressure gradient force. It has magnitude G and components u_g and v_g in the x - and y -directions given by

$$u_g = -\frac{1}{f\rho_r} \frac{\partial P_0}{\partial y} \quad (2.4)$$

$$v_g = +\frac{1}{f\rho_r} \frac{\partial P_0}{\partial x} \quad (2.5)$$

CHAPTER 2: LES OF THE CBL

where f is the Coriolis parameter which has a value of 10^{-4}s^{-1} at 45°N . Note that in this Boussinesq framework it will sometimes be useful to consider buoyancy, $\bar{b} = \left(\frac{g}{\theta_r}\right) \bar{\theta}$, rather than potential temperature. Also, mention of density is suppressed (equivalent to choosing units of mass so that the density is unity), so that both energy and stress have units of $(\text{m}^2\text{s}^{-2})$.

τ_{ij} , the subgrid stress tensor, and H_i , the subgrid heat flux, have to be parametrized. This is usually done deterministically, often using the Smagorinsky model (Smagorinsky, 1963) which is essentially a 3-dimensional mixing length closure

$$\tau_{ij} = -\nu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \quad (2.6)$$

$$H_i = -\nu_h \frac{\partial \bar{\theta}}{\partial x_i} \quad (2.7)$$

The eddy viscosity (ν) and diffusivity (ν_h) are given by:

$$\nu = \lambda^2 S f_m(Ri_p) \quad (2.8)$$

$$\nu_h = \lambda^2 S f_h(Ri_p) \quad (2.9)$$

where

$$S^2 = \frac{1}{2} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right)^2 \quad (2.10)$$

and λ is a length scale which, in the interior of the flow, has a constant value, λ_0 , which is related to the filter-scale. Stability dependence is introduced through $f_m(Ri_p)$ and $f_h(Ri_p)$ which are functions of local gradient Richardson number (calculated pointwise). For details see Brown *et al.* (1994).

Close to the surface the length scale of the subgrid motions must decrease so that λ is proportional to the distance from the wall (z). The rigid lid at the top of the domain ($z = h$) forces $w = 0$ so it is reasonable to impose a similar decrease in length scale to the top of the domain. The matching relation is written

$$\frac{1}{\lambda^2} = \frac{1}{\lambda_0^2} + \frac{1}{(\kappa z)^2} + \frac{1}{(\kappa(h-z))^2} \quad (2.11)$$

CHAPTER 2: LES OF THE CBL

where κ is the von Karman constant. This match is fairly arbitrary, but was found to give the best results by Mason and Thomson (1992). The backscatter model (see below) is also sensitive to this match, and Mason and Brown (1994) showed that approximately the correct amount of energy was backscattered when using this matching relation.

Note that the approach taken has followed Mason and Callen (1986) by considering the filter to be defined by the subgrid model, and to be independent of the finite-difference grid. Indeed, the closure model would be better termed the ‘subfilter model’ than the ‘subgrid model’, but the latter is almost invariably used and has been adopted here. The filter determines which eddies are to be resolved, and the grid is then chosen so as to be able to properly resolve those eddies. No particular value of the Smagorinsky constant ($C_s = \lambda_0/\Delta$ where Δ is a measure of the resolution) is correct in any sense. Small values will lead to finite-difference errors as the filter-scale becomes smaller than the mesh spacing. Large values, implying a mesh much finer than the filter, are fine in principle but are wasteful of computational resources. The values chosen are therefore compromises, and the use of different values for different flows results from trying to make the best use of resources in each case, rather than any fundamental association of particular values with different flow types.

The boundary conditions used are periodic in the horizontal. The lower boundary is a no-slip wall, with imposed surface heat flux (characterized by roughness lengths, $z_0 = 0.1\text{m}$ for momentum, and $z_{0t} = 0.01\text{m}$ for heat). The surface layer is considered to be in local equilibrium between the surface and each of the lowest grid points, and Monin-Obukhov similarity is applied pointwise. Provided that this is applied sufficiently close to the surface for the large-scale acceleration terms to have a negligible effect on the stress budget then this approach is justified and results will be independent of the exact height of the lowest grid points. The top boundary is a rigid lid at height h where the stress and heat flux are set to zero.

Deterministic models such as the Smagorinsky model have been used extensively and with considerable success in modelling the atmospheric boundary layer. However, Mason

and Thomson (1992) pointed out that previous simulations of the neutral static-stability boundary layer had all shown excessive shear in the semi-resolved near-wall region. They argued, following Chasnov (1991), that the subgrid model should not be deterministic as the subgrid motions are influenced but not fully determined by resolved motions. The addition of stochastic subgrid stress fluctuations to the model has the effect of transferring some energy from small to large scales, against the turbulent energy cascade (hence 'backscatter') and was shown to lead to a much more realistic simulated velocity profile. Mason and Brown (1994) performed various tests concerning the implementation of the backscatter process in the model, studying for example the effects of changing the spatial and time scales of the stochastic variations. They concluded that the proposed model of Mason and Thomson (1992) was fairly optimum, and used it to perform a high resolution simulation of the neutral boundary layer. The backscatter model was extended to include buoyancy effects by Brown *et al.* (1994). They showed in simulations of the stable boundary layer that the use of backscatter led to non-dimensional velocity and temperature gradients in much better agreement with observations. Only a very brief description of the model is given here as full details can be found in the aforementioned papers.

The backscatter process is modelled by adding random stress fluctuations to the standard Smagorinsky model. The space and time scales of these variations (which should be the implied filter scale and subgrid turbulence time scale) are dealt with approximately by using a 1:2:1 filter and changing the random numbers every two timesteps. The model ensures that the rates of backscatter of energy and scalar variance are given by:

$$\left(\frac{\partial \langle \overline{u_i'^2} / 2 \rangle}{\partial t} \right)_{SCT} = C_B \left(\frac{\lambda_r}{\lambda_0} \right)^5 \epsilon \quad (2.12)$$

$$\left(\frac{\partial \langle \overline{\theta'^2} / 2 \rangle}{\partial t} \right)_{SCT} = C_{B\theta} \left(\frac{\lambda_r}{\lambda_0} \right)^5 \epsilon_\theta \quad (2.13)$$

where ϵ is the dissipation, ϵ_θ is the dissipation of scalar variance, and λ_r is a typical subgrid length scale defined through:

$$\nu = \lambda_r^2 S (1 - Rf_p)^{1/2} \quad (2.14)$$

physics
behind
it
explain
more
thoroughly
place

CHAPTER 2: LES OF THE CBL

where Rf_p is the flux Richardson number, calculated pointwise. C_B and $C_{B\theta}$ are constants whose magnitude can be estimated using EDQNM theory. However, their exact values depend on the (unknown) filter shape, and the amount of backscatter is sensitive to the precise form of the matching relation so there is a degree of empiricism. Mason and Brown found that good results were obtained using matching relation (2.11) along with the values $C_B = 1.4$, $C_{B\theta} = 0.45$ and this has been adopted here. Subgrid estimates of energy and scalar variance are made using Equations (13) and (14) of Brown *et al.* (1994).

In view of the theoretical arguments that the subgrid model should be stochastic, and the evidence that more realistic velocity and temperature gradients are obtained with such a model, the use of backscatter has been adopted as standard in the present study. Backscatter has not previously been used in simulations of the convective boundary layer, and although its effect is expected to be less marked than in neutral flows, this must be tested. Accordingly additional runs have been carried out using the basic Smagorinsky model in the limiting cases of pure shear flow and free convection, so that the impact of backscatter can be assessed.

The numerical methods used are similar to those discussed by Mason and Callen (1986). The variables are stored on a staggered mesh and the standard model uses the Piacsek and Williams (1970) form of the non-linear terms which, with the leapfrog time-stepping scheme, ensures conservation of energy and scalar variance. S and ν are calculated and stored on w -points to avoid averaging of vertical derivatives.

Slightly different numerical formulations were used in some of the simulations. Some of the early simulations used a three-level locally implicit scheme for vertical diffusion terms (Hobson *et al.*, 1995), while the simulations involving temperature inversions used a total variance diminishing (TVD) scheme for advection of temperature (Leonard, 1991). More details on these schemes, and discussion of problems encountered in implementing them consistently, can be found in Appendices 2.A.1 and 2.A.2 at the end of this chapter.

2.2 Energy Transfers in LES

Many authors have studied the various terms in the turbulence kinetic energy budget using large-eddy simulation (e.g. Mason and Thomson (1987), Andrn *et al.* (1994), Moeng and Sullivan (1994)). However, there are various possible ways of incorporating the effects of the subgrid model in to the budget, and the method used has not always been made clear. Here the budget equation is derived, starting from the filtered Boussinesq approximation to the Navier-Stokes equations which are used in the model. This leads to a clearer understanding of the transfers that occur between energy of the mean flow (MKE), resolved turbulent kinetic energy (RKE) and subgrid-scale turbulent kinetic energy (SKE).

Equation (2.1) reads

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{1}{\rho_r} \frac{\partial p}{\partial x_i} - \frac{1}{\rho_r} \frac{\partial P_0}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) (\bar{\theta} - \theta_r) - \frac{\partial \tau_{ij}}{\partial x_j} - 2\epsilon_{ijk} \Omega_j \bar{u}_k \quad (2.15)$$

where the subgrid stress tensor, τ_{ij} , is defined as in Equation (2.6). Now writing $\bar{u}_i = \langle \bar{u}_i \rangle + \bar{u}'_i$, $\tau_{ij} = \langle \tau_{ij} \rangle + \tau'_{ij}$, $p = \langle p \rangle + p'$, $\bar{\theta} = \langle \bar{\theta} \rangle + \bar{\theta}'$ and substituting in Equation (2.15) leads to

$$\begin{aligned} \frac{\partial (\langle \bar{u}_i \rangle + \bar{u}'_i)}{\partial t} + \frac{\partial ((\langle \bar{u}_i \rangle + \bar{u}'_i) (\langle \bar{u}_j \rangle + \bar{u}'_j))}{\partial x_j} = \\ - \left(\frac{1}{\rho_r} \right) \frac{\partial (P_0 + \langle p \rangle + p')}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) (\langle \bar{\theta} \rangle + \bar{\theta}' - \theta_r) - \frac{\partial (\langle \tau_{ij} \rangle + \tau'_{ij})}{\partial x_j} - 2\epsilon_{ijk} \Omega_j (\langle \bar{u}_k \rangle + \bar{u}'_k) \end{aligned} \quad (2.16)$$

Next averaging the whole of this equation gives

$$\begin{aligned} \frac{\partial \langle \bar{u}_i \rangle}{\partial t} + \frac{\partial (\langle \bar{u}_i \rangle \langle \bar{u}_j \rangle + \langle \bar{u}'_i \bar{u}'_j \rangle)}{\partial x_j} = \\ - \left(\frac{1}{\rho_r} \right) \frac{\partial (P_0 + \langle p \rangle)}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) (\langle \bar{\theta} \rangle - \theta_r) - \frac{\partial \langle \tau_{ij} \rangle}{\partial x_j} - 2\epsilon_{ijk} \Omega_j \langle \bar{u}_k \rangle \end{aligned} \quad (2.17)$$

and subtracting Equation (2.17) from (2.16) leads to

$$\frac{\partial \bar{u}'_i}{\partial t} + \frac{\partial (\langle \bar{u}_i \rangle \bar{u}'_j + \bar{u}'_i \langle \bar{u}_j \rangle + \bar{u}'_i \bar{u}'_j - \langle \bar{u}'_i \bar{u}'_j \rangle)}{\partial x_j} = -\frac{1}{\rho_r} \frac{\partial p'}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) \bar{\theta}' - \frac{\partial \tau'_{ij}}{\partial x_j} - 2\epsilon_{ijk} \Omega_j \bar{u}'_k \quad (2.18)$$

CHAPTER 2: LES OF THE CBL

From Equations (2.17) and (2.18) expressions can be obtained for the rates of change of the energy of the mean flow (MKE), and of the resolved scale turbulent kinetic energy (RKE). The first of these is calculated by multiplying Equation (2.17) by $\langle \bar{u}_i \rangle$, and noting that the use of periodic boundary conditions in the horizontal directions in the large-eddy model means that $\partial \langle a \rangle / \partial x_1 = \partial \langle a \rangle / \partial x_2 = 0$ for all $\langle a \rangle$ (except for $\langle a \rangle = P_0$), and $\langle \bar{u}_3 \rangle = 0$. After some manipulation the following equation is obtained

$$\frac{\partial \langle \bar{u}_i^2 / 2 \rangle}{\partial t} = -\langle \bar{u}_i \rangle \frac{1}{\rho_r} \frac{\partial P_0}{\partial x_i} + \langle \bar{u}_i' \bar{u}_3' \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} - \frac{\partial (\langle \bar{u}_i \rangle \langle \tau_{i3} \rangle)}{\partial x_3} + \langle \tau_{i3} \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} \quad (2.19)$$

The boundary layer wind is generally backed relative to the geostrophic wind, and the pressure gradient term then leads to production of MKE. The second term describes the transfer from MKE to RKE. The third term is a transport term, and the last term represents the effects of the subgrid stresses on the mean fields (i.e. direct transfer from MKE to SKE).

To obtain the RKE budget, both sides of Equation (2.18) are multiplied by $\bar{u}_i'$, and then the mean is taken of the resulting equation. This gives

$$\frac{\partial \langle \bar{u}_i'^2 / 2 \rangle}{\partial t} + \langle \bar{u}_i' \frac{\partial \langle \bar{u}_i \rangle \bar{u}_j'}{\partial x_j} \rangle + \langle \bar{u}_i' \frac{\partial \bar{u}_i' \langle \bar{u}_j \rangle}{\partial x_j} \rangle + \langle \bar{u}_i' \frac{\partial \bar{u}_i' \bar{u}_j'}{\partial x_j} \rangle = -\langle \frac{\bar{u}_i'}{\rho_r} \frac{\partial p'}{\partial x_i} \rangle + \delta_{i3} \left(\frac{g}{\theta_r} \right) \langle \bar{u}_i' \bar{\theta}' \rangle - \langle \bar{u}_i' \frac{\partial \tau_{ij}'}{\partial x_j} \rangle \quad (2.20)$$

Some rearrangement, and use of the continuity equation ($\partial \bar{u}_i / \partial x_i = \partial \bar{u}_i' / \partial x_i = 0$) leads to

$$\frac{\partial \langle \bar{u}_i'^2 / 2 \rangle}{\partial t} + \langle \bar{u}_j \rangle \frac{\partial \langle \bar{u}_i'^2 / 2 \rangle}{\partial x_j} = -\langle \bar{u}_i' \bar{u}_j' \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_j} - \frac{\partial \langle \bar{u}_j' \bar{u}_i'^2 / 2 \rangle}{\partial x_j} - \frac{\partial \langle \bar{u}_i' p' / \rho_r \rangle}{\partial x_i} + \delta_{i3} \left(\frac{g}{\theta_r} \right) \langle \bar{u}_i' \bar{\theta}' \rangle - \langle \bar{u}_i' \frac{\partial \tau_{ij}'}{\partial x_j} \rangle \quad (2.21)$$

This looks very like the turbulence kinetic energy budget of Stull (1988), although the last term in this equation represents the effect of the subgrid model on the resolved turbulence, whilst that of Stull represents the molecular dissipation of turbulence.

Noting the constraints imposed by the horizontal periodicity of the LES, Equation (2.21) can be simplified to

$$\frac{\partial \langle \bar{u}_i'^2 / 2 \rangle}{\partial t} = -\langle \bar{u}_i' \bar{u}_3' \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} - \frac{\partial \langle \bar{u}_3' \bar{u}_i'^2 / 2 \rangle}{\partial x_3} - \frac{\partial \langle \bar{u}_3' p' / \rho_r \rangle}{\partial x_3} + \left(\frac{g}{\theta_r} \right) \langle \bar{u}_3' \bar{\theta}' \rangle - \langle \bar{u}_i' \frac{\partial \tau_{ij}'}{\partial x_j} \rangle \quad (2.22)$$

CHAPTER 2: LES OF THE CBL

The first four terms on the right hand side of (2.22) are commonly known as the shear production, turbulent transport, pressure transport and buoyancy production terms. Note that the shear production term represents the transfer of energy from the mean flow and so is equal and opposite to the loss term in the MKE budget.

All subgrid effects are contained in the last term. Andrn *et al.* (1994) used this 'resolved kinetic energy budget' and referred to the last term as the 'dissipation'. However, there are other ways of presenting the budget. The last term in Equation (2.22) can be expanded as follows

$$\begin{aligned}
 -\langle \bar{u}_i' \frac{\partial \tau_{ij}'}{\partial x_j} \rangle &= -\langle \bar{u}_i' \frac{\partial (\tau_{ij} - \langle \tau_{ij} \rangle)}{\partial x_j} \rangle = -\langle \bar{u}_i' \frac{\partial \tau_{ij}}{\partial x_j} \rangle = -\frac{\partial \langle \bar{u}_i' \tau_{ij} \rangle}{\partial x_j} + \langle \tau_{ij} \frac{\partial \bar{u}_i'}{\partial x_j} \rangle \\
 &= -\frac{\partial \langle \bar{u}_i' \tau_{i3} \rangle}{\partial x_3} - \left(\langle \nu S^2 \rangle + \langle \tau_{i3} \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} \right)
 \end{aligned}
 \tag{2.23}$$

Handwritten notes: "this is the subgrid dissipation", "the first term is the transport of RKE by the subgrid model", "the term in brackets is a dissipative term, representing the transfer of energy from RKE to subgrid scale (SKE)".

The first term on the right hand side of (2.23) integrates vertically to zero. It is a transport term, representing the transport of resolved kinetic energy (RKE) by the subgrid model. The term in brackets is a dissipative term, representing the transfer of energy from RKE to subgrid scale (SKE).

An estimate of the true molecular dissipation rate, $\langle \epsilon \rangle$, can be obtained by assuming local equilibrium in the budget of subgrid-scale turbulent kinetic energy (SKE). Then the sum of the inputs from MKE and RKE, plus that from subgrid buoyancy effects, must equal the dissipation. Therefore

$$\langle \epsilon \rangle = \left(\langle \nu S^2 \rangle + \langle \tau_{i3} \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} \right) - \langle \tau_{i3} \rangle \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} + \left(\frac{g}{\theta_r} \right) \langle H_3 \rangle = \langle \nu S^2 \rangle + \left(\frac{g}{\theta_r} \right) \langle H_3 \rangle \tag{2.24}$$

where $H_3 = -\nu_h \partial \bar{\theta} / \partial x_3$ is the subgrid heat flux (Equations (2.3) and (2.7)).

A summary of these energy transfers can be found in Figure 2.1. *Trans* represents all of the terms describing transport of RKE (grouped together here for clarity). It is equal to the sum of the turbulent and pressure transport terms (Equation (2.22)), and the term describing the transport of RKE by the subgrid viscosity (Equation (2.23)).

Stull (1988) discusses how the action of molecular viscosity on the mean flow is negligible in the atmosphere (due to the very large Reynolds number). In large-eddy simu-

Figure 2.1: Schematic diagram of energy transfers in LES between kinetic energy of the mean flow (MKE), turbulent kinetic energy (RKE) and subgrid kinetic energy (SKE). $\langle \epsilon \rangle$ represents the molecular dissipation from the smallest scales.

lations, the terms involving direct transfer of energy from the mean flow to the subgrid scale are often non-negligible, particularly close to the surface, suggesting that the effective Reynolds number of the simulations is only moderately high. Mason (1994) discusses how a large-eddy simulation can be viewed as a moderate Reynolds number direct simulation of the flow interior patched with a high Reynolds number boundary condition. If computer resources permitted the filter scale to be made progressively smaller (increasing effective Reynolds number), then the transfer of energy directly from MKE to SKE would be expected to reduce and eventually become negligible, whilst that from MKE through RKE to SKE would increase. Similarly, the subgrid buoyancy flux would steadily decrease in magnitude, whilst the resolved flux increased. However, if the model results do converge successfully with increasing resolution, then the total production of turbulent kinetic energy ($TKE = \langle E \rangle = RKE + SKE$) should be insensitive to resolution, as should the dissipation. Hence it was decided to adopt the following budget equation, obtained by diagnostic rearrangement of the terms in (2.22), using (2.23) and (2.24), and noting that the rate of change of TKE is equal to that of RKE as equilibrium is assumed in the

SKE equation

$$\frac{\partial \langle E \rangle}{\partial t} = -(\langle \bar{u}'_i \bar{u}'_3 \rangle + \langle \tau_{i3} \rangle) \frac{\partial \langle \bar{u}_i \rangle}{\partial x_3} - \frac{\partial (\langle \bar{u}'_3 \bar{u}'_i{}^2 / 2 \rangle + \langle \bar{u}'_3 p' \rangle + \langle \bar{u}'_i \tau_{i3} \rangle)}{\partial x_3} + \left(\frac{g}{\theta_r} \right) (\langle \bar{u}'_3 \bar{\theta}' \rangle + \langle H_3 \rangle) - \langle \epsilon \rangle \quad (2.25)$$

This budget equation was also used, without being explicitly presented, by Mason and Thomson (1987). The four terms on the right hand side are, respectively, total shear production, total transport, total buoyancy production and dissipation. In general the production terms will be referred to simply as shear and buoyancy production, but it should be borne in mind that the subgrid contributions are included unless explicitly stated otherwise. The dissipation is still diagnosed using (2.24). It is sometimes useful to look at the three components of the transport term separately. Note however that the definition of pressure used here implicitly includes two-thirds of the subgrid energy, and any attempts to calculate a ‘true’ pressure transport term would require use of the purely diagnostic estimate of subgrid variance and are not advised (Andrn *et al.* , 1994).

The introduction of backscatter (shown dashed in Figure 2.1) does not have a major complicating influence, as the rate of backscatter of energy is related to the viscous drain of energy. A net dissipation can be diagnosed (viscous drain minus backscatter), and the budget equation used as before.

At this point the rather cumbersome overbar notation which has been used to indicate resolved quantities, is dropped. Unless otherwise stated in the text, all turbulence statistics presented are total quantities i.e. the sum of the resolved and subgrid contributions. For example, profiles of $\langle u'w' \rangle$ show the sum of the resolved part, $\langle \bar{u}'\bar{w}' \rangle$, and the subgrid part, $\langle \tau_{13} \rangle$. Similarly, $\langle w'\theta' \rangle$ is the sum of $\langle \bar{w}'\bar{\theta}' \rangle$ and $\langle H_3 \rangle$, $\langle w'w' \rangle$ is the sum of $\langle \bar{w}'\bar{w}' \rangle$ and two-thirds of the estimate of subgrid energy, and so on.

2.3 Simulations performed

A large number of simulations have been performed with flows driven by imposed geostrophic wind and surface buoyancy flux. These simulations fall into three main categories:

1. 'Lid runs'.

These simulations used the stress-free rigid lids at height $h = 1000$ m to form the boundary layer tops (i.e. $z_i = h$). They were designed to study the direct effects of the interaction of shear and buoyancy forcing, without the complicating influence of entrainment of air from above the boundary layer. The absence of inversion rise also meant that these simulations could be run for a long time, which is useful in studies of the mean fields which only slowly approach inertial equilibrium.

2. 'Inversion runs'.

These simulations were set up with capping inversions in the initial temperature profiles. They were run until the boundary layers had grown to depths of around 1000 m and are used to study the effects on the entrainment flux on boundary layer turbulence, and also the factors affecting the entrainment flux itself. In these simulations the stress-free rigid lids were placed well above the inversion region, with damping layers to dissipate gravity waves.

3. 'Baroclinic runs'.

Simulations in which the imposed geostrophic wind varied with height. For simplicity these also used the stress-free lids to form the boundary layer tops.

The baroclinic runs are discussed separately in Chapter 5. However, results from the main lid and inversion runs are used repeatedly throughout the remainder of this thesis, and so more details of these simulations are given in this chapter in Sections 2.3.3 and 2.3.4. First consideration is given to some issues which are of importance for all simulations, including the choices made for the initial conditions, the lengths of the runs, and the domain sizes used.

2.3.1 Initial conditions and the inertial oscillation

Ideally, all of the model simulations would be run to long enough time that the results were independent of the initial conditions chosen. Unfortunately, the mean flow only adjusts very slowly on the Coriolis time scale ($2\pi/f \simeq 63000$ s at 45° N), and it is impractical to run high resolution simulations to inertial equilibrium. The possible approaches are to run at relatively low resolution for long time, or to use high resolution and accept that the flows will not be in geostrophic balance. The former approach is useful for quantities which depend sensitively on the mean fields (e.g. geostrophic drag coefficients). The latter approach is suitable for studies of scaled turbulence statistics as the turbulence time scale, $t_* = z_i / \max(u_*, w_*)$ (where w_* is the convective velocity scale defined in (3.1)), is typically of order 1000 s i.e. $t_* \ll 2\pi/f$. This means that the turbulence can be approximately in equilibrium with the mean flow even when the mean flow is not in equilibrium with the geostrophic forcing.

Both approaches are used in the present study. In general when studying scaled turbulence statistics this study will concentrate on results from high resolution runs (typically $80 \times 80 \times 64$ mesh points) as these simulations resolve as large a range of scales as possible. However low resolution runs are also useful for sensitivity studies, choosing the best cases to run at high resolution and, in conjunction with high resolution simulations, assessing the resolution dependence of the results.

Although useful turbulence statistics can be obtained from simulations which are not in geostrophic balance, it is obviously desirable to be as close to balance as possible. For this reason, in most cases initial mean velocity and temperature fields were obtained using a one-dimensional boundary layer model. The large-eddy simulations were then initialized using these fields and a random perturbation. Comparison of results from a run started in this way, and from one started from more arbitrary initial conditions, showed a smaller acceleration term in the momentum budget of the former, as expected.

2.3.2 Choice of domain

With current computing resources it is not possible to resolve much more than two decades of scales ($80 \times 80 \times 80$ points gives only 1.6 decades). For a given number of mesh points, a 'small' domain run will have 'high' resolution so should resolve small scale features relatively well, but must miss the contribution from the largest eddies. Conversely a run with a 'large' domain will capture these eddies but must give a poorer representation of the small-scale motions due to an increase in filter-scale.

One approach to the problem, used by Mason and Thomson (1987), is to perform several simulations of the same flow, each using a different domain. No one simulation captures all the relevant scales, but looking at all together gives some idea of the relative importance of the different scales of motion and may help with the choice of the best 'compromise' domain. In the present study the choices were based on past work and on some low resolution test runs, with extra simulations performed to test sensitivity to domain size (and orientation) where thought applicable.

In neutral conditions, Mason and Thomson used domains with horizontal extents of $24 \text{ km} \times 12 \text{ km}$, $6 \text{ km} \times 3 \text{ km}$ and $3 \text{ km} \times 1.5 \text{ km}$. The largest of these was designed to encompass large-scale roll vortices as found in a two-dimensional study by Mason and Sykes (1980). However, no evidence for such motions was found, although the eddies were found to be elongated in the streamwise direction. This is consistent with other evidence which suggests that the formation of coherent vortices in the atmosphere requires a mixed shear-buoyancy regime (see chapter 1). Therefore a domain was chosen for the neutral simulations which it is recognized is too small to encompass these rolls, but which, at $3 \text{ km} \times 2 \text{ km}$, is nevertheless slightly larger relative to the boundary layer depth ($z_i = 1000 \text{ m}$) than domain B ($6 \text{ km} \times 3 \text{ km}$) of Mason and Thomson.

Mason (1989) examined the sensitivity of large-eddy simulations of the convective boundary layer to domain size and resolution. Simulations FL6.4 and M had the same mesh spacing, but square domains of sides $6.4z_i$ and $3.2z_i$ respectively. The statistics

obtained (e.g. for the velocity variances $\langle u'u' \rangle$ and $\langle w'w' \rangle$) were similar in the two cases. This led Mason to the conclusion that the domain of side $3.2z_i$ was adequate, while a similar test suggested that a domain of side $1.6z_i$ was too small. Sykes and Henn (1989) modelled convection between moving flat plates and used domains of side 4 and 8 times the plate separation. They found similar results using these two domains, and therefore advocated the use of the smaller domain as it enables higher resolution to be used. In the light of these findings a square domain of side $4z_i$ was chosen for the convective simulations. The slight increase in domain size from that advocated by Mason is made without compromising his resolution as the present study uses an increased number of mesh points.

In the intermediate cases (i.e. mixed shear and buoyancy regime) it was decided to use the domains described for use in the neutral and free convective simulations. These cannot accurately represent large roll vortices, with aspect ratios of $2 - 3z_i$, due to the periodic boundary conditions. However, there is evidence (see Chapter 1) that these rolls are simply an organized form of convection and that the existence or otherwise of these large scale features does not have a major effect on turbulence statistics. Note that even the domain of Moeng and Sullivan (1994), a square of side approximately 6 times the boundary layer depth, severely restricts the possible numbers and orientations of rolls. For this reason the use of smaller domains for good resolution of the smaller-scale features is preferred. In order to reduce the influence of the periodic boundary conditions, in many of the simulations the geostrophic wind was imposed 13° to the right of the x -axis (rather than parallel to it) in order to make the average boundary layer flow more closely parallel to the model axis. Some sensitivity tests which used much larger domains and different angles of geostrophic wind relative to the model axes are described in Chapter 3.

2.3.3 Lid runs

The high resolution simulations used $80 \times 80 \times 64$ grid points. The mesh was non-uniform in the vertical, with smaller grid intervals close to the surface and to the upper boundary.

CHAPTER 2: LES OF THE CBL

The lowest points were at 1.8 m from the surface, and the spacing gradually increased from 3.6 m at this height to $\simeq 20$ m at 200 m. The separation was then constant at this value until about 800 m, above which there was a gradual decrease to 4 m at the top of the domain. The horizontal mesh spacings resulted from spreading the points evenly throughout the chosen domain. Initial mean fields were obtained using a one-dimensional boundary layer model, and the simulations were run for long enough for the turbulence to become approximately in equilibrium with the mean fields (typically for around 20000 s, or 15-20 eddy turnover times). The low resolution simulations used only $40 \times 40 \times 32$ points, so that the spacing was approximately doubled in all directions. These simulations were run for 100000 s.

A summary of the main lid runs can be found in Table 2.1. Various additional sensitivity tests are described at the relevant points in the text.

2.3.4 Inversion runs

The initial state for the inversion runs was a uniform potential temperature gradient of 0.003 Km^{-1} ($N^2 = (g/\theta_r)\partial(\theta)/\partial z \simeq 0.01 \text{ s}^{-2}$) from the surface to the top of the domain, with the wind components set equal to their geostrophic values at all heights. In most cases a one-dimensional model was used to grow the boundary layer from this initial state to a depth of between 600 and 900 m, and the resulting mean fields were used to initialize the large-eddy model. However, in some of the most convective cases (in which inversion rise was rapid) the large-eddy model was used to grow the boundary layer from the surface without using the one-dimensional model. Boundary layer depths were diagnosed by using a parabolic fit to estimate the height at which the maximum downward flux occurred.

Table 2.2 gives a summary of the main inversion runs. The horizontal resolution was chosen to be the same as in the lid runs. The vertical spacing was non-uniform, with enhanced resolution close to the surface and in the target region for the inversion (between around 800 m and 1300 m). The low resolution simulations used a spacing of

CHAPTER 2: LES OF THE CBL

high resolution ($80 \times 80 \times 64$ points)

run	L_x/km	L_y/km	λ_0/m	New diffusion	$ \mathbf{G} /\text{ms}^{-1}$	$\langle w'b' \rangle_0/\text{m}^2\text{s}^{-3}$
BNHR	3	2	5.0	No	10	0
M04HR	3	2	5.0	No	10	10^{-4}
M09HR	4	4	11.5	Yes	$10^\dagger$	3×10^{-4}
M23HR	4	4	11.5	Yes	$10^\dagger$	10^{-3}
M40HR	4	4	11.5	Yes	$10^\dagger$	2×10^{-3}
M68HR	4	4	11.5	Yes	$10^\dagger$	4×10^{-3}
M147HR	4	4	11.5	Yes	10	10^{-2}
BCHR	4	4	11.5	Yes	0	10^{-2}

low resolution ($40 \times 40 \times 32$ points)

BNLR	3	2	10.0	No	10	0
M03	3	2	10.0	Yes	10	10^{-4}
M09	4	4	23.0	Yes	$10^\dagger$	3×10^{-4}
M21	4	4	23.0	Yes	$10^\dagger$	10^{-3}
M35	4	4	23.0	Yes	$10^\dagger$	2×10^{-3}
M64	4	4	23.0	Yes	$10^\dagger$	4×10^{-3}
M134	4	4	23.0	Yes	10	10^{-2}
BCLR	4	4	23.0	No	0	10^{-2}

Table 2.1: Summary of lid runs. L_x (L_y) is the size of domain in the x - (y -) direction. λ_0 is the basic mixing length. Runs which used the new diffusion scheme of Hobson *et al.* (1995) are indicated. The geostrophic wind, $\mathbf{G}$, was imposed in the x -direction except in those runs marked † in which it was 13° to the right of the x -axis. $\langle w'b' \rangle_0$ is the surface buoyancy flux which was imposed.

CHAPTER 2: LES OF THE CBL

high resolution ($80 \times 80 \times 100$ points)					
run	L_x/km	L_y/km	λ_0/m	$ \mathbf{G} /\text{ms}^{-1}$	$\langle w'b' \rangle_0/\text{m}^2\text{s}^{-3}$
INHR	3	2	5.0	10	0
I10HR	4	4	11.5	$10^\dagger$	3×10^{-4}
ICHR	4	4	11.5	0	2×10^{-3}

low resolution ($40 \times 40 \times (64 - 72)$ points)					
IN	3	2	10.0	10	0
I03	3	2	10.0	$10^\dagger$	10^{-4}
I10	4	4	23.0	$10^\dagger$	3×10^{-4}
I27	4	4	23.0	$10^\dagger$	10^{-3}
I77	4	4	23.0	$6^\dagger$	10^{-3}
IC	4	4	23.0	0	2×10^{-2}

Table 2.2: Summary of inversion runs. All used ^{the} standard diffusion scheme, but advection of θ was performed using the TVD scheme of Leonard (1991). As before, the † symbol indicates that the geostrophic wind was rotated 13° to the right of the x -axis.

12 m close to the surface, increasing to 38 m in mid boundary layer and then decreasing again to around 27 m in the inversion region. Higher up the spacing increased to as much as 230 m towards the domain top which was at 5000 m in most cases. The extra levels in the high resolution simulations were placed largely in the inversion region, reducing the spacing there to around 18 m.

As mentioned earlier, the inversion runs used a damping layer to dissipate gravity waves before they could reflect back off the domain top. The layer took the form of a Newtonian relaxation term on all prognostic variables, damping them back towards their mean values with timescale γ_D given by

$$\gamma_D(z) = \begin{cases} \gamma_{D0} \left(\exp \left(\frac{z-z_D}{H_D} \right) - 1 \right) & \text{for } z > z_D \\ 0 & \text{for } z \leq z_D \end{cases} \quad (2.26)$$

Some experimentation was required in finding suitable values of γ_{D0} , z_D and H_D - too

weak a damping layer does not serve its purpose, while too rapid an increase in γ_D with height can lead to unwanted reflections. Also z_D must be safely above the inversion layer at all times. Satisfactory results were obtained in the high resolution simulations using $\gamma_{D0} = 0.005 \text{ s}^{-1}$, $z_D = 2000 \text{ m}$ and $H_D = 1500 \text{ m}$, and similar values were used in the low resolution runs.

2.A Appendices to Chapter 2

2.A.1 New diffusion scheme

Here a brief description is given of the diffusion scheme of Hobson *et al.* (1995) which was used in a few of the large-eddy model simulations. In an explicit diffusion scheme any point is only influenced in any one timestep by the immediately neighbouring points. A linear stability analysis shows that this imposes a limitation on the timestep, Δt

$$C = \frac{4\nu\Delta t}{\min(\Delta x^2, \Delta y^2, \Delta z^2)} \leq 1 \quad (2.27)$$

C is a viscous Courant number which would typically be maintained at a value of 0.3 or less. This relatively stringent criterion ensures that the simulations do not suffer instabilities due to non-linear effects, and also leads to some increase in accuracy. In practice it is vertical diffusion which restricts the timestep (as the mesh-spacing is smallest in the vertical direction, especially close to the surface). The scheme of Hobson *et al.* (1995) replaces the standard formulation for the double vertical derivative at level k , with a form that uses implicit values for terms at the $k+1$ and $k-1$ levels and explicit values for terms at the $k+2$ and $k-2$ levels.

For every level (e.g. the k^{th}) the following three equations can be written. Note that the notation has been simplified by assuming constant mesh spacing and viscosity. As described above, the terms at $k+2$ and $k-2$ (labelled ($\mathcal{A}$) and ($\mathcal{B}$) below) are evaluated

explicitly at time $t - 1$. All other terms are at time $t + 1$.

$$\frac{u_{k+1}^{t+1} - u_{k+1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta z} \left(\frac{(u_{k+2}^{t-1} - u_{k+1}^{t+1})}{\Delta z} - \frac{(u_{k+1}^{t+1} - u_k^{t+1})}{\Delta z} \right) \quad (2.28)$$

$$\frac{u_k^{t+1} - u_k^{t-1}}{2\Delta t} = \frac{\nu}{\Delta z} \left(\frac{(u_{k+1}^{t+1} - u_k^{t+1})}{\Delta z} - \frac{(u_k^{t+1} - u_{k-1}^{t+1})}{\Delta z} \right) \quad (2.29)$$

$$\frac{u_{k-1}^{t+1} - u_{k-1}^{t-1}}{2\Delta t} = \frac{\nu}{\Delta z} \left(\frac{(u_k^{t+1} - u_{k-1}^{t+1})}{\Delta z} - \frac{(u_{k-1}^{t+1} - u_{k-2}^{t+1})}{\Delta z} \right) \quad (2.30)$$

A 3x3 matrix can then be written for every k level and solved for u_k^{t+1} . It is a little more computationally expensive than explicit methods, but is very much cheaper than a fully implicit scheme. A linear stability analysis shows that this scheme is unconditionally stable. However it is wise to continue to place some limit on the timestep as the scheme does show some time lag when compared with an analytical solution for a simple problem. This lag increases with increasing Courant number so it is insisted that $C \leq 1$ on all points.

The other viscous terms are still calculated using the standard explicit scheme. The stability criteria on these will generally not be restrictive as the grid spacings are larger in the horizontal directions. However, in runs where the horizontal mesh spacing is comparable to that in the vertical, it would probably be wise to define a separate 'horizontal Courant number' based on the horizontal grid spacing and to insist that this remain below some threshold value (e.g. 0.3) to ensure that no instabilities result from these terms.

This scheme was coded into the large-eddy model and was used for some of the lid runs (see Table 2.1). The increase in computation time per step was more than offset by the increase in timestep in all cases. However it was realized that the diagnosed dissipation was no longer consistent with the model formulation. Estimates of the true dissipation for these runs were made by assuming stationarity in the energy budget, (2.25), and were typically smaller by around 25%. This means that these runs will typically have had a

backscatter rate around 25% greater than originally intended. This is not thought to be a particularly serious problem as the most appropriate backscatter rate is not well known in any event (Mason and Brown, 1994). Furthermore, backscatter is not found to have a major impact in convective conditions (see Chapter 3), so the results of the runs seem unlikely to be sensitive to small changes in the backscatter rate. Nevertheless, in view of these uncertainties it was decided not to continue with this scheme in the present study, although it is planned to return to it in the future when a consistent method of diagnosing dissipation has been developed.

2.A.2 TVD advection scheme

For the simulations involving capping temperature inversions it was decided to use the TVD scheme of Leonard (1991) for advection of θ . This was done because the basic Piacsek-Williams (1970) scheme is linearly and quadratically conserving but not positive definite and can perform poorly in regions with sharp scalar gradients. The Leonard scheme is linearly conserving and positive definite, and although it is not quadratically conserving, it is less diffusive than the TVD scheme of van Leer (1974). Strictly speaking the use of a diffusive scheme means that the diagnosis of dissipation of scalar variance is in error, and this affects the scalar backscatter rates. In practice the errors are found to be small, and the effects on the backscatter are insignificant compared with the uncertainties in the tuning of the scalar backscatter parametrization.

Recently it has been pointed out (M.K. MacVean, private communication) that there is an inconsistency in using TVD for advection of θ , while still using a centred form in the buoyancy term of the w -equation. This means that the loss (gain) of kinetic energy due to buoyancy effects is not exactly equal to the gain (loss) of potential energy. This error appears to be common to a number of large-eddy models and may be significant in studies of cloudy boundary layers which can be topped by very sharp inversions where the TVD and centred schemes operate quite differently. To assess whether this inconsistency is significant in the present simulations, profiles of $\langle w'\theta' \rangle$ were diagnosed consistent with

CHAPTER 2: LES OF THE CBL

both the TVD and centred formulations for simulations IC and IN. The profiles from IC were indistinguishable from one another, showing that the two schemes behave almost identically in this case and that any inconsistency is insignificant. Simulation IN might be expected to be a 'worst case' as it is a low resolution run with a relatively sharp inversion, but even here the two profiles were very similar up to around z_i , with maximum discrepancies of around 20% at $z/z_i = 1.1$. The conclusion is that the inversions in the present study are insufficiently sharp for this problem to be significant.

Chapter 3

Turbulent structure of the CBL

In this chapter the variation of boundary layer flow fields and scaled turbulence statistics with stability is examined. The large-eddy model results are presented, and, where possible, are compared with atmospheric and laboratory observations (and other published LES results). Comparison of results from the LES lid and inversion runs allows an assessment to be made of the impact of entrainment on the boundary layer turbulence structure.

3.1 Preliminary simulations

Although the large-eddy simulations cover the whole range of stabilities between neutral and free convective conditions, results from the two extreme cases are presented first. This approach is taken for the following reasons:

1. Many studies have dealt with pure shear flow and free convection. It is useful to check that the results are broadly consistent with earlier findings in these cases, before looking at the more complex cases in which both shear and buoyancy are important.

CHAPTER 3: CBL TURBULENCE

run	mesh points	L_x/km	L_y/km	λ_0/m	backscatter
SNLR	$40 \times 40 \times 32$	3	2	10	No
SNHR	$80 \times 80 \times 64$	3	2	5	No
BNLR	$40 \times 40 \times 32$	3	2	10	Yes
BNHR	$80 \times 80 \times 64$	3	2	5	Yes

Table 3.1: Summary of neutral runs. L_x (L_y) is the size of domain in the x - (y -) direction. λ_0 is the basic mixing length.

2. This study uses a variety of runs with different resolutions. It is therefore important to check the sensitivity of the results to resolution, and ‘high’ and ‘low’ resolution results are compared here.
3. This is the first modelling study of the convective boundary layer to use backscatter. The effects of the process in highly convective conditions are not expected to be as significant as they are in a shear flow due to the dominance of large well-resolved thermals in the convective case. However, this must be tested and some results from simulations using the standard Smagorinsky model are presented for comparison.

3.1.1 Neutral simulations

In addition to the high and low resolution simulations performed with backscatter (BNHR and BNLR), two additional simulations were performed without backscatter for comparison. These will be referred to as ‘Smagorinsky Model simulations’. Table 3.1 shows a summary of these four neutral static-stability simulations. All flows were driven by imposed geostrophic winds of 10 ms^{-1} in the x -direction.

Figure 3.1 shows the evolution of vertically averaged total kinetic energy with time for these four runs. The non-backscatter runs showed very little energy for approximately the first 5000 s and then a large overshoot, while the turbulence initialization was much more

Figure 3.1: Volume averaged kinetic energy versus time for the four neutral runs.

smooth with backscatter. However it can^{be} seen that all runs had reached quasi-steady state by 15000 s. Statistics were taken from the Smagorinsky model runs between 15000 s and 20000 s. This relatively short averaging period ($\approx 2t_*$) where t_* is the large-eddy turnover time) is sufficient for the present comparison. The results from the backscatter runs represent averages over 10000 s ($\approx 4t_*$). Slow geostrophic adjustments will still have been occurring, but should have little influence on the statistics. Note that in order to minimize their influence perturbations were taken relative to instantaneous rather than time-averaged mean quantities.

Before considering any turbulence statistics, a brief examination is made of flow structures resolved. Figure 3.2 shows horizontal sections of u fluctuations (x -axis aligned with the geostrophic wind) at four different heights in the high resolution Smagorinsky model simulation (SNHR). Figure 3.3 shows the same information for the corresponding backscatter simulation (BNHR). The contour interval is 0.3 ms^{-1} with contours of positive perturbation shown in bold. Irregular streaky structures can be seen close to the surface, elongated roughly in the direction of the mean shear. These streaks become

CHAPTER 3: CBL TURBULENCE

Figure 3.2: Horizontal sections of u fluctuations after 20000 s in high resolution Smagorinsky model neutral simulation (SNHR). The contour interval is 0.3 ms^{-1} with the contours of positive perturbation shown in bold.

CHAPTER 3: CBL TURBULENCE

Figure 3.3: Horizontal sections of u fluctuations after 30000 s in high resolution neutral simulation with backscatter (BNHR). The contour interval is 0.3 ms^{-1} with the contours of positive perturbation shown in bold.

Figure 3.4: $\langle u'u' \rangle$ velocity variances, normalized by surface stress, for the four neutral runs. The x -axis is aligned with the geostrophic wind.

less easily distinguishable higher up the boundary layer. These findings are consistent with many previous large-eddy simulations (e.g. Moin and Kim, 1982; Moeng and Sullivan, 1994). The inclusion of backscatter does not appear to have a major impact on the flow fields, although the structures at 47 m appear to be slightly less coherent in the backscatter simulation due to the small scale random forcing.

Figure 3.4 shows the profiles of total $\langle u'u' \rangle$ velocity variance (resolved plus subgrid) obtained in these four simulations. The x -axis is aligned with ^{the} geostrophic wind. The subgrid estimates are made ~~using~~ assuming equal energy in each component. This must be erroneous close to the surface, but should give a reasonable estimate in the flow interior. Results from both runs using the standard Smagorinsky model show an unrealistic elevated maximum which is not present in the backscatter runs. This effect of backscatter was noted by Mason and Thomson (1992).

The effect of model resolution is now discussed. One of the key tests of the large-eddy simulation technique is that the results should converge to the correct limit with

CHAPTER 3: CBL TURBULENCE

increasing resolution (i.e. decreasing filter-scale) and become insensitive to the subgrid parametrization. The hope is that this convergence will occur rapidly so that the best possible results are obtained for a given computational expense. It has already been noted that both the Smagorinsky model runs show unrealistic elevated peaks in $\langle u'u' \rangle$. The profiles from the two runs also differ significantly. In contrast the results from the low and high resolution backscatter runs are in good agreement with each other and with the expected profile.

The differences between the results of the four runs are less marked for the other variances and are not shown here. Instead, in Figure 3.5, results from simulation BNHR are compared with data obtained in flights in near neutral conditions over the sea (Grant, 1986). Two of the flights were made during the 1981 KONTUR experiment over the North Sea, and a third was over the Atlantic Ocean to the northwest of the United Kingdom.

The experimental data show inversion-capped boundary layers with z_i between 350 m and 675 m, giving values of $u_*/(fz_i)$ of around 10. The LES boundary layer is relatively deep ($u_*/(fz_i) \simeq 4.5$), but it can be seen that the total stress profile is still fairly linear and not inconsistent with that observed. The modelled $\langle u'u' \rangle/u_*^2$ and $\langle v'v' \rangle/u_*^2$ profiles (x -axis aligned with mean boundary layer wind) have similar shapes to the experimental curves, but tend to be towards the low side of the data scatter. This is not unexpected, as the experimental values might be increased by mesoscale motions, although the spectra do not show much evidence for such motions with relatively well defined peaks at wavelengths of $O(z_i)$. Additionally the simulation results might be expected to be low as the limited domain size must exclude some of the larger-scale turbulent motions.

The agreement between modelled and observed values of $\langle w'w' \rangle/u_*^2$ is generally good. Close to the surface the LES has a larger variance, although there is some evidence that the aircraft data may be low. Panofsky and Dutton (1984) tabulated the results of a number of surface layer experiments and found a range of values for $\langle w'w' \rangle/u_*^2$ from 1.2 to 2.0 with a mean of 1.6, in better agreement with the LES result.

CHAPTER 3: CBL TURBULENCE

Figure 3.5: Comparison between LES results and observations (Grant, 1986). $\langle \tau \rangle$ is the total stress, and $\langle u'u' \rangle$, $\langle v'v' \rangle$ and $\langle w'w' \rangle$ are the velocity variances. The x -axis is aligned with the mean boundary layer wind. Solid lines : BNHR (stress-free rigid lid at z_i); dashed lines : IN (temperature inversion at z_i); diamonds : aircraft data

CHAPTER 3: CBL TURBULENCE

run	mesh points	L_x/km	L_y/km	λ_0/m	backscatter
SCLR	$40 \times 40 \times 32$	4	4	23	No
SCHR	$80 \times 80 \times 64$	4	4	11.5	No
BCLR	$40 \times 40 \times 32$	4	4	23	Yes
BCHR	$80 \times 80 \times 64$	4	4	11.5	Yes

Table 3.2: Summary of convective runs. L_x (L_y) is the size of domain in the x - (y -) direction. λ_0 is the basic mixing length.

The dashed lines show on Figure 3.5 show the results of inversion run IN. The profiles are very similar, suggesting that the impact of entrainment on turbulence statistics in the interior of the neutral boundary layer of simulation IN is minimal. Note that a more marked effect might be found for a shallower boundary layer in which the entrainment rate was more rapid.

3.1.2 Free convective simulations

Simulations of the boundary layer in free convective conditions are now examined. As in the neutral case, extra simulations were performed using the Smagorinsky model without backscatter. Table 3.2 shows a summary of the four simulations performed using stress-free rigid lids to cap the boundary layers. In all cases the flows were driven by an imposed surface buoyancy flux, $\langle w'b' \rangle_0$, of $10^{-2} \text{m}^2 \text{s}^{-3}$, with the geostrophic wind set to zero. The time evolution of the turbulent kinetic energy (not shown) was much more similar for all runs than in the neutral case. Statistics were taken from 15000-20000 s ($\simeq 10t_*$) in the low resolution simulations and from 10000-12000 s ($\simeq 4t_*$) in the high resolution cases.

Figure 3.6 shows the vertical velocity fields at various heights in the high resolution backscatter simulation, BCHR. There is a very different structure to that observed in the neutral flow as the regions of ascending air form a cellular structure close to the surface, which gradually changes with height into more isolated thermals. The strongest of these

CHAPTER 3: CBL TURBULENCE

Figure 3.6: Horizontal sections of w fluctuations after 12000 s in high resolution convective run with backscatter (BCHR). The contour interval is 0.4 ms^{-1} with positive contours shown in bold as before.

CHAPTER 3: CBL TURBULENCE

updraughts occur above the ‘junctions’ of the spokes in the cellular pattern. A very similar flow structure is found in the other convective runs and it is consistent with observations in the atmosphere using dual Doppler radars and also with observations of Rayleigh-Bénard convection in the laboratory. It is also consistent with the simulation results of Mason (1989), and the much higher resolution simulation of Schmidt and Schumann (1989). This is not surprising as the large thermals which dominate in the free convective boundary layer are easily resolved by all models.

Figure 3.7 shows the velocity and temperature variance profiles from the four runs. Note that they have been scaled using the convective velocity and temperature scales, w_* and θ_f , defined through

$$w_* = \left(\left(\frac{g}{\theta_r} \right) \langle w'\theta' \rangle_0 z_i \right)^{1/3} \quad (3.1)$$

and

$$\theta_f = (\langle w'\theta' \rangle_0 / w_*) \quad (3.2)$$

It can be seen that the variances for all four runs are encouragingly consistent. Note also that the differences between the scaled $\langle u'u' \rangle$ and $\langle v'v' \rangle$ profiles are of comparable magnitude to the differences between the profiles from the various runs, suggesting that such differences as do exist may be largely statistical in origin. The present results are also close to those obtained by Krettenauer and Schumann (1992) in similar simulations. It is concluded that LES results in free convective conditions are, for second moments at least, relatively insensitive to resolution and the use of backscatter.

Figure 3.7 also shows the approximate spread in the laboratory measurements of Adrian *et al.* (1986). This study dealt with convection between fixed plates, driven by a heat flux at the lower plate but with zero flux through the upper. The stress-free rigid lid at the top of the domain acts as a plate of zero roughness, leading to a large peak in horizontal variance due to the spreading out of updraughts impinging on the lid. The LES simulations of Sykes and Henn (1989) which used a rough plate at the upper boundary, showed that the assumed roughness of the plates does affect the magnitude of the horizontal velocity variance, particularly close to the upper boundary, but also to

Figure 3.7: Velocity and temperature variances for the four simulations of the convective boundary layer capped by stress-free rigid lids. The variances have been normalized using the convective velocity and temperature scales, w_* and θ_f . The shaded regions enclose the experimental results of Adrian *et al.* (1986).

CHAPTER 3: CBL TURBULENCE

some extent in mid boundary layer. Therefore, although the shape of the profile seems reasonable, the quantitative agreement between the LES results for $\langle u'u' \rangle / w_*^2$ and the experimental data in mid boundary layer may be somewhat fortuitous. Sykes and Henn found that results for the vertical velocity and temperature variances were considerably less sensitive to the boundary conditions, and the present LES results are in reasonable agreement with the experimental data, the model values of $\langle w'w' \rangle / w_*^2$ lying on the upper side of the spread of data points, while the $\langle \theta'\theta' \rangle / \theta_f^2$ results follow the lowest measured values.

Figure 3.5 showed that in the neutral case, similar variance profiles are obtained when using stress-free rigid lids and temperature inversions to form the boundary layer top. More marked differences are found in the convective case. Figure 3.8 shows the results from simulations IC (inversion) and BCHR (lid). In simulation IC overshooting updraughts perform work entraining fluid from above the boundary layer (heat flux at the inversion of $\simeq -0.13\langle w'\theta' \rangle_0$) and the large upper peak in $\langle u'u' \rangle / w_*^2$ is entirely absent. Mid boundary layer values of the horizontal velocity variance are also reduced to around $0.2w_*^2$. There has been a considerable amount of debate over whether LES predictions of $\langle u'u' \rangle / w_*^2$ in the free convective boundary layer are reliable. The present results are broadly consistent with previous LES studies, lying just on the upper edge of the spread of results in the intercomparison study of Nieuwstadt *et al.* (1992). As can be seen from Figure 3.8 they also agree reasonably well with the aircraft measurements over the sea from the AMTEX experiment of Lenschow *et al.* (1980), although showing slightly smaller values in the upper half of the boundary layer. Other atmospheric data (e.g. Caughey and Palmer, 1979) tend to show larger variances. However, it does seem plausible that such data might be contaminated by the presence of a mean wind, with shear production near the surface acting as an additional source of turbulence (see Section 3.4.2). Surface inhomogeneity over land might also lead to enhanced variances. For example, Schmidt (1988) found, using LES, that sinusoidal surface heat flux variations of amplitude 50% of the mean led to a 30% increase in horizontal velocity variance. It has also been suggested (Andreas Dörnbrack, private communication) that atmospheric variances in the boundary

CHAPTER 3: CBL TURBULENCE

Figure 3.8: Variances predicted by large-eddy simulation of the free convective boundary layer capped by a temperature inversion (IC). The symbols show the results of the tank experiments of Deardorff and Willis (1974) and Willis and Deardorff (1985), and the aircraft measurements of Lenschow *et al.* (1980). The dotted line on the vertical velocity variance plot is the interpolation curve, $\langle w'w' \rangle / w_*^2 = 1.8(z/z_i)^{2/3}(1 - 0.8z/z_i)^2$. Also shown for comparison, are the results of simulation BCHR in which the boundary layer is capped by a stress-free rigid lid.

layer might be increased by forcing from gravity waves in and above the inversion layer.

Figure 3.8 also shows that the $\langle u'u' \rangle / w_*^2$ profiles are in good agreement with case S1 of the convection tank experiments of Willis and Deardorff (1974) which used an aspect ratio of two, but tend to be low compared to the experiments of Deardorff and Willis (1985) which used an aspect ratio of five. However it has been suggested (Schmidt and Schumann, 1989) that at least some of the increase in the latter study was due to horizontal variations in the surface heat flux, so the impact of the change in aspect ratio is not clear. A test LES run with the same mesh spacing as BCLR but with a domain of $6.4z_i \times 6.4z_i \times z_i$ (instead of $4z_i \times 4z_i \times z_i$) was performed and gave almost identical variance profiles. This result is consistent with those of the similar tests performed by Sykes and Henn (1989) and Mason (1989) and suggests that use of the smaller domain, while forcing more energy onto smaller scales, does not have a significant impact on the total variances.

A more recent laboratory study by Hibberd and Sawford (1994) which used a saline tank, again produced horizontal velocity variances significantly larger than LES ($0.34w_*^2$ in mid boundary layer). A full explanation is not offered, although the discrepancy may be in part due to their relatively strong inversion ($Nt_* = 23$ compared to around 8 in the LES inversion runs, IC and ICHR). This leads to a strong upper maximum in $\langle u'u' \rangle$, in many ways reminiscent of the LES results with a rigid lid. Some low resolution LES tests failed to show any significant variation of $\langle u'u' \rangle / w_*^2$ with the strength of the overlying inversion, but arguably much higher resolution is required to obtain credible results with stronger inversions.

In summary, the LES results for the horizontal velocity variance do seem to be credible for the idealized case studied, but the wide scatter in observational results indicates sensitivity to a large number of factors. In contrast, results for the vertical velocity variance are much less scattered and good agreement is found with the interpolation curve proposed by Lenschow *et al.* (1980) and with the laboratory experiments of Willis and Deardorff (1974) and Deardorff and Willis (1985). Note that the effect of allowing entrain-

ment is much less marked than for $\langle u'u' \rangle / w_*^2$, although the process does lead to a slight lowering of the height of the maximum of $\langle w'w' \rangle / w_*^2$, and reduced values in the upper half of the boundary layer. The temperature variance results with and without entrainment are very similar, except close to the inversion where entrainment of warm air from aloft leads to a large peak in $\langle \theta'\theta' \rangle$. The shapes of the LES profiles are encouragingly consistent with observations, and although the mixed layer values are slightly low compared to most observations, it should be noted, following Schmidt and Schumann (1989), that the magnitude of the temperature fluctuations in this region is small (typically of order 0.1K) making any observations prone to error.

3.1.3 Summary to Section 3.1

In this section results have been presented from a variety of simulations of the boundary layer in neutral conditions and in free convective conditions. The main conclusions are as follows:

1. The agreement with observations, both from the field and the laboratory, has generally been good and increases the level of confidence in the ability of the model to produce credible simulations of turbulence in the convective boundary layer.
2. The results have been shown to be relatively insensitive to model resolution. This is encouraging as it provides at least limited evidence for convergence of results with increasing resolution. Also it increases confidence in the value of low resolution simulation results. This is important as it means that additional sensitivity tests can be performed relatively cheaply, and also because results from low resolution simulations (which have been run to long time) are used extensively when studying drag coefficients in Chapter 4.
3. Entrainment appears to have minimal impact in simulations of the neutral boundary layer. However some statistics, most notably $\langle u'u' \rangle / u_*^2$, are significantly affected by

the use of a rigid lid (rather than a temperature inversion) to cap the boundary layer in convective conditions.

4. As expected, the impact of backscatter in conditions of free convection is minimal.

3.2 Simulations in the mixed shear and buoyancy regime

As discussed in Chapter 1, the stability of the convective boundary layer is characterized by $-z_i/L$, or alternatively by the ratio of the convective velocity scale, w_* , to the friction velocity, u_* . Values of these quantities for the high and low resolution lid runs can be found in Table 3.3. Note that the naming convention is designed so that the approximate stability of each simulation can be ascertained from the the name of that simulation – M03 has $-z_i/L \simeq 0.3$, M21 has $-z_i/L \simeq 2.1$, M64 has $-z_i/L \simeq 6.4$ and so on. Also shown in the table are the angles between the surface and geostrophic winds (α_0), the eddy turnover times (t_*), and the averaging periods used. In the high resolution simulations, the averages are typically over four eddy turnover times.

Table 3.4 gives results for the inversion runs. These simulations all show a negative buoyancy flux at the top of the boundary layer. The magnitude of this entrainment flux is found to be around 13% of the size of the surface buoyancy flux in simulation IC, and about 60% of the surface value in I03. However, a discussion of the factors affecting the size of the entrainment flux and the rate of inversion rise is deferred until Chapter 6. The present chapter concentrates on the effects of entrainment on turbulence in the boundary layer interior by comparing the results of the lid and inversion runs.

Note that relatively short averaging periods were used in the more unstable runs. This was done in order to prevent excessive inversion rise within any one averaging period, but makes the results rather more prone to statistical error, with profiles from successive averaging periods sometimes showing considerable scatter. This is most noticeable when

CHAPTER 3: CBL TURBULENCE

high resolution ($80 \times 80 \times 64$ points)							
run	w_*/ms^{-1}	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	$-z_i/L$	t_*/s	Averaging time /s	Total time /s
BNHR	0.00	0.42	20.0	0.00	2390	10000	30000
M04HR	0.46	0.46	17.8	0.40	2160	10000	30000
M09HR	0.69	0.52	17.5	0.95	1440	6000	24000
M23HR	1.00	0.55	17.4	2.35	1000	4000	20000
M40HR	1.26	0.59	19.5	3.99	794	3000	18000
M68HR	1.59	0.62	22.1	6.83	630	3000	18000
M147HR	2.15	0.65	24.5	14.7	464	3000	14000
BCHR	2.15	0.08	—	7300	464	3000	12000

low resolution ($40 \times 40 \times 32$ points)							
run	w_*/ms^{-1}	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	$-z_i/L$	t_*/s	Averaging time /s	Total time /s
BNLR	0.00	0.45	18.0	0.00	2220	10000	100000
M03	0.46	0.52	18.5	0.28	1920	10000	100000
M09	0.69	0.54	17.5	0.87	1440	10000	100000
M21	1.00	0.58	18.6	2.06	1000	10000	100000
M35	1.26	0.61	20.8	3.51	794	10000	100000
M64	1.59	0.63	23.0	6.35	630	10000	100000
M134	2.15	0.67	25.8	13.4	464	10000	100000
BCLR	2.15	0.05	—	25000	464	5000	20000

Table 3.3: Results of high and low resolution simulations of the boundary layer capped by a stress-free rigid lid at $z_i = 1000$ m. w_* is the convective velocity scale, u_* is the friction velocity, and α_0 is the angle between the surface stress and the geostrophic wind. $-z_i/L = \kappa(w_*/u_*)^3$ is used to characterize a particular flow. Note that the averaging period for statistics in the high resolution simulations is typically four times the eddy turnover time, t_* .

CHAPTER 3: CBL TURBULENCE

high resolution ($80 \times 80 \times 100$ points)								
run	w_*/ms^{-1}	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	z_i/m	$-z_i/L$	t_*/s	Averaging time /s	Total time /s
INHR	0.00	0.43	21.3	879	0.00	2040	5000	40000
I10HR	0.68	0.51	18.3	962	0.95	1410	5000	30000
ICHR	1.27	0.03	—	1030	26000	810	1000	11000

low resolution ($40 \times 40 \times (64 - 72)$ points)								
run	w_*/ms^{-1}	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	z_i/m	$-z_i/L$	t_*/s	Averaging time /s	Total time /s
IN	0.00	0.44	19.7	847	0.00	1940	10000	50000
I03	0.47	0.49	18.5	1007	0.35	2060	10000	50000
I10	0.69	0.52	18.2	1003	0.97	1450	5000	40000
I27	1.07	0.57	17.7	1239	2.70	1150	2000	50000
I77	0.98	0.36	21.1	934	7.69	960	2000	30000
IC	1.28	0.03	—	1052	37000	820	1000	11000

Table 3.4: Results of high and low resolution simulations of the boundary layer capped by a temperature inversion. Values shown are for the final averaging period in each run.

looking at third order moments such as $\langle w'w'w' \rangle$, particularly in the moderately unstable runs which show considerable wave activity around the inversion and fluctuations in the entrainment flux. Accordingly, turbulence statistics from successive averaging periods in the inversion runs have been averaged together (as functions of z/z_i) to form ‘long averages’, and it is these which are shown in the section on turbulence statistics. They typically represent averages over around $10t_*$, although rather shorter in INHR and ICHR ($7t_*$ and $4t_*$ respectively). Note that this approach is not quite equivalent to having taken a single long average over time, as each individual profile is normalized using the value of z_i appropriate at that time, and so the final averages should be less sensitive to changes in z_i over time.

First some flow fields from these simulations are presented, and then the variation of some turbulence statistics with stability is examined.

3.3 Flow fields

Figure 3.9 shows horizontal sections of the w fields at $0.2z_i$ from a selection of the high resolution lid runs. BNHR shows the irregular pattern characteristic of neutral flows, and the structures in M04HR do not appear to be significantly different. However, the flow fields change markedly with increasing instability. M09HR shows a large convective roll, aligned with the x -axis and spanning the entire domain. M23HR and M40HR (not shown) appear similar, although by M68HR there are signs that the roll structure is beginning to break up. Indeed, by M147HR there is a cellular structure not dissimilar to that in the free convective simulation, BCHR. Therefore these results suggest that the transition from the regime favouring roll vortices to that favouring cellular convection occurs at a value of $-z_i/L$ of around 7. This is reasonably consistent with the LES results of Sykes and Henn (1989) which showed the transition at $-z_i/L \simeq 9$, and also the BOMEX data (see Chapter 1).

The flow fields from the low resolution lid runs show a similar variation with stability. Figure 3.10 shows results from some of the inversion runs. Note that the horizontal sections shown are all at 207 m, which is around $0.25z_i$ although there is a slight variation between runs due to differing values of z_i . In these runs there is some evidence of a rather broken roll structure with $-z_i/L$ as small as 0.4, and simulation I10 shows two main bands of ascent (cf the single band in M09HR). Nevertheless the tendency of the regions of ascent in the lower CBL to become organized into bands at intermediate values of stability does not appear to have been significantly affected by inclusion of the entrainment process. Rather more marked differences between the flows in the lid and inversion runs can be seen higher in the boundary layer. Figure 3.11 shows wind vectors in vertical sections from simulations M09HR and I10HR. The sections are in the $y-z$ plane and are therefore perpendicular to the roll axes. In M09HR a single strong roll can be seen. On approaching the stress-free upper boundary, the updraught simply spreads out horizontally giving rise to a large peak in $\langle v'v' \rangle$. Almost horizontal outflow continues until two opposing flows meet, at which point the downdraught is observed. In I10HR there is a two roll pattern,

CHAPTER 3: CBL TURBULENCE

Figure 3.9: Horizontal sections of w fluctuations at $z/z_i = 0.21$ from a selection of the high resolution lid runs. The contour interval is 0.3 ms^{-1} for BNHR, M04HR, M09HR and M68HR, and 0.4 ms^{-1} for M127HR and BCHR.

CHAPTER 3: CBL TURBULENCE

Figure 3.10: Horizontal sections of w fluctuations at height 207 m ($z/z_i \simeq 0.25$) from a selection of the inversion runs. The contour interval is 0.3 ms⁻¹ in all cases.

Figure 3.11: Vertical slices in the $y-z$ plane showing velocity vectors from simulations M09HR and I10HR.

CHAPTER 3: CBL TURBULENCE

with rather weaker horizontal outflow around the temperature inversion at z_i . Above the inversion there is evidence of gravity wave motions induced by updraughts impinging on the inversion. Moeng and Rotunno (1990) suggest that updraughts in the free convective boundary layer lose most of their energy by setting the inversion into motion, and therefore induce only weak return flow. It is not immediately clear from Figure 3.10 that the roll downdraughts in I10HR are weaker than those in M09HR, but note that the skewness of the vertical velocity field is larger in this simulation, consistent with the downdraughts being relatively weak and diffuse compared to the updraughts (see Section 3.4.4). Hence it seems plausible that the entrainment process, while not preventing the formation of large-scale structures such as rolls, might place a restriction on the strength and size of these circulations.

The presence of roll structures in these simulations is clear, and it is encouraging that they appear over a range of stabilities broadly consistent with that observed in the atmosphere. However, the use of periodic boundary conditions with a small domain severely constrains their possible spacings and orientations, and it is not obvious how much this constraint affects the turbulence statistics. Indeed, it is not impossible that their very formation in the model is due to the periodic boundary conditions. Accordingly two additional test simulations were performed to examine the sensitivity of the results to domain size and orientation.

The first test aimed to reduce the influence of the periodicity by using a much larger domain. It was run using the same geostrophic wind and surface heat flux as M09HR, but had a horizontal mesh spacing of 200 m (a factor of four larger than in M09HR) so that the domain was a square of size 16 km. In view of the degradation of the horizontal resolution, the number of mesh points in the vertical was reduced with 40 points below the rigid lid at 1 km, and the basic mixing length, λ_0 , was increased to 46 m. Figure 3.12 shows that rolls are still observed in this large domain, and in this case they do not span the entire domain which should mean that the boundary conditions have less influence. The spacing of between 2 and 3 times the boundary layer depth is also encouragingly consistent with atmospheric observations (see Chapter 1). Note however that there are

Figure 3.12: Horizontal sections of w fluctuations at $z/z_i = 0.2$ from additional runs performed as sensitivity tests. Both should be compared with M09HR. The first plot shows results using a much larger domain; the second shows results obtained with the geostrophic wind aligned with the x -axis (rather than rotated 13 degrees). The contour interval is 0.3ms^{-1} in both cases.

still a very limited number of possible orientations, and once again the rolls are aligned with the x -axis. In order to realistically simulate roll orientation a still larger domain would be needed. However, even with this domain the simulation is very poorly resolved (the vertical velocity variance is less than 50% resolved at $0.3z_i$). Hence the smaller domains are preferred, even though the roll structure is undoubtedly dependent on the grid geometry.

The second plot in Figure 3.12 shows results of a test simulation, similar to M09HR in all respects except that the geostrophic wind is parallel to the x -axis, rather than rotated 13 degrees. Rolls are still observed, although this time there is two roll pattern rather than the single roll of M09HR. Interestingly, the vertical profiles of turbulence statistics (e.g. velocity variances) from the two runs are found to be similar. Moeng and Sullivan (1994) noted similar statistics from two simulations, one at $-z_i/L = 1.6$ which had a clear two roll pattern, and another at $-z_i/L = 1.4$ in which rolls were not visible. These results suggest that scaled turbulence statistics are not strongly affected by the organization of convection into large roll structures.

Figure 3.13: Mean wind profiles from runs BNLR, M03, M21, and M134. The x -axis is aligned with the geostrophic wind.

It is concluded that the formation of roll structures by the model is broadly realistic, although their orientation and spacing are undoubtedly affected by the use of relatively small domains with periodic boundary conditions. Nevertheless, there is at least limited evidence that LES turbulence statistics at a given stability are not particularly sensitive to the presence or otherwise of large roll structures, so any unrealistic spacings or orientations of such structures should not have a major effect.

3.4 Turbulence statistics

Figure 3.13 shows the mean wind profiles from a selection of the low resolution lid simulations. They are shown at this point to confirm that the simulations capture the expected changes with stability, with significant shear at all levels in BNLR but reasonably well mixed profiles in the more convective runs. However, a detailed examination of the mean fields and attempts to model them with simple mixed layer and closure models is post-

Figure 3.14: Variation of $\langle w'w' \rangle / w_*^2$ with stability. The first plot shows profiles from some of the high resolution runs of the boundary layer capped by a rigid lid (free convective and $-z_i/L \simeq 6.8, 2.3, 0.9, 0.4$). The second plot shows profiles from runs using a temperature inversion (free convective and $-z_i/L \simeq 7.7, 2.7, 0.9, 0.3$), and also some atmospheric observations. Squares : Lenschow *et al.* (1980); Triangles : flight H467 of Grant (1986); Diamonds : class A of Nicholls and Readings (1979).

poned until Chapter 4. Instead, this section looks at the variation with stability of scaled turbulence statistics from both the lid and inversion simulations.

3.4.1 Vertical velocity variance

Figure 3.14 shows profiles of $\langle w'w' \rangle / w_*^2$ from a selection of the simulations. The results obtained using a stress-free rigid lid will be considered first. The variance in these simulations is typically between 80 and 90% resolved for $z/z_i \gtrsim 0.2$, so the results should not be sensitive to the subgrid estimates. The free convective profile of BCHR is that which was compared with the laboratory data of Adrian *et al.* (1986) in Figure 3.7. Addition of a mean wind rapidly leads to increased variances close to the surface due to shear production of turbulence. However the variances in the interior of the boundary layer are shown to be insensitive to the presence of a mean wind, at least up to some threshold value of stability. The profiles from simulations M146HR (not shown) and M68HR are very similar to that from BCHR, while even at $-z_i/L = 2.3$ (M23HR) the mid boundary layer maximum is

CHAPTER 3: CBL TURBULENCE

only about 25% larger than the free convective value. Analysis of the energy budgets (not shown) reveals that this is due to buoyant mixing keeping the velocity profiles reasonably well mixed, so that buoyancy production of turbulence dominates over shear production throughout most of the CBL. Furthermore, while buoyancy forcing contributes directly to $\langle w'w' \rangle$, shear production can only contribute to $\langle u'u' \rangle$. Energy could be transferred from the horizontal to the vertical velocity component by the pressure forces, but the LES shows that for $-z_i/L \gtrsim 1$, $\langle p'\partial w'/\partial z \rangle$ is negative throughout the CBL, indicating that the transfer is in the opposite direction. In contrast, the $\langle w'w' \rangle$ profile from simulation M04HR is similar in shape to that obtained in the neutral simulation, BNHR. It seems that the transition between essentially free convective and neutral regimes for the vertical velocity variance occurs relatively rapidly, over a range of $-z_i/L$ between around 3 and 0.5. This is consistent with the finding of Deardorff (1972a) that the boundary layer root mean square vertical velocity scales with w_* for $-z_i/L \gtrsim 4.5$.

The results obtained in the simulations using a more realistic temperature inversion show a similar dependence on stability, with interior values of $\langle w'w' \rangle$ remaining close to free convective for $-z_i/L \gtrsim 3$. Interestingly there does appear to be a slight minimum in $\langle w'w' \rangle/w_*^2$ around $-z_i/L = 7$. Some of the decrease relative to the free convective result of ICHR might be due to the relatively poor resolution of simulation I77, although the discrepancy between the high and low resolution results of ICHR and IC is smaller by a factor of about three, suggesting that at least some of the decrease may be real. Note that Mason (1992) also found a slight minimum of $\langle w'w' \rangle/w_*^2$ in his R7 ($-z_i/L = 6.3$). The change in behaviour close to the surface is an artefact of the procedure used to average profiles from the inversion runs, and has no physical significance.

The result that relatively small values of $-z_i/L$ are required before the vertical velocity variance increases significantly above its free convective value, is supported by atmospheric data. Also shown in Figure 3.14 are the highly convective results of Lenschow *et al.* (1980), and data from flight H467 of Grant (1986) for which $-z_i/L = 5.9$, and class A of Nicholls and Readings (1979) for which the average value of $-z_i/L$ is 3.9. These data are generally consistent and show little or no trend with stability.

CHAPTER 3: CBL TURBULENCE

Parametrization of $\langle w'w' \rangle$ is of particular importance for dispersion modelling. Højstrup (1982) and Hunt (1984) argue for the statistical independence of shear and buoyancy produced turbulence close to the surface, and therefore advocate addition of separately modelled contributions to the variance. Their ideas find support in the works of Panofsky *et al.* (1977) and Wayland and Raman (1994) which both showed reasonable agreement between atmospheric measurements and the empirical curve

$$\langle w'w' \rangle = \left(1.6 + 2.9 \left(\frac{z}{-L} \right)^{2/3} \right) u_*^2 = 1.6u_*^2 + 5.3 \left(\frac{z}{z_i} \right)^{2/3} w_*^2 \quad (3.3)$$

Note that the first term on the right hand side of Equation (3.3) represents the contribution to the variance of shear-generated turbulence, and the second term represents the buoyancy contribution. The large-eddy simulations are poorly resolved close to the surface and therefore not suitable for critical evaluation of parametrizations such as this. However, it is encouraging that the results show a steady increase in $\langle w'w' \rangle$ with increasing shear, and are broadly consistent with (3.3).

One possible approach to parametrizing the vertical velocity variance in the boundary layer interior is to apply the assumption that shear and buoyancy generated turbulence are independent of each other at all heights. This leads to a parametrization of the form

$$\langle w'w' \rangle = f_N u_*^2 + f_C w_*^2 \quad (3.4)$$

where f_N and f_C are shape functions describing the profiles of $\langle w'w' \rangle / u_*^2$ and $\langle w'w' \rangle / w_*^2$ as functions of (z/z_i) in neutral and free convective conditions respectively. This is attractively simple and also has the advantage of being consistent with (3.3) in the surface layer. However, it implies that any non-zero value of u_* will lead to an increase in $\langle w'w' \rangle$ relative to free convective values at all levels, which has been shown not to be the case. Another possibility is to take

$$\langle w'w' \rangle^{3/2} = (f_N u_*^2)^{3/2} + (f_C w_*^2)^{3/2} \quad (3.5)$$

This has the potential advantage over (3.4) that u_* loses its influence more quickly as $-z_i/L$ increases. In fact, Panofsky *et al.* (1977) found that an interpolation formula based on adding cubes rather than squares performed better for large $-z/L$ in the surface layer.

Figure 3.15: w_B/w_* for LES lid runs. Diamonds : high resolution; Squares : low resolution. Note that results from BCHR and BCLR are plotted at $-z_i/L = 16$ to show the convective limit. Also shown are the results of three possible parametrizations, involving linear, quadratic and cubic combinations of u_* and w_* , as described in the text.

Also it could be argued that the shear and buoyancy production terms in the turbulence kinetic energy budget scale with u_*^3/z_i and w_*^3/z_i respectively, giving this interpolation formula some physical justification.

w_B is defined to be the square root of the average value of $\langle w'w' \rangle$ between the surface and z_i i.e. a boundary layer average root mean square vertical velocity. The variation with stability of w_B/w_* for the LES lid runs is shown in Figure 3.15. As expected, it is almost constant from $-z_i/L = \infty$ until $-z_i/L \simeq 3$, and then increases sharply as shear effects become significant. Also shown are the results of three possible parametrizations, all of which have been tuned to give $w_B = 0.9u_*$ when $w_* = 0$ and $w_B = 0.6w_*$ when $u_* = 0$ to be consistent with the LES results in the neutral and convective limits. That labelled 'linear' represents the curve, $w_B = 0.6(w_* + 1.5u_*)$, and can be seen to systematically overestimate the root mean square vertical velocity. In contrast, the parametrization $w_B = 0.6(w_*^2 + 2.25u_*^2)^{1/2}$, which is consistent with vertical integration of Equation (3.4),

CHAPTER 3: CBL TURBULENCE

is in much better agreement with the LES results, although still overestimating w_B by $\simeq 15\%$ when $-z_i/L \simeq 2$. Note however that the cubic combination, $w_B = 0.6(w_*^3 + 3.4u_*^3)^{1/3}$ which is consistent with (3.5), performs better still.

Consistent with these findings for the root mean square velocity, it is found that Equation (3.5) is more successful than (3.4) in reproducing the LES variance profiles. Using results from BNHR and BCHR to give f_N and f_C , it predicts variances within 20% of the LES values in most cases, with the largest error being a 50% overestimate at $z/z_i = 0.3$ for $-z_i/L = 1$. Interpolation formula (3.4) shows a rather larger overestimate ($\simeq 100\%$) at this point, and generally shows a greater influence of u_* on the variance in mid boundary layer in convective conditions. Neither formula is capable of reproducing the slight minimum in $\langle w'w' \rangle$ found around $-z_i/L = 7.7$ in the inversion runs, but once again the agreement of (3.5) with the LES inversion run results is slightly more satisfactory than that of (3.4).

In conclusion, for practical dispersion models requiring a profile of $\langle w'w' \rangle$ in the CBL, the use of Equation (3.5) is advocated. This requires specification of the shape functions, f_N and f_C , and $f_N = 1.3(1 - 0.8z/z_i)$ and $f_C = 1.8(z/z_i)^{2/3}(1 - 0.8z/z_i)^2$ are suggested, consistent with LES and observational results. Note that the variances predicted will be sensitive to the values of u_* , w_* and z_i , which may not be known accurately. Therefore it may be that any additional errors brought about by the use of interpolation formula (3.4) instead of (3.5) are not significant in practice.

3.4.2 Horizontal velocity variances

The effect of shear on the horizontal velocity variance profiles is rather different. Shear production contributes directly to $\langle u'u' \rangle$ (strictly to the component aligned with the mean shear at that height), but can only have an effect on $\langle w'w' \rangle$ through transfer of kinetic energy via the pressure forces. Deardorff (1972a) found that this transfer was relatively slow so that shear had more effect on $\langle u'u' \rangle$ than $\langle w'w' \rangle$ or, alternatively, larger values of

CHAPTER 3: CBL TURBULENCE

$-z_i/L$ were required before $\langle u'u' \rangle$ scaled convectively.

Figure 3.16 shows the results for the horizontal velocity variances scaled using the convective velocity scale. In the inversion runs $\langle u'u' \rangle / w_*^2$ increases monotonically with increasing geostrophic wind, having a value in mid boundary layer of around four times the free convective value for $-z_i/L \simeq 1$. The increase in $\langle v'v' \rangle$ is less rapid (as energy has to be transferred from $\langle u'u' \rangle$ by the pressure forces) although still monotonic. There is some evidence of slight upper maxima in the profiles from the moderately unstable runs, consistent with the presence of roll structures in these simulations.

The most unstable lid runs tend to show larger values of $\langle u'u' \rangle$ than the corresponding inversion runs as the transfer of energy from $\langle w'w' \rangle$ is more significant as updraughts impinge on the stress-free lid. However, the profiles show a similar increase in variance as shear production becomes increasingly important. The $\langle v'v' \rangle$ statistics are dominated by the presence of very strong roll circulations in these runs and are probably not relevant to the atmospheric boundary layer.

It is concluded that free convective scaling does not appear to be appropriate for the horizontal velocity variance profiles. They might be expected to scale more successfully with u_*^2 when shear production is important. Indeed Figure 3.17 shows that the neutral and moderately unstable inversion run profiles do collapse reasonably successfully when this scaling is used. Apart from I03, which behaves somewhat anomalously, increasing instability tends to reduce the scaled variances in the lower boundary layer as the smaller mean velocity gradients lead to reduced shear production. At the same time variances aloft tend to increase due to transfer from the buoyancy driven $\langle w'w' \rangle$. With increasing instability this transfer becomes more important and eventually the scaled variances exceed their neutral values at all heights. Note however that the pressure forces mainly transfer energy into $\langle v'v' \rangle$ rather than $\langle u'u' \rangle$, consistent with the presence of roll structures in the simulations. Similar behaviour was observed by Grant (1986) who found that $\langle v'v' \rangle / u_*^2$ increased significantly between neutral conditions and $-z_i/L = 5.8$, while $\langle u'u' \rangle / u_*^2$ was little changed in the lower part of the boundary layer.

CHAPTER 3: CBL TURBULENCE

Figure 3.16: Variation of horizontal velocity variances with stability. The x -axis is aligned with the mean boundary layer wind. Profiles are shown from lid runs, BC_{HR}, M68_{HR}, M23_{HR}, M09_{HR} and M04_{HR}, and inversion runs, IC_{HR}, I77, I27, I09_{HR} and I03, as in Figure 3.14.

Figure 3.17: Horizontal velocity variances from the inversion runs, scaled by u_*^2 . The x-axis is aligned with the mean boundary layer wind.

3.4.3 Temperature variance

Figure 3.18 shows profiles of the total temperature variance (i.e. resolved plus subgrid), scaled using the convective temperature scale, $\theta_f = (\langle w'\theta' \rangle_0 / w_*)$. There is considerable uncertainty in the subgrid estimates but note that the high (low) resolution simulation variances are all 80% (60%) resolved at $z/z_i = 0.1$ and 90% (80%) resolved for $z/z_i \gtrsim 0.2$, and so errors in these estimates are not expected to significantly affect the results quantitatively except in the surface layer.

Very close to the surface a large peak in $\langle \theta'\theta' \rangle / \theta_f^2$ is expected, and found, as the production term in the temperature variance budget ($-\langle w'\theta' \rangle \partial \langle \theta \rangle / \partial z$) becomes large. The size of the surface peak does vary with stability, as the near surface temperature gradients depend on u_* , and the temperature variance is expected to scale with $\theta_* (= \langle w'\theta' \rangle_0 / u_*)$ rather than θ_f . However, experimental results from the atmospheric surface layer suggest that u_* loses its influence on the variance relatively quickly as distance from the surface increases. For example, Ohtaki (1985) found that the variance scaled convectively for $-z/L \gtrsim 0.1$, and Hicks (1981) found that this was the case for $-z/L \gtrsim 0.3$. Accordingly it is not surprising to find that the profiles of $\langle \theta'\theta' \rangle / \theta_f^2$ from simulations M09HR, M23HR

Figure 3.18: Variation of $\langle \theta' \theta' \rangle / \theta_i^2$ with stability. The first plot shows profiles from some of the high resolution runs of the boundary layer capped by a rigid lid. The second plot shows profiles from runs using a temperature inversion.

and M68HR are in good agreement throughout most of the boundary layer, although the values from the free convective simulation, BCHR, do appear to be anomalously low. Convective inversion run ICHR is in better agreement with the less unstable runs I77, I27 and I09HR in mid CBL. It is concluded that the LES results are broadly consistent with the experimental results mentioned above, although the inversion runs clearly show that values of $\langle \theta' \theta' \rangle$ above about $0.7z_i$ are highly sensitive to the entrainment process.

3.4.4 Skewness

The vertical velocity skewness, $\langle w'w'w' \rangle / \langle w'w' \rangle^{3/2}$ provides important information on flow structure and energy transport. It has a value zero for Gaussian turbulence, while positive values indicate relatively strong, narrow updraughts and weak, diffuse downdraughts. For $\langle w'w' \rangle$ the sum of the resolved and subgrid parts is taken as before. Following Mason (1989), total $\langle w'w'w' \rangle$ is estimated by adding two-thirds of $\langle w'(SKE) \rangle$ (where SKE is the subgrid energy) to the resolved value. This 'mixed scale' contribution has a large effect near the surface, but typically contributes less than 20% of the total for $z/z_i > 0.2$.

Figure 3.19: Variation of vertical velocity skewness with stability.

The entirely subgrid scale contribution is neglected but it is not expected to be significant in the flow interior.

The results in Figure 3.19 show the skewness increasing at first with increasing instability in the lid runs, but tending to become constant in mid CBL with a value of around 0.5 for $-z_i/L \gtrsim 1$. It has already been shown that $\langle w'w' \rangle$ scales approximately convectively in the CBL interior for moderate values of $-z_i/L$ and this result suggests that $\langle w'w'w' \rangle$ behaves similarly. This is consistent with the triple moment being dominated by large-scale thermals, with approximately Gaussian shear turbulence having little influence even in the surface layer as shown in the measurements of Hunt *et al.* (1988).

The inversion runs show similar profiles in the lower halves of the boundary layers, although tending to show slightly larger values. The increase in values is more marked higher up, particularly in simulation ICHR. The change relative to the lid runs is associated with updraughts losing some of their energy entraining fluid from above the inversion resulting in weaker downdraughts as discussed in Section 3.3. Observations in the upper CBL generally show rather smaller skewness values ($\simeq 0.6$) than LES results. This has sometimes been interpreted as a failing of the simulations, but Mason (1989) and Moeng and Rotunno (1990) have suggested that observations might be contaminated by

Figure 3.20: Variation of dissipation length scale (normalized by boundary layer depth) with stability.

larger-scale mesoscale structures or gravity waves which contribute to $\langle w'w' \rangle$ but have little effect on $\langle w'w'w' \rangle$. These ideas were supported by the analysis of experimental data performed by LeMone (1990). Thus it is concluded that the LES skewness profiles are credible, although only directly comparable with observations made in conditions close to the idealized ones which are simulated.

3.4.5 Dissipation length scale

Almost all boundary layer parametrization schemes require specification of a turbulent length scale, and here the variation of the dissipation length, λ_E , with stability is examined (Figure 3.20). It is defined through

$$\lambda_E = \frac{(\langle u'u' \rangle + \langle v'v' \rangle + \langle w'w' \rangle)^{3/2}}{\langle \epsilon \rangle} \quad (3.6)$$

where ϵ is the dissipation rate. The first plot shows the results of some of the lid runs. Due to a diagnostic error, the dissipation rate in some of these runs had to be estimated as a residual in the turbulent kinetic energy budget, assuming stationarity. This approach makes the profiles rather rough, and prone to errors near the boundaries where any inconsistencies in the diagnostic evaluation of the budget terms have most effect. Nevertheless,

CHAPTER 3: CBL TURBULENCE

it is clear that the length scale has a tendency to approach a constant value (which depends on stability) in mid boundary layer. That value is around $2z_i$ in the neutral run, and between $3.5z_i$ and $4z_i$ for the simulations with $-z_i/L \gtrsim 1$.

The profiles from the inversion runs are now considered. Looking again at Figure 3.20, it can be seen that inclusion of entrainment does not have a major effect on the neutral length scale, and that moderate instability still brings about a significant increase in λ_E . However, the mid CBL values do appear to be rather smaller in the unstable runs with inversions than in those with lids, consistent with the earlier suggestion that entrainment tends to reduce the importance of large scale motions. The values of λ_E in the upper CBL are subject to considerable statistical uncertainty, even after averaging of successive profiles (the six averaging periods used from simulation I27 gave values of λ_E at $0.6z_i$ ranging between $2.2z_i$ and $3.8z_i$). However the values of λ_E in the upper CBL in the moderately unstable simulations, do appear to be significantly larger than in the free convective simulation. This is presumably associated with the presence of large roll structures in these runs and it is interesting that a similar result was found by Moeng and Sullivan (1994).

3.4.6 Non-dimensional gradients

Monin-Obukhov similarity theory relates the mean gradients of wind and temperature in the surface layer to the surface fluxes:

$$\left(\left(\frac{\partial \langle u \rangle}{\partial z} \right)^2 + \left(\frac{\partial \langle v \rangle}{\partial z} \right)^2 \right)^{1/2} = \frac{u_*}{\kappa z} \phi_m \quad (3.7)$$

and

$$\left(\frac{\partial \langle \theta \rangle}{\partial z} \right) = \frac{\theta_*}{\kappa z} \phi_h \quad (3.8)$$

where $\theta_* = \langle w' \theta' \rangle_0 / u_*$. The non-dimensional gradients of velocity and temperature, ϕ_m and ϕ_h , are functions of stability and have to be determined empirically. An accurate knowledge of these functions is of vital importance as they are often prescribed to enable the calculation of bulk transfer coefficients relating surface fluxes to mean gradients in

CHAPTER 3: CBL TURBULENCE

numerical models. Furthermore, observed surface layer stability functions are often used to provide the stability dependence of simple one-dimensional parametrizations of the entire boundary layer.

Unfortunately, the determination of the stability functions, ϕ_m and ϕ_h , has proved to be difficult experimentally. Högström (1988) discusses some of the issues involved, and tabulates some widely used formulations. There has been much debate in the literature over questions such as the correct asymptotic form of the functions in the free convective limit, the value of the Prandtl number ($Pr = \phi_h/\phi_m$) in neutral conditions and even the value of the von Karman ‘constant’ (defined so that ϕ_m is unity in neutral conditions). $\kappa = 0.4$ is now widely accepted, and Högström (1988) calculated revised forms for the results of some previous experiments (most notably the Kansas experiment (Businger *et al.*, 1971) which gave $\kappa = 0.35$). However, some have doubted the validity of recalculating experimental results nearly twenty years after the event, and it is common, although strictly inconsistent, to use the stability functions of Businger *et al.* in conjunction with $\kappa = 0.4$. Most authors have assumed that the Prandtl number is unity in neutral conditions, although, as pressure terms feature in the momentum but not the scalar budget equations, it is not clear that ϕ_h should be equal to ϕ_m . In fact, the Kansas value of $\phi_h \simeq 0.7$ has found some support in the results of large-eddy simulations, and whilst noting the need for a continuing program of experiments in the field, a discussion is now given of what has been, and can be learnt from model results.

As discussed earlier, a large-eddy model aims to resolve much of the boundary layer turbulence parametrizing only the smaller-scale (‘subgrid’) eddies. In well resolved regions of the flow, such a model should be capable of giving results which are relatively insensitive to the subgrid model. For example, Mason and Derbyshire (1990) found a turbulent Prandtl number of around 0.7 in the interior of a simulated neutral boundary layer using a constant subgrid Prandtl number of 0.5, whilst Mason and Brown (1994) obtained a similar result using a subgrid value of 0.7. Obtaining information on the surface layer similarity functions, ϕ_m and ϕ_h , is more problematical as the characteristic scale of turbulent eddies decreases close to the surface and so the turbulence is inevitably less well resolved

Figure 3.21: Profiles of ϕ_m from the high resolution runs. The lines are dotted where the turbulent fluxes are less than two-thirds resolved.

in this region. Indeed, it has been usual to regard the level of agreement between model results and observations in this region as a measure of the success of the subgrid model. In this way, Mason and Thomson (1992) used the improved logarithmic profiles simulated in the neutral surface layer when using backscatter as evidence for the importance of modelling that process. Similarly, Brown *et al.* (1994) showed much greater success in reproducing observed surface layer non-dimensional gradients in stable conditions when using backscatter. Large-eddy model results for the behaviour of the stability functions in the convective surface layer are now presented.

The approach taken is to consider only points which are high enough for the turbulence to meet some arbitrary resolution criterion, whilst being low enough for surface layer theory to be judged applicable. These requirements are obviously conflicting, and a compromise is sought with reference to Figure 3.21 which shows profiles of ϕ_m from the high resolution lid runs. There is an almost monotonic decrease in surface layer non-dimensional velocity gradients with increasing instability. Note, however, that ϕ_m increases significantly with height in the neutral simulation BNHR, and so it was decided

CHAPTER 3: CBL TURBULENCE

Businger <i>et al.</i>	:	$\phi_m = (1 - 15z/L)^{-1/4}$	,	$\phi_h = 0.74(1 - 9z/L)^{-1/2}$
Dyer and Bradley	:	$\phi_m = (1 - 28z/L)^{-1/4}$	,	$\phi_h = (1 - 14z/L)^{-1/2}$

Table 3.5: Stability functions of Businger *et al.* (1971) and Dyer and Bradley (1982).

not to consider data from above $z/z_i = 0.1$ (where ϕ_m has a value of around 1.35, compared to 1.0 for an exactly logarithmic profile). For the resolution criterion it was decided to demand that the total fluxes of momentum and heat should be at least two-thirds resolved. Figure 3.21 shows that this excludes a large fraction of the data for $z/z_i < 0.1$ (profiles are dotted where this criterion is not met), but this is accepted in order to reduce the dependence of the results on the subgrid model.

Figure 3.22 shows the variation of ϕ_m and ϕ_h with z/L . Results are shown from both high and low resolution simulations, although the requirement that fluxes should be 2/3 resolved excludes almost all of the points from the low resolution runs. Also shown for comparison are the experimental results of Businger *et al.* (1971) and Dyer and Bradley (1982) (see Table 3.5). These are chosen as giving a reasonable impression of the variation in experimental results, the expression of Businger *et al.* having the weakest stability dependence of those tabulated by Högström (1988), whilst that of Dyer and Bradley has the strongest. Note that the original expressions of Businger *et al.* are being used in conjunction with $\kappa = 0.4$, rather than the modified functions of Högström.

The agreement between the LES and experimental results is good. Arguably the resolution criterion is not strict enough for these simulations to be regarded as an independent source of data and, as mentioned above, it is probably best to regard the agreement as evidence of successful operation of the subgrid model. However, it does seem plausible that more powerful computers in years to come will enable simulations to be performed which are sufficiently well resolved in the surface layer to give independent information on the behaviour of ϕ_m and ϕ_h .

Figure 3.22: Non-dimensional gradients, ϕ_m and ϕ_h , against z/L . Points plotted are from high and low resolution LES lid runs, where $z < 0.1z_i$ and fluxes are at least 2/3 resolved. Also shown for comparison are the results of Businger *et al.* (1971) and Dyer and Bradley (1982).

3.5 Summary

Results have been presented from large-eddy simulations of the atmospheric boundary layer for a range of stabilities between neutral and free convective conditions. Results in the extreme cases have been shown to be in good agreement with observations, and relatively insensitive to resolution (see Section 3.1.3 for a more detailed summary of these results). In cases with both shear and buoyancy forcing, the flow fields show the expected changes with stability. Observational datasets showing changes in turbulence statistics with stability in this intermediate regime are scarce, but those that have been used are broadly consistent with the LES results. The latter indicate that many statistics (e.g. $\langle w'w' \rangle$, $\langle \theta'\theta' \rangle$ and skewness) continue to scale approximately convectively in mid boundary layer even in the presence of a considerable mean wind, with the change to an essentially neutral regime not occurring until $-z_i/L$ is around 1. However the horizontal velocity variances are not found to scale similarly as shear production contributes directly to $\langle u'u' \rangle$ leading to an increase over free convective values. There is little evidence for any abrupt changes in turbulence statistics associated with the formation of rolls, consistent with these structures being no more than an organized form of convection.

Entrainment does not appear to have a major impact on turbulence in the interior of the near neutral boundary layer. In more convective conditions, lid and inversion run results in the lower half of the boundary layer remain similar for most statistics (obvious exceptions are $\langle u'u' \rangle$ and $\langle v'v' \rangle$ which are larger at all levels in the lid runs). In the upper CBL the differences are more marked and can often be directly related to entrainment effects. For example it has been argued that the larger skewness values in the inversion runs result from updraughts losing most of their energy when they impinge on the inversion and so inducing only a weak return flow.

Chapter 4

Mean structure of the CBL and its parametrization

Chapter 3 looked at the turbulence structure of the LES boundary layers, and showed it to be credible across a wide range of conditions, and relatively insensitive to model resolution. This chapter concentrates on the variation with stability of the profiles of the mean fields ($\langle u \rangle$, $\langle v \rangle$ and $\langle \theta \rangle$) and fluxes ($\langle u'w' \rangle$, $\langle v'w' \rangle$ and $\langle w'\theta' \rangle$) – the quantities which are most immediately relevant for large-scale NWP and climate prediction models.

First of all the LES results for the mean wind and temperature structure are presented, and their credibility is established by reference to the predictions of a simple mixed layer model and observational results for various similarity coefficients. Then the ability of various simple closure models to reproduce the results of the LES lid runs is examined. This approach is taken as it is argued that entrainment affects the mean profiles mainly indirectly through its effects on z_i . It is supported by the generally good agreement found between the mean profiles from the lid and inversion runs, given similar values of z_i and $-z_i/L$. It also provides a convenient way of testing the equilibrium performance of closure models against LES, as, with entrainment excluded, they too can be run to long time without problems associated with inversion rise. Factors affecting the entrainment

rate are studied separately in Chapter 6.

Note that in cases where entrainment is particularly rapid (e.g. shallow unstable boundary layers in summer mornings), the direct effects of entrainment on the boundary layer averaged momentum budget may be non-negligible (Garratt *et al.*, 1982). However, in these cases the mean fields are likely to be highly non-stationary and so it is probably not useful to attempt to obtain any ‘equilibrium solution’ and any attempt to compare future LES results with closure model results for these conditions would have to consider the time evolution of the fields.

4.1 Variation of mean wind profiles with stability

Figure 4.1 shows mean wind profiles from the low resolution lid runs (solid lines), which are in quasi-steady state after 100000 s. The neutral simulation shows significant shear throughout the boundary layer. However, with increasing instability, the velocity profiles rapidly become well mixed, with relatively little shear in the CBL interior. Interior values of $\langle u \rangle / u_*$ decrease monotonically with increasing instability, while $\langle v \rangle / u_*$ becomes close to zero for $-z_i / L \gtrsim 1$.

Although this chapter concentrates on the results of the lid runs, it is encouraging to note that the profiles from the low resolution inversion runs (shown dotted in Figure 4.1) show very similar behaviour. In particular, the $\langle u \rangle / u_*$ profiles are very similar throughout most of the boundary layer to those obtained at similar stabilities in the lid runs. The $\langle v \rangle / u_*$ profiles also become well mixed, although they tend to show more shear than the lid run results in the upper CBL as the temperature inversion cannot sustain infinite shear at z_i .

The well mixed velocity profiles in the CBL are amenable to description using a simple mixed layer model. Sometimes (e.g. Garratt *et al.*, 1982) these comprise three layers – a thin surface layer, a deep mixed layer and a transition or inversion layer. However it

Figure 4.1: Mean wind profiles from low resolution lid runs, BNLR, M03, M09, M21, M35, M64 and M134 (solid lines). The x -axis is aligned with the surface stress. $\langle u \rangle / u_*$ decreases monotonically with increasing instability between neutral (N) and more convective (C) conditions. $\langle v \rangle / u_*$ is negative throughout most of the boundary layer in the most neutral runs, but becomes close to zero for $-z_i/L \gtrsim 1$. Also shown for comparison are the profiles from low resolution inversion runs, IN, I03, I10, I27 and I77 (dotted lines).

CHAPTER 4: MEAN STRUCTURE

is common practice to use a simplified two-layer model which assumes that the inversion layer is negligibly thin as in the lid runs.

With the x -axis aligned with the surface stress, it is assumed that the wind profile is given by

$$\kappa \langle u \rangle / u_* = \ln(z/z_0) - \psi(z/L), \quad z_0 < z \leq z_s \quad (4.1)$$

$$\kappa \langle u \rangle / u_* = \ln(z_s/z_0) - \psi(z_s/L), \quad z_s < z \leq z_i \quad (4.2)$$

$$\langle v \rangle = 0, \quad z_0 < z \leq z_i \quad (4.3)$$

where z_s is the surface layer depth and $\psi(z/L)$ is a surface layer stability function, obtained by integration of Equation (3.7) (Paulson, 1970). The model of Garratt *et al.* uses

$$\psi(z_s/L) = \ln\left((1+x^2)(1+x)^2\right) - 2\tan^{-1}x + (\pi/2 - \ln 8) \quad (4.4)$$

with

$$x = 1/\phi_m = (1 - 15z_s/L)^{1/4} \quad (4.5)$$

and $z_s = 0.1z_i$, although tests reveal that the results are relatively insensitive to changing the stability function and surface layer depth. As $z_s \ll z_i$, the mixed layer averaged wind, $\langle u \rangle_m$, is approximately equal to $\langle u \rangle$ at height z_s , and so

$$\kappa \langle u \rangle_m / u_* = \ln(z_s/z_0) - \psi(z_s/L) = \ln(z_i/z_0) - \Psi(z_i/L) \quad (4.6)$$

$$\kappa \langle v \rangle_m / u_* = 0 \quad (4.7)$$

where

$$\Psi(z_i/L) = \psi(0.1z_i/L) + 2.3 \quad (4.8)$$

Hence predictions can be made for the behaviour of the similarity coefficients, A_m and B_m , which are defined through

$$\kappa \langle u \rangle_m / u_* = \ln(z_i/z_0) - A_m \quad (4.9)$$

$$\kappa \langle v \rangle_m / u_* = -B_m \quad (4.10)$$

Figure 4.2 shows the variation with stability of A_m and B_m predicted by this model, and also some of the large-eddy model results. They are in good agreement for $-z_i/L \gtrsim 2$.

Figure 4.2: Variation of similarity coefficients, A_m and B_m , with stability. Open squares : low resolution lid runs; closed squares : high resolution lid runs; crosses : inversion runs. The solid lines are the predictions of the mixed layer model described in the text.

The discrepancies for smaller values of $-z_i/L$ are not surprising because the assumption of well mixed velocity profiles is clearly erroneous in near neutral conditions.

The similarity coefficients, A_m and B_m , are often used because they are relatively insensitive to the effects of non-stationarity, entrainment, subsidence and baroclinicity (Garratt *et al.*, 1982). However, they relate the surface stress to the mean mixed layer wind. The coefficients A_i and B_i , which relate the surface stress to the surface geostrophic wind (regarded here as the external parameter), are defined through (e.g., Arya, 1975)

$$\frac{\kappa u_{g0}}{u_*} = \ln \left(\frac{z_i}{z_0} \right) - A_i \quad (4.11)$$

$$\frac{\kappa v_{g0}}{u_*} = -B_i \quad (4.12)$$

Here u_{g0} and v_{g0} are the surface geostrophic wind components. A_i and B_i are functions of the scale-height ratio, $u_*/(fz_i)$, stability (z_i/L) and baroclinicity. In practice, these empirical coefficients are extremely difficult to determine directly from atmospheric data. In part this is due to the difficulty of isolating the effects of changes in scale-height ratio from those of changes in stability and baroclinicity (see e.g. Grant and Whiteford, 1987). Also, these coefficients are sensitive to non-stationarity, entrainment and subsidence effects, as discussed by Garratt *et al.* (1982). However, many of these difficulties

Figure 4.3: Variation of friction velocity, u_* , with time for four of the low resolution lid runs.

are not relevant to model simulations. For example, the low resolution lid runs are not influenced by baroclinicity, entrainment or subsidence, and have been run to long time to reduce the effects of non-stationarity. Figure 4.3 shows time series of u_* from four of these simulations, and confirms that, although the inertial oscillation causes u_* to oscillate with period $2\pi/f$ ($\simeq 63000$ s), the fields appear close to achieving inertial equilibrium after 100000 s. The diagnosed values of A_i and B_i are shown in Figure 4.4. In fact the plot shows $(B_i - \kappa u_*/(fz_i))$ as vertical integration of the equations of motion, assuming stationarity and no entrainment fluxes at z_i , leads to

$$\frac{\langle u \rangle_m}{u_*} = \frac{u_{gm}}{u_*} \quad (4.13)$$

$$\frac{\langle v \rangle_m}{u_*} = \frac{v_{gm}}{u_*} + \frac{u_*}{fz_i} \quad (4.14)$$

where the subscript m indicates an average over the mixed layer as before. Note that in the non-baroclinic case considered here, the geostrophic wind components are constant with height so that the mixed layer averaged values (e.g. u_{gm}) are simply equal to the surface values. Hence $A_i = A_m$ and $(B_i - \kappa u_*/(fz_i)) = B_m$, and the similarity of the LES results in Figures 4.4 and 4.2 gives further evidence of the closeness of the fields

Figure 4.4: Variation of A_i and $B_i - \kappa u_* / (f z_i)$, with stability. Open squares : low resolution lid runs; closed squares : high resolution lid runs; crosses : inversion runs. The solid lines are the predictions of the mixed layer model assuming stationarity and no entrainment fluxes at z_i (i.e. $A_i = A_m$ and $B_i - \kappa u_* / (f z_i) = B_m$). The dotted lines are the predictions of Arya (1977), assuming $(u_* / (f z_i)) \simeq 4$.

to steady state. As discussed above, observational results for the similarity coefficients, A_i and B_i , are very scattered and, in convective conditions, the predictions of mixed layer models are probably as representative as any. Therefore the agreement between the LES results and mixed layer model predictions shown in Figure 4.4 for $-z_i/L \gtrsim 2$ is encouraging. In more neutral conditions these models are not valid, but the LES results can be compared more directly with observations. Grant and Whiteford (1987) tabulated various published estimates of the Rossby A and B coefficients in neutral conditions. These can be related to A_i and B_i using $A_i = A - \ln(u_* / (f z_i))$ and $B_i = B$. Thus, assuming $u_* / (f z_i) \simeq 4$ (which is broadly consistent with the LES), these estimates imply a range of values of A_i between around -1.4 and $+1.0$, and of $(B_i - \kappa u_* / (f z_i))$ between 1.7 and 3.5. These do not compare unfavourably with the LES results (BNLR gives $A_i = 0.8$, $(B_i - \kappa u_* / (f z_i)) = 1.0$), although the slightly smaller value of B_i from the LES implies a surface ageostrophic angle a few degrees smaller than observed.

Finally the LES results are compared with the functions proposed by Arya (1977), which are shown dotted in Figure 4.4. The agreement for B_i is generally good, but note

that the functions of Arya predict values of A_i smaller than those given by the LES and the mixed layer model in convective conditions.

4.2 Variation of temperature profiles with stability

Temperature profiles are commonly presented as non-dimensionalized differences from the surface temperature. However the LES surface temperature values are purely diagnostic. Temperature differences between the lowest interior grid point and the surface were diagnosed using Monin-Obukhov similarity with $\phi_h = (1 - 12z/L)^{-1/2}$ (Högström, 1988). However, in view of evidence from these (and other) LES for $\phi_h = 0.7$ in neutral conditions (see Chapter 3), these temperature differences were later reduced by 30%. This means that $\phi_h = 0.7(1 - 12z/L)^{-1/2}$ has effectively been used. Note that, for small z/L , this is close to the function of Businger *et al.* (1971) and in reasonable agreement with the interior LES results.

Figure 4.5 shows profiles of $\langle \theta - \theta_0 \rangle / \theta_*$, (where θ_0 is the adjusted surface temperature and $\theta_* = \langle w'\theta' \rangle_0 / u_*$) from the low resolution lid runs (solid lines). The profile labelled 'N', shows the behaviour of a passive scalar in simulation BNLR to give the neutral limit, and it shows significant gradient throughout the entire boundary layer. With increasing instability the potential temperature profiles rapidly become well mixed throughout most of the mixed layer. Interestingly, the unstable runs actually show slightly stable profiles in the upper CBL. It has been suggested that this can only be caused by entrainment, but note that Deardorff (1972a) and Krettenauer and Schumann (1992) found similar results in their convective runs using rigid lids. Nevertheless, the inversion runs (dotted) show that entrainment of warm air from aloft does lead to enhanced gradients, particularly above about $0.8z_i$.

Figure 4.6 shows high and low resolution lid run predictions for the similarity coefficient

Figure 4.5: Dimensionless potential temperature profiles from low resolution lid runs BNL, M03, M09, M21, M35, M64 and M134 (solid lines). In the boundary layer interior there is a monotonic decrease of $\langle \theta - \theta_0 \rangle / \theta_0$ with increasing instability between neutral (N) and more convective (C) conditions. In mid boundary layer the profiles from inversion runs IN, I03, I10, I27 and I77 (dotted lines) also show a monotonic decrease of $\langle \theta - \theta_0 \rangle / \theta_0$ with increasing instability.

C_i , which is defined through

$$\frac{\langle \theta_\infty - \theta_0 \rangle}{\theta_0} = \frac{\phi_{hN}}{\kappa} \left[\ln \left(\frac{z_i}{z_{0t}} \right) - C_i \right] \quad (4.15)$$

where $\langle \theta_\infty \rangle$ is the potential temperature at the top of the mixed layer, ϕ_{hN} is the neutral value of ϕ_h ($= 0.7$ to be consistent with that used in the surface temperature diagnosis) and z_{0t} is the roughness length for temperature ($= 0.01$ m). C_i increases from around -1 in neutral conditions to $\simeq 3$ at $-z_i/L = 2$, and then shows only a slow increase with further increase in $-z_i/L$. Values of C_i for the inversion runs are not shown as the results are sensitive to the height used for $\langle \theta_\infty \rangle$ due to the increase of $\langle \theta \rangle$ towards the inversion which is caused by entrainment and does not scale with θ_0 .

For comparison, the predictions of a simple mixed layer model are also shown (solid line). This assumes that the potential temperature is constant above $0.1z_i$, and that below this height the non-dimensional gradient is given by $\phi_h = 0.7(1 - 9z/L)^{-1/2}$. The

Figure 4.6: Variation with stability of similarity coefficient C_i . Open squares : low resolution lid runs; closed squares : high resolution lid runs; solid line : mixed layer model; dotted line : Arya (1977); dashed line : Arya (1977), adjusted to be consistent with $\phi_{hN} = 0.7$.

agreement with LES is good for $-z_i/L \gtrsim 2$. Note however that much of the temperature difference, $\langle \theta - \theta_0 \rangle / \theta_*$, in the LES runs occurs between the lowest interior grid level and the surface ($\simeq 70\%$ for M21, 80% for M134), so this agreement is dependent upon using a stability function in the mixed layer model broadly consistent with that used in the large-eddy model lower boundary condition (in particular $\phi_{hN} = 0.7$.) The dotted line is the curve proposed by Arya (1977) and shows consistently higher values of C_i . However it was calculated using $\phi_{hN} = 1.0$, and using this value in Equation (4.15) the Arya predictions for the variation of $\langle \theta - \theta_0 \rangle / \theta_*$ with stability can be calculated. From these adjusted values of C_i can be diagnosed using (4.15) with $\phi_{hN} = 0.7$. The results of this procedure are shown in Figure 4.6 (dashed line) and can be seen to be in fair agreement with the LES results.

4.3 Comparison of LES and closure model results

The LES results are now used to assess the performance of various one-dimensional parametrization schemes which could be used in large-scale NWP and climate models. Obviously a scheme should produce good results for given test cases, but it must also be robust and computationally inexpensive. This last requirement precludes the use of many high order closure schemes developed for boundary layer studies.

One possibility is to use a bulk model which assumes a boundary layer structure below z_i . For example, mixed layer models can perform well in convective conditions by directly incorporating our knowledge of boundary layer structure. Also, their performance is not adversely affected by the limited vertical resolution which can be used in large-scale models. Nevertheless, there are major disadvantages with bulk methods of boundary layer parametrization. Different structures have to be assumed for all the different boundary layer types – for example, it has been shown that a simple mixed layer model does not perform well in neutral conditions. Also, it is necessary to use uncertain prognostic equations for the boundary layer depth. For these reasons almost all NWP and climate models use closures which attempt to parametrize the fluxes on a finite difference grid.

The equations which have to be solved are as follows

$$\frac{\partial \langle u \rangle}{\partial t} = f \langle v - v_g \rangle - \frac{\partial \langle u'w' \rangle}{\partial z} \quad (4.16)$$

$$\frac{\partial \langle v \rangle}{\partial t} = -f \langle u - u_g \rangle - \frac{\partial \langle v'w' \rangle}{\partial z} \quad (4.17)$$

$$\frac{\partial \langle \theta \rangle}{\partial t} = - \frac{\partial \langle w'\theta' \rangle}{\partial z} \quad (4.18)$$

where $\langle u'w' \rangle$, $\langle v'w' \rangle$ and $\langle w'\theta' \rangle$ are the fluxes which need to be parametrized. Note that although θ is the only scalar considered, it is usual to parametrize the fluxes of all scalars in similar ways, so the results for temperature are also relevant to the parametrization of other scalar fluxes, notably that of humidity.

The tests performed compare the equilibrium performance of different closure schemes with the results of the low resolution lid runs (which themselves are close to equilibrium).

Figure 4.7: Variation of u_* , and α_0 , with stability for a constant geostrophic windspeed (G) of 10 ms^{-1} , with $z_i = 1000 \text{ m}$ and $z_0 = 0.1 \text{ m}$. Open squares : LES results; solid lines : mixed layer model predictions.

The various closure models described in this chapter were set up to be driven by imposed geostrophic wind and surface heat flux, and with the fluxes at z_i set to zero, in order to be directly comparable with the large-eddy simulations. All used Monin-Obukhov similarity to provide the no-slip lower boundary condition (with $\phi_m = (1 - 16z/L)^{-1/4}$, $\phi_h = (1 - 12z/L)^{-1/2}$, $z_0 = 0.1 \text{ m}$ and $z_{0t} = 0.1 \text{ m}$). Unless otherwise stated, they were run with 40 points in the vertical, and for 240000 seconds to ensure equilibrium was reached.

Clearly the results could be presented by comparing LES and closure model predictions for the similarity coefficients, A_i and B_i . However, it was decided to compare values of u_* and α_0 (related to A_i and B_i through Equations 4.11 and 4.12), as they are more directly relevant both for forecasting boundary layer winds and for synoptic scale development (t_{sd} , the time scale for filling of low pressure systems through Ekman pumping, is inversely proportional to $u_*^2 \cos \alpha_0$, as explained in Chapter 1). Figure 4.7 shows the LES results which the simpler models will be compared against. Note that u_* shows a sharp increase as $-z_i/L$ increases from zero, but the ageostrophic angle does not show nearly such a marked change with stability. The slight decrease in α_0 between simulations M03 and M09 is probably related to the change in domain size and is not thought to be a real

CHAPTER 4: MEAN STRUCTURE

effect. For comparison, Figure 4.7 also shows the predictions of the mixed layer model (solid lines). These are obtained by taking Equations (4.6), (4.7), (4.13) and (4.14), and rearranging to obtain

$$\frac{\kappa^2 G^2}{u_*^2} = \left[\ln \left(\frac{z_i}{z_0} \right) - \Psi \right]^2 + \kappa^2 \left(\frac{u_*^2}{f^2 z_i^2} \right) \quad (4.19)$$

This can be solved iteratively for u_* . α_0 can then be obtained by calculating v_{g0} using Equation (4.12), and noting that $\sin \alpha_0 = -v_{g0}/G$.

The ability of the closure models to model correctly the boundary layer wind profiles which are an important forecast product will also be discussed. For temperature, the flux profiles are effectively imposed by the boundary conditions in equilibrium (i.e. conditions of uniform heating), but the temperature gradients across the boundary layer are of interest. This is because errors in temperature (and humidity) profiles may lead to poor forecasts of boundary layer clouds. In turn this will lead to errors in the modelled radiative fluxes which may be very significant, particularly in a climate model. Once again the results could be presented in terms of similarity coefficients (C_i in this case), but it was decided that the potential significance of any discrepancy between the LES and closure model results could be assessed more easily by looking directly at the temperature profiles.

It is believed that the LES results are credible, and suitable for evaluation of the performance of closure models. However, even if they were 'perfect' in some sense, it is worth asking how precisely a parametrization should seek to reproduce them. This is because the errors introduced by the closure may be less significant in practice than those associated with uncertainties in quantities such as z_0 and z_i which are imposed in the simulations. For example, Annex 4.A.1 suggests that the errors in u_* associated with uncertainties in choosing the most appropriate values of z_0 are of order 5 or 10 per cent. Hence the benefits of trying to improve on a closure model which gave errors in u_* , for given z_0 , of only 1 or 2 per cent are likely to be small. Conversely, errors of 5 or 10 per cent probably are significant and deserving of attention. Annex 4.A.2 attempts to ascertain the sensitivity of u_* to z_i , which might be in error due to poor representation of surface and entrainment fluxes, or to poor vertical resolution. At least in convective conditions, it is found that, other than for shallow boundary layers, the sensitivity is relatively weak.

CHAPTER 4: MEAN STRUCTURE

It is more difficult to quantify the importance of errors in the temperature (and humidity) profiles, but it is stressed again that realistic simulation of clouds is of vital importance, so any improvement in mean temperature (and humidity) structure is potentially significant.

4.4 CBL parametrization : mixing length models

The starting point for many low-order closure models is to relate the turbulent shear stress to the mean velocity gradient using a turbulent viscosity, K_m :

$$\langle u'w' \rangle = -K_m \frac{\partial \langle u \rangle}{\partial z} \quad (4.20)$$

$$\langle v'w' \rangle = -K_m \frac{\partial \langle v \rangle}{\partial z} \quad (4.21)$$

Similarly the heat flux is related to the temperature gradient through

$$\langle w'\theta' \rangle = -K_h \frac{\partial \langle \theta \rangle}{\partial z} \quad (4.22)$$

where K_h is the diffusivity. The viscosity and diffusivity have to be expressed in terms of known or calculable quantities. The mixing length approach writes the viscosity as the product of a turbulent length scale, l_M , and velocity scale, $l_M |\partial \langle \mathbf{u} \rangle / \partial z|$, i.e.

$$K_m = l_M^2 \left| \frac{\partial \langle \mathbf{u} \rangle}{\partial z} \right| \quad (4.23)$$

The mixing length, l_M , is prescribed algebraically and will typically be related to height, boundary layer depth and the local stability. Often (e.g. Louis, 1979) l_M^2 is written as the product of the square of a basic mixing length, λ_M , and a function of stability, $F_m(Ri)$ i.e.

$$l_M^2 = \lambda_M^2 F_m \quad (4.24)$$

The diffusivity is set equal to the viscosity divided by a Prandtl number (Pr) which is itself a function of stability

$$K_h = \frac{K_m}{Pr} = K_m \frac{F_h(Ri)}{F_m(Ri)} \quad (4.25)$$

CHAPTER 4: MEAN STRUCTURE

The UK Meteorological Office Unified Model boundary layer scheme (Smith, 1993) uses a mixing length scheme of this type. In unstable conditions ($Ri \leq 0$), the stability functions are set so as to be broadly consistent with observations in the atmospheric surface layer

$$F_m = 1 - \frac{g_m Ri}{1 + (g_m/e_m)(-Ri)^{-1/2}} \quad (4.26)$$

$$F_h = 1 - \frac{g_m Ri}{1 + (g_m/e_h)(-Ri)^{-1/2}} \quad (4.27)$$

where $g_m = 10$, $e_m = 4$ and $e_h = 25$. In stable conditions the scheme uses

$$F_h = F_m = \frac{1}{1 + g_m Ri} \quad (4.28)$$

The basic length scale, λ_M is written

$$\frac{1}{\lambda_M} = \frac{1}{\lambda_{M0}} + \frac{1}{\kappa z} \quad (4.29)$$

Note that the Smagorinsky subgrid model used in the large-eddy simulations is a 3-dimensional version of this model. However, whereas the length scale λ_0 is associated with the filter-scale in large-eddy modelling, λ_{M0} is associated here with the size of the turbulent eddies, and is therefore related to the boundary layer depth, z_i through

$$\lambda_{M0} = \beta z_i \quad (4.30)$$

The present scheme uses $\beta = 0.15$, although tests using other values will also be described.

4.4.1 Performance in neutral conditions

Equations (4.20) and (4.21) imply that the local stress is parallel to the local shear. This is expected to be the case in neutral conditions when the transport terms in the budget equations for the second order moments are small (Grant, 1992). The first plot in Figure 4.8 shows the angles of the mean wind, mean shear and turbulent stress relative to the geostrophic wind direction for simulation BNLR, and confirms that the stress is indeed closely parallel to the shear. The second plot shows a profile of the neutral mixing length, $\lambda_M (= l_M)$, diagnosed using (4.20) and (4.23). Its variation can be seen to be well

Figure 4.8: Results from neutral simulation, BNLr. The first plot shows the variation with height of the directions of the mean wind (VEL), mean shear and stress. Positive values indicate anticlockwise rotation relative to the geostrophic wind. The second plot shows the diagnosed length scale, λ_M/z_i , and three possible parametrizations of that length scale using $1/\lambda_M = 1/(\beta z_i) + 1/(\kappa z)$ with $\beta = 0.09, 0.15$ and 0.33 .

represented by Equation (4.29) with a value of β of 0.15 , as used in the Meteorological Office model.

Having found that the mixing length model assumptions are well supported by diagnostic analysis of LES simulation BNLr, it is expected that a run of such a model should produce velocity and stress profiles similar to those from LES given the same external forcing. Figure 4.9 confirms that this is the case, showing that the equilibrium velocity and stress profiles from the mixing length model with $\beta = 0.15$ are in excellent agreement with those from the large-eddy simulation. Increasing (decreasing) the value of β causes the velocity profiles to become more (less) uniform, with some increase (decrease) in the surface stress.

Of course, many practical models will have much poorer vertical resolution. For example, the mesoscale version of the Meteorological Office Unified Model (used for forecasting weather over the British Isles) has nine grid points below 1000 m, while the global version has only four. Hence it is important to assess the sensitivity of the results both to changes

Figure 4.9: Velocity and stress profiles in neutral conditions with $G = 10 \text{ ms}^{-1}$, $z_i = 1000 \text{ m}$ and $z_0 = 0.1 \text{ m}$. Results are shown from large-eddy simulation BNLr, and from the mixing length model described in the text with $\beta = 0.09, 0.15$ and 0.33 . Note that the dashed profiles ($\beta = 0.15$) are very similar to the solid profiles (LES) so that they are indistinguishable in some places. The x -axis is aligned with the geostrophic wind.

in the closure and to changes in the model resolution. Table 4.1 shows values of u_* and α_0 predicted by the mixing length model when run using four different values of β and with four different numbers of grid points (the values from the corresponding large-eddy simulation (BNLR) are $u_* = 0.45 \text{ ms}^{-1}$ and $\alpha_0 = 18^\circ$). Encouragingly the predicted values are not particularly sensitive to resolution – changing from 1000 points to 4 points leads to only a 2% change in u_* (for the same inversion height) which is probably not significant compared to other uncertainties, although in practice there are also likely to be larger errors in the modelled inversion height when using coarse resolution. The sensitivity of u_* to the asymptotic length scale $\lambda_{M0} (= \beta z_i)$ is potentially more significant, although even here the use of any value between $0.09z_i$ and $0.33z_i$ leads to a predicted u_* value within 6% of that from the LES.

Finally note that the behaviour of a passive scalar in simulation BNLr indicates a Prandtl number of around 0.7 throughout most of the neutral boundary layer. This is consistent with the results of earlier large-eddy simulations (e.g. Mason and Brown, 1994), but smaller than the usually quoted value of 1 (see Chapter 3). Although the adoption of

β	1000 points	40 points	9 points	4 points
0.05	0.391 (22.2)	0.395 (22.0)	0.404 (21.1)	0.424 (19.6)
0.09	0.418 (18.8)	0.421 (18.5)	0.427 (17.6)	0.438 (16.3)
0.15	0.441 (17.3)	0.444 (17.0)	0.447 (16.1)	0.451 (14.9)
0.33	0.466 (16.6)	0.468 (16.3)	0.468 (15.5)	0.467 (14.4)

Table 4.1: Values of u_* (in ms^{-1}) predicted by the mixing length model in neutral conditions for $G = 10 \text{ ms}^{-1}$, $z_i = 1000 \text{ m}$, $z_0 = 0.1 \text{ m}$. Also shown, in parentheses, are values of α_0 (in degrees). Results are presented for four different values of β , and with various numbers of grid points.

$Pr = 0.7$ (implying $F_h = 1.4$) in near neutral conditions would not have a major impact on the temperature structure (as the heat fluxes would remain small), it is common practice to use a diffusivity of water vapour equal to that of heat and so the transport of moisture would be affected (increased flux for the same gradient).

4.4.2 Performance in convective conditions

It has been shown that a simple mixing length model can perform well in neutral conditions. However, the success of mixed layer models provides a warning that the mixing length approach must run into difficulties in convective conditions, for linear flux profiles with zero mean gradients could only be achieved through the use of infinite viscosity and diffusivity. In fact, if profiles of K_m and K_h are diagnosed from the more convective LES runs, then they are found to pass through $\pm\infty$ and become negative in the upper part of the CBL where the fluxes are counter-gradient. Clearly then, the mixing length parametrization, which can only represent down-gradient fluxes using viscosity and diffusivity which are specified in terms of a geometric length scale and the local stabil-

Figure 4.10: Variation of u_* , and α_0 , with stability for a constant geostrophic windspeed (G) of 10 ms^{-1} , with $z_i = 1000 \text{ m}$ and $z_0 = 0.1 \text{ m}$. Results are shown from the mixing length model with three values of β , and also from the LES (open squares) and the mixed layer model (solid lines).

ity, is not going to be able to accurately reproduce the LES results. However, it is not clear whether the discrepancies are significant and, if so, whether other models perform sufficiently better to justify any additional computational cost.

The mixing length model described above was run to equilibrium with $G = 10 \text{ ms}^{-1}$, $z_i = 1000 \text{ m}$, $z_0 = 0.1 \text{ m}$ and a variety of different values of surface heat flux. The 40 grid points were distributed non-uniformly so that the mesh spacing was $\simeq 4 \text{ m}$ at the surface, increasing to 30 m in the boundary layer interior. This was done so that the results were relatively insensitive to the stability dependence of the lower boundary condition, and more dependent on the interior turbulence parametrization. Tests in neutral conditions showed that the slow stretching ($\leq 10\%$ change in spacing per grid point) caused no degradation of the results. Figure 4.10 shows the variation with stability of u_* and α_0 predicted by this model with three values of β , and also the LES and mixed layer model results. The mixing length model correctly predicts increases in surface stress and ageostrophic angle as $-z_i / L$ increases, but the rates of increase are too small – for $\langle w'\theta' \rangle_0 = 0.3 \text{ Kms}^{-1}$ the mixing length model with $\beta = 0.15$ predicts $u_* = 0.59 \text{ ms}^{-1}$ and $\alpha_0 = 22^\circ$, while the mixed layer model gives 0.65 ms^{-1} and 25° and the LES gives

CHAPTER 4: MEAN STRUCTURE

0.67 ms^{-1} and 26° . This behaviour can be understood by reference to Figure 4.11 which shows LES and mixing length model results for the profiles of $\langle u \rangle$ and $\langle v \rangle$, and the fluxes $\langle u'w' \rangle$ and $\langle v'w' \rangle$. The mixing length model shows velocity profiles which are insufficiently well mixed, as it requires a velocity gradient to produce the stress needed to balance the geostrophic departure (Equations (4.16) and (4.17)). The errors are most marked in the upper CBL, and the wind close to the surface is predicted with errors of around 8% in the speed, and of only a few degrees in the direction, which may be adequate for most forecasting purposes. Nevertheless, u_* controls the boundary layer cross-isobaric flow and thus affects large-scale development (see Chapter 1), and an 8% underestimate is potentially significant compared with other uncertainties. Accurate wind forecasts are probably most important in strong wind conditions, such as when a deep Atlantic low pressure system approaches the British Isles. Strong winds will usually be associated with relatively small values of $-z_i/L$, particularly over the ocean where heat fluxes tend to be small (while 0.3 Kms^{-1} might be observed over Britain in summer, fluxes over the Atlantic will typically be an order of magnitude smaller). Therefore, while a comparison between LES and mixing length model results has been shown for $-z_i/L \simeq 14$, it is important to realize that comparable fractional errors in u_* are found for all $-z_i/L \gtrsim 1$. Similar discrepancies between mixed layer and mixing length model predictions were also found for $z_i = 600 \text{ m}$, and only slightly smaller differences for $z_i = 2000 \text{ m}$, suggesting that the mixing length model performance is not strongly dependent on boundary layer depth. Further tests suggested that the results remain largely independent of resolution, for the same boundary layer depth – 4 points evenly spaced with $\langle w'\theta' \rangle_0 = 0.3 \text{ Kms}^{-1}$ and $\beta = 0.15$ gave $u_* = 0.60 \text{ ms}^{-1}$, only 0.01 ms^{-1} greater than the value obtained using 40 points.

Figure 4.11 also shows LES and mixing length model results for the mean temperature profile and heat flux. Note that the temperatures have been adjusted to be the same at $0.02z_i$ rather than at the surface to remove differences resulting from the different boundary condition formulations used by the two models (different z_{0t}). In order to achieve a linear flux profile (which is necessary for uniform boundary layer heating), $\langle \theta \rangle$

Figure 4.11: Mean profiles and fluxes from convective large-eddy simulation M134, and attempts to reproduce them using the mixing length model described in the text.

CHAPTER 4: MEAN STRUCTURE

in the mixing length model has to decrease with height throughout the CBL. This is in contrast to the LES profile which shows an almost constant value in the boundary layer interior, and actually increases slightly with height in the upper part of the CBL where the flux is counter-gradient. The net result is that the temperature difference predicted between $0.08z_i$ and z_i by the closure model is of order 1 K too large (actually 0.7 K for $\beta = 0.15$). With smaller heat fluxes the error in the temperature difference tends to be reduced, as smaller temperature gradients are required to produce the smaller fluxes (in the unstable limit, $F_h \propto (-Ri)^{1/2}$ and it can be shown that $(\partial\langle\theta\rangle/\partial z) \propto \langle w'\theta'\rangle^{2/3}$). Thus errors in the temperature profiles resulting from the use of mixing length closures will not usually be large, although they may be significant if the cold bias in the upper boundary layer is sufficient to cause condensation which would not otherwise have occurred. In fact the situation tends to be more complicated than this, as humidity profiles also tend to be insufficiently well mixed. This often leads to excessive amounts of low cloud in models which use a local mixing length formulation (Holtslag and Boville, 1993).

It is possible that the results might be improved by making changes to the stability dependence of the functions F_m and F_h . Indeed, a run with $\beta = 0.15$, and e_m in Equation (4.26) arbitrarily changed to 10, gave $u_* = 0.65 \text{ ms}^{-1}$ for $\langle w'\theta'\rangle_0 = 0.3 \text{ Kms}^{-1}$, in good agreement with the mixed layer model prediction. This had relatively little effect on the temperature profile, so additionally, e_h in Equation (4.27) was increased to 62.5 (a factor of 2.5 increase as with e_m). As expected, this led to a slightly improved temperature profile ($\simeq 20\%$ reduction in $\Delta\langle\theta\rangle$ across the boundary layer), but only at the cost of making the wind profiles less well mixed once again (u_* reduced to 0.63 ms^{-1}). This highlights the fundamental problem with models of this type, namely that the results are sensitive to local values of Richardson number, while the stability of the CBL is better characterized through some bulk measure such as $-z_i/L$. It might be possible to produce better results in any given case by further arbitrary tuning of F_m and F_h , but it seems unlikely that they would be robust given their very weak physical basis. Also, the use of stability functions inconsistent with those observed in the atmospheric surface layer and used in the model lower boundary condition might degrade the near surface results in a

high resolution run and also lead to increased sensitivity to resolution. If a more accurate parametrization of the CBL is sought, then it seems likely to be more profitable to look at other types of model rather than to continue with further tuning of the local mixing length model.

Finally note that while $\beta = 0.15$ appears most successful in neutral conditions, slightly better results are obtained in convective conditions when using $\beta = 0.33$. This is because larger viscosities and diffusivities are obtained for given gradients when using the larger basic length scale. This is the first suggestion that it might be better to make the mixing length, l_M , sensitive to a non-local measure of stability (e.g. $-z_i/L$) rather than to the local Richardson number. Non-local models will be discussed in Section 4.6.

4.5 CBL parametrization : TKE models

The next level of complexity is the TKE model, or $1\frac{1}{2}$ order closure as it is commonly known. In TKE models, the turbulent diffusivities are related to the TKE, for which a prognostic equation is carried. Such models have been widely used, both for boundary layer modelling (e.g. Therry and Lacarrère, 1983; Schilling, 1991) and in general circulation models (e.g. Myakoda and Sirutis, 1977). Many attempt to allow for some non-local effects by incorporation of counter-gradient fluxes of scalars and by careful choice of length scales (e.g. the model of Therry and Lacarrère (1983) which is discussed in the next section). However, the present section concentrates on the simplest possible TKE model, where the fluxes are all down-gradient and stability effects are incorporated by relating the length scale to the local stability.

Equations (4.20), (4.21) and (4.22) are still used to relate the fluxes to the mean gradients, but the velocity scale is taken to be proportional to the square root of the turbulent kinetic energy, $\langle E \rangle$, and so

$$K_m = C_k l_{T1} \langle E \rangle^{1/2} \quad (4.31)$$

CHAPTER 4: MEAN STRUCTURE

where l_{T1} is a length scale. The following prognostic equation for energy is carried

$$\frac{\partial \langle E \rangle}{\partial t} = -\frac{\partial}{\partial z} \langle w' E' + w' p' / \rho_r \rangle - \langle u' w' \rangle \frac{\partial \langle u \rangle}{\partial z} - \langle v' w' \rangle \frac{\partial \langle v \rangle}{\partial z} + \frac{g}{\theta_r} \langle w' \theta' \rangle - \langle \epsilon \rangle \quad (4.32)$$

with the following closure assumptions

$$\langle w' E' + w' p' / \rho_r \rangle = -\frac{K_m}{\sigma_E} \frac{\partial \langle E \rangle}{\partial z} \quad (4.33)$$

$$\langle \epsilon \rangle = C_k^3 \langle E \rangle^{3/2} / l_{T2} \quad (4.34)$$

$$K_h = K_m / Pr \quad (4.35)$$

where C_k^2 is the stress-energy ratio, Pr is the Prandtl number as before, σ_E can be thought of as a Prandtl number for diffusion of energy, and l_{T2} is a dissipation length scale.

Note that this model attempts to take some account of non-local effects by inclusion of a simple parametrization of the transport term in the prognostic equation for E . In order to be able to make a direct comparison with the results of the mixing length model the two formulations need to be made identical in the steady state when this term is set equal to zero. Hence, assuming local balance between production and dissipation of energy

$$\langle \epsilon \rangle = K_m \left| \frac{\partial \langle u \rangle}{\partial z} \right|^2 (1 - Rf) \quad (4.36)$$

where Rf is the flux Richardson number defined through

$$Rf = \frac{\left(\frac{g}{\theta_r} \right) \langle w' \theta' \rangle}{\langle u' w' \rangle \frac{\partial \langle u \rangle}{\partial z} + \langle v' w' \rangle \frac{\partial \langle v \rangle}{\partial z}} \quad (4.37)$$

Eliminating $\langle \epsilon \rangle$ and $\langle E \rangle$ (using (4.34) and (4.31)) leads to

$$K_m = \left(l_{T1}^{3/2} l_{T2}^{1/2} \right) \left| \frac{\partial \langle u \rangle}{\partial z} \right| (1 - Rf)^{1/2} \quad (4.38)$$

Looking for consistency with Equation (4.23), this leads to

$$l_M = l_{T1}^{3/4} l_{T2}^{1/4} (1 - Rf)^{1/4} \quad (4.39)$$

Hence, taking the simplest possible model in which $l_{T1} = l_{T2} = l_T$, l_T is set equal to $l_M / (1 - Rf)^{1/4}$, where l_M is defined as in the mixing length model to be a function of height and local stability (Equations (4.24), (4.26), (4.29) and (4.30)). The Prandtl

Figure 4.12: Turbulence kinetic energy budgets for simulation M134 and for TKE model given the same forcing. All terms are normalized by (w_*^3/z_i) . Solid lines : shear production; dotted lines : dissipation; dashed lines : total transport; dot-dash lines : buoyancy production.

number is set equal to F_h/F_m as before. This model was run (with $C_k^2 = 0.25$, $\sigma_E = 1.0$) in the same way as the mixing length model in an attempt to reproduce the LES results.

In neutral conditions, both the LES and TKE model show an almost exact balance between shear production and dissipation of energy and so, as expected, the equilibrium wind profiles from the closure model are almost identical to those from the mixing length model and LES. In convective conditions the TKE model profiles remain almost identical to those from the mixing length model, suggesting that the inclusion of the transport term in Equation (4.32) is having little effect. Figure 4.12 shows the energy budgets from convective simulation M134 and from the TKE model run with $\langle w'\theta' \rangle_0 = 0.3 \text{ Kms}^{-1}$, and although they are broadly similar, it is clear that the magnitude of the transport term is underestimated by the TKE model. Accordingly, a test simulation was performed in which σ_E was arbitrarily reduced to 0.1 (i.e. eddy coefficient for energy transfer ten times greater than that for momentum). This had the effect of making the energy budget more similar to that from LES, but made the TKE profile almost uniform with height which is probably less realistic as although $\langle u'u' \rangle$ and $\langle v'v' \rangle$ may be roughly constant in the CBL, $\langle w'w' \rangle$ shows a maximum in mid boundary layer (see Chapter 3). Clearly more

sophisticated closures could be used for the energy transport term (e.g. a counter-gradient correction as described in the next section) but already there is an indication that this may not be important as the mean fields from this test simulation remained very similar to those from the mixing length model. This is presumably because K_m and K_h are far more sensitive to the parametrization of the length scale, l_T , than they are to the parametrization of the energy equation (as K_m depends only on the square root of the energy). TKE models will be studied again in the next section on non-local models.

4.6 CBL parametrization : Non-local models

As described above, stability dependent mixing length models are highly sensitive to small changes in mean profiles, through the dependence of the diffusivities on local Richardson number. This section examines the performance of two classes of models in which K_m and K_h are related to some non-local measure of stability. The first class calculates K_m in terms of the TKE (as in Section 4.5), but with the length scales l_{T1} and l_{T2} defined using a non-local measure of stability. In the second class of model, the eddy coefficients are prescribed directly as functions of z/z_i and the boundary layer stability.

Once the viscosity and diffusivity profiles are determined non-locally, the equilibrium solutions for the mean wind and temperature profiles are to a much greater extent decoupled from one another – a small change in the mean temperature gradient at any given level will no longer have a large direct impact on the wind profiles as K_m is no longer sensitive to local Richardson number. Moreover, it is now possible to introduce some modifications to the heat flux formulation to allow upward heat flux even with slightly stable local temperature gradient, as occurs in the upper CBL. This should alleviate some of the errors in the temperature profiles obtained using the mixing length model where unstable gradients are required at all heights to allow an upward flux. Accordingly, Equation (4.22) is replaced with

$$\langle w'\theta' \rangle = -K_h \left(\frac{\partial \langle \theta \rangle}{\partial z} - \gamma_c \right) \quad (4.40)$$

CHAPTER 4: MEAN STRUCTURE

where γ_c is the counter-gradient term. This form was derived by Deardorff (1972b) by neglecting the transport term in the heat flux budget. More recently, Holtslag and Moeng (1991) applied a different set of closure assumptions (based partly on LES) to the heat flux equation and obtained the same form although the physical interpretation is different as their counter-gradient term results from the third-moment transport effect (while that of Deardorff comes from the buoyancy production term).

Although many models have adopted the use of a counter-gradient term for heat (and humidity) transport (e.g. Therry and Lacarrère, 1983; Troen and Mahrt, 1986; Holtslag and Boville, 1993), almost all have continued to use (4.20) and (4.21) for the momentum fluxes without counter-gradient correction. In part this is due to the scarcity of data of suitable quality for developing and testing a model incorporating such a correction, although Troen and Mahrt (1986) argued that counter-gradient transports of momentum are less significant than those of heat, as pressure effects make the transport of momentum over large distances by thermals relatively inefficient. Also, Therry and Lacarrère (1983), performed a similar analysis on the momentum flux budget to that performed by Deardorff (1972b) and Holtslag and Moeng (1991) on the heat flux budget. Although the transport term is not negligible in convective conditions, a third order closure model suggested that the buoyancy production term is of opposite sign but of roughly equivalent magnitude. Accordingly both terms were neglected simultaneously, leading to flux parametrizations of the form given in Equations (4.20) and (4.21).

4.6.1 Non-local TKE models

The model of Therry and Lacarrère (1983) is now examined as an example of a model which attempts to improve upon the performance of the basic TKE model. It can be difficult to ascertain whether differences between the performance of different models are fundamentally related to the type of closure, or are simply related to the particular choice of closure coefficients used (Cuxart *et al.*, 1994). Accordingly results are presented from the full model of Therry and Lacarrère (1983) using the coefficients proposed by the

CHAPTER 4: MEAN STRUCTURE

authors, and also from some tests which attempt to ascertain whether the carrying of energy and use of the counter-gradient correction have a significant impact on the mean fields.

Full details of the model can be found in Therry and Lacarrère (1983), and only a brief summary of the main differences from the basic TKE model (described in Section 4.5) is given here. The length scale l_{T1} is given by

$$\frac{1}{l_{T1}} = \frac{1}{\kappa z} + \frac{C_1}{z_i} - \left(\frac{1}{\kappa z} + \frac{C_2}{z_i} \right) m_1 m_2 + \frac{C_5}{l_s} \quad (4.41)$$

where

$$m_1 = 1 / (1 + C_3 z_i / (\kappa z)) \quad (4.42)$$

$$m_2 = \begin{cases} 1 / (1 - C_4 L / z_i) & \text{for } L < 0 \\ 0 & \text{for } L \geq 0 \end{cases} \quad (4.43)$$

$$1/l_s = \begin{cases} 0 & \text{for local } \partial\langle\theta\rangle/\partial z < 0 \\ ((g/\langle\theta_r\rangle) (\partial\langle\theta\rangle/\partial z) / \langle E \rangle)^{1/2} & \text{for local } \partial\langle\theta\rangle/\partial z > 0 \end{cases} \quad (4.44)$$

and C_{1-5} are empirical constants based on atmospheric observations. Note that in the unstable cases considered in this study, the last term is usually negligible (although not exactly zero in the upper CBL where the use of the counter-gradient term enables the model to sustain an upward heat flux even for $\partial\langle\theta\rangle/\partial z > 0$). Thus the length scale is sensitive to stability through the value of z_i/L (in the definition of m_2), but not dependent on local stability. The same form is used in the definition of the dissipation length scale, l_{T2} , but with different values for the empirical constants.

Equation (4.40) is used to parametrize the heat flux, with K_h calculated from K_m using a constant Prandtl number of 0.77, and the counter-gradient correction term, γ_c given by

$$\gamma_c = 5\langle w'\theta' \rangle_0 / (w_* z_i) \quad (4.45)$$

for $\langle w'\theta' \rangle_0 > 0$. This has the desirable property of vanishing in neutral conditions when $\langle w'\theta' \rangle_0 = 0$. The parametrization (4.33) of the transport term in the energy Equation (4.32), is also replaced by one incorporating a counter-gradient correction.

Figure 4.13: Variation of u_* , and α_0 , with stability for a constant geostrophic windspeed (G) of 10 ms^{-1} , with $z_i = 1000 \text{ m}$ and $z_0 = 0.1 \text{ m}$. Results are shown from the model of Therry and Lacarrère (TL) and the mixing length model (ML) with $\beta = 0.15$. The squares are the LES results and the solid lines are the mixed layer model predictions as before.

Figure 4.13 shows the equilibrium values of u_* and α_0 predicted by this model (TL), for $G = 10 \text{ ms}^{-1}$, $z_i = 1000 \text{ m}$, $z_0 = 0.1 \text{ m}$, using 40 grid points as before. The behaviour can be seen to be quite different from that of the mixing length model. In neutral conditions, this model predicts a value of u_* rather low compared to the mixing length model (and LES), but the sharper increase in u_* with increasing $-z_i/L$ is more reminiscent of the LES results. In highly convective conditions, this model gives values of u_* (and α_0) rather high relative to the LES and mixed layer model predictions, while the mixing length model gives lower values.

The behaviour in neutral conditions is easily understood. The transport term in the energy equation is negligible and so local production is equal to local dissipation and Equation (4.38) is valid. Setting $Rf = 0$ and substituting for l_{T1} and l_{T2} leads to

$$K_m = \left(\left(\frac{1}{\kappa z} + \frac{1}{0.067 z_i} \right)^{-1} \right)^2 \left| \frac{\partial \langle u \rangle}{\partial z} \right| \quad (4.46)$$

This is exactly the same as the viscosity given by the mixing length model with $\beta = 0.067$ (see Equations (4.23), (4.24), (4.26), (4.29) and (4.30)). Thus the differences between the Therry and Lacarrère and mixing length model results for mean wind profiles in neutral

Figure 4.14: Mean profiles from convective large-eddy simulation M134, and attempts to reproduce them using the mixing length model (ML) with $\beta = 0.15$, and the model of Therry and Lacarrère (TL). The profiles labelled TL2 are from a test simulation of the Therry and Lacarrère model, as described in the text. Note that the velocity profiles which are almost indistinguishable are those from TL and TL2.

conditions are due to the particular choice of constants used rather than to the different closures.

Figure 4.14 shows mean wind and temperature profiles from the LES, mixing length and non-local TKE model for the case with $\langle w'\theta' \rangle_0 = 0.3 \text{ Kms}^{-1}$. Both closure models predict wind profiles which show too much shear in the boundary layer, and the discrepancies between the results of each model and the LES are of roughly comparable magnitude. Nevertheless, the LES temperature profile is much better reproduced by the non-local model due to the inclusion of the counter-gradient term.

Therry and Lacarrère (1983) commented that removal of the counter-gradient correction in the parametrization of the transport term in the energy budget has little effect on the mean profiles of velocity and temperature (although it does affect the TKE profile). This is consistent with the finding in Section 4.5 that arbitrarily changing the transport term parametrization has little impact on the mean fields. In fact, test simulations revealed that removal of the entire transport term in the Therry and Lacarrère model makes almost no difference to the equilibrium velocity and temperature profiles, even in

CHAPTER 4: MEAN STRUCTURE

convective conditions. When the model is run in this mode, Equation (4.38) must hold exactly in the steady state. Noting that the heat flux (which appears in the numerator of Rf) must be linear in the steady state, the profiles of K_m and the wind components must be independent of $\partial\langle\theta\rangle/\partial z$ as none of the terms in the equation depend on that gradient (ignoring the very weak dependence of l_{T1} and l_{T2} on that gradient for cases where $\partial\langle\theta\rangle/\partial z > 0$). Thus, although the counter-gradient term (γ_c) has a direct impact on the equilibrium temperature profile, it is not expected to affect the velocity profiles. To confirm that this is the case, further test simulations were performed in which the counter-gradient term was set to zero. The profiles labelled TL2 in Figure 4.14 are from such a test with $\langle w'\theta'\rangle_0 = 0.3 \text{ Kms}^{-1}$. The shape of the temperature profile changes as expected, becoming similar to that obtained with the mixing length model, as it has to show non-zero gradient throughout the CBL in order to support the upward heat flux. However, the velocity profiles are indeed almost identical to those obtained with the full model (TL).

The main conclusion is that this model is less different from the mixing length model than it might first appear, as the equilibrium velocity profiles are entirely determined by the choices made for l_{T1} and l_{T2} , and are not influenced by the carrying of a parametrized form of the energy equation. However, it is important to note that the way in which these length scales are parametrized depends on a bulk measure of stability, while the mixing length model used has eddy coefficients which depend on local Richardson number. It is this change which allows us to introduce the counter-gradient correction which does appear to fundamentally alter the character of the solutions for temperature by allowing upward heat fluxes even when $\partial\langle\theta\rangle/\partial z > 0$, as occurs in the upper CBL.

The potential advantages of using a model which carries a prognostic equation for energy in a parametrization would seem to be in non-homogeneous or non-stationary conditions. For example, TKE generated at the crest of a hill might be advected downwind by the mean wind in a three-dimensional model. Also, changes in mean shear will not lead to an instantaneous change in energy (which will change with a time scale of order the eddy turnover time, $t_* \simeq z_i^2/K_m$), and this may be advantageous in time-dependent problems.

CHAPTER 4: MEAN STRUCTURE

Considerations of this kind have made TKE models popular for detailed boundary layer and mesoscale modelling. Note however that the sensitivity of the eddy coefficients to the length scale parametrization may mask these benefits, as K_m depends only on the square root of the TKE. Furthermore, a larger scale model (e.g. global) may have insufficient horizontal resolution for advection of TKE from a neighbouring grid point to be significant (or even desirable). It may also run with a timestep comparable to, or larger than, the eddy turnover time (the climate version of the Meteorological Office Unified Model uses 1800 s). In this case the advantages of carrying energy in non-stationary conditions are lost. Therefore, in such a model, using a mixing length parametrization with non-locally determined length scale and counter-gradient term for heat may be more cost effective than using a more expensive TKE model. Presumably the results of such a mixing length model could be brought into closer agreement with LES by careful tuning of the length scale. For example, if the form of Equation (4.41) were used, then setting $C_1 = 6.7$ (instead of 15) would make the length scale in neutral conditions consistent with that diagnosed from LES.

4.6.2 Specified viscosity profiles

This section considers models in which the profiles of the eddy coefficients, K_m and K_h , are specified. The most appropriate profiles are not well established, and it is not clear that any chosen profile will be able to perform satisfactorily across a wide range of conditions (changing stability, baroclinicity etc.). However, there has been some success in using these very simple models. For example, Chrobok *et al.* (1992) found that a parametrization using eddy diffusivities based on the dimensionless gradient functions of Moeng and Wyngaard (1984) performed better than a local mixing length model, and as well as a more complicated transilient turbulence model, for the case of a cold air outbreak. Also, Holtslag and Boville (1993) found that a scheme (based on one proposed by Troen and Mahrt, 1986) using prescribed profiles and counter-gradient corrections for scalar fluxes, transported moisture away from the surface more realistically than a local

CHAPTER 4: MEAN STRUCTURE

mixing length model in a global climate model. A scheme of this type (but without the counter-gradient terms) has recently been introduced into the operational model of the European Centre for Medium Range Weather Forecasting (ECMWF).

As an example of a parametrization which uses specified viscosity profiles, the performance of the extension of the scheme of Troen and Mahrt (1986) described by Holtslag and Boville (1993) is considered here. Momentum fluxes are related to local mean gradients as before (Equations (4.20) and (4.21)) but with K_m given by

$$K_m = \kappa w_m z \left(1 - \frac{z}{z_i}\right)^2 \quad (4.47)$$

where w_m is a turbulent velocity scale. Equation (4.40) is used to parametrize the heat flux, with diffusivity

$$K_h = \kappa w_t z \left(1 - \frac{z}{z_i}\right)^2 \quad (4.48)$$

where w_t is another velocity scale, and the counter-gradient term, γ_c is given by

$$\gamma_c = a \frac{w_* \langle w' \theta' \rangle_0}{w_m^2 z_i} \quad (4.49)$$

In the surface layer ($z/z_i \leq 0.1$), $w_m = u_*/\phi_m$, $w_t = u_*/\phi_h$ and $a = 0$ (i.e. no counter-gradient correction). For, $z/z_i > 0.1$, w_m and w_t are constant. w_m is set equal to the value of u_*/ϕ_m at $z/z_i = 0.1$, and w_t is determined by ensuring that the flux equation, (4.40), is continuous at this height. Finally the constant a is set equal to 7.2, which gives $\gamma_c = 10 \langle w' \theta' \rangle_0 / (w_* z_i)$ in highly unstable conditions, consistent with Troen and Mahrt (1986), but twice as large as that used by Therry and Lacarrère (1983).

The mean fields near the top of the boundary layer are highly sensitive to the form chosen for the eddy coefficients. In particular, the cubic profiles of (4.47) and (4.48) cannot sustain a discontinuity in velocity across the inversion and lead to large shears below the inversion (Nieuwstadt, 1983). Similarly, in cases without entrainment, substituting for K_h (using (4.48)) and $\langle w' \theta' \rangle$ (by assuming a linear profile) in Equation (4.40), and rearranging leads to

$$\frac{\partial \langle \theta \rangle}{\partial z} = \gamma_c - \frac{\langle w' \theta' \rangle_0}{\kappa w_t z (1 - z/z_i)} \quad (4.50)$$

Figure 4.15: Variation of u_* and α_0 with stability for a constant geostrophic windspeed (G) of 10 ms^{-1} , with $z_i = 1000\text{m}$ and $z_0 = 0.1\text{m}$. Results are shown from the model of Holtslag and Boville (HB) and the mixing length model (ML) with $\beta = 0.15$. The squares are the LES results and the solid lines are the mixed layer model predictions as before.

Thus this diffusivity profile implies that $\partial\langle\theta\rangle/\partial z \rightarrow -\infty$ as $z/z_i \rightarrow 1$. Accordingly, near the top of the boundary layer, the model of Holtslag and Boville (1993) uses K_m and K_h calculated based on local gradients, as in the mixing length model, if those values are larger than those given by (4.47) and (4.48). For the tests with this model (HB), the same mixing length formulation was used as in Section 4.4. Additional tests (HB2) were also performed in which this modification was not made i.e. eddy coefficients given by (4.47) and (4.48) at all heights.

Figure 4.15 shows u_* and α_0 predicted by this model (HB). Almost identical results (not shown) were given by HB2. The performance appears to be comparable to, or slightly better than that of the mixed layer model, although the sharp increase in u_* shown by LES as $-z_i/L$ increases from zero is not captured.

It has already been shown (Figure 4.9) that the velocity profiles from simulation BNLr are well reproduced by the local mixing length model (with $\beta = 0.15$). Figure 4.16 shows that the predictions of the full Holtslag and Boville model (HB) are also highly satisfactory. Note though that the viscosities applied are actually from the mixing length

Figure 4.16: Velocity profiles from neutral large-eddy simulation BNLR, and attempts to reproduce them using the full model of Holtslag and Boville (HB), and the test version of this model described in the text (HB2).

formulation for all $z/z_i \gtrsim 0.5$. Nevertheless, the use of the viscosity given by (4.47) at all heights HB2 gives similar velocity profiles for $z/z_i \lesssim 0.8$. Above this height, the wind components are expected to become geostrophic but, while this appears to be the case for $\langle v \rangle$, it does not occur for $\langle u \rangle$. Tests revealed that this is because the vertical resolution used (40 points) is not sufficient to resolve the shear in $\langle u \rangle$ just below the inversion. In fact, most large-scale models will have much coarser resolution than used here and may not resolve the differences between HB and HB2 at all.

In convective conditions, the HB2 model profiles show more shear than LES throughout most of the CBL (Figure 4.17). This time the discrepancy is not removed by using the full model (HB), as the mixing length derived viscosities are smaller except for $z/z_i \gtrsim 0.9$ (due to the counter-gradient term reducing the local instability). The same discrepancy is also likely to be seen at much lower resolution as the shear is no longer restricted to a narrow region just below the inversion. Neglecting the modifications made by this model to the velocity scales in the surface layer, the analytic solutions of Nieuwstadt (1983) for the cubic viscosity profile suggest that this unrealistic behaviour should be expected in the limit $fz_i/(\kappa w_m) \rightarrow 0$. The convective case described here has $fz_i/(\kappa w_m) \simeq 0.1$

Figure 4.17: Mean profiles from convective large-eddy simulation M134, and attempts to reproduce them using the mixing length model (ML) with $\beta = 0.15$, and both versions of the model of Holtslag and Boville (HB and HB2). The velocity profiles which are almost indistinguishable for $z/z_i \lesssim 0.9$ are those from HB and HB2.

(compared to 0.6 for the neutral case), but note that the performance of the model of Holtslag and Boville remains at least comparable to, and arguably slightly better, than that of the mixing length model. Also, the temperature profile is improved, HB showing almost no gradient above $z/z_i = 0.1$. The small remaining discrepancy with LES is mainly associated with different behaviour in the surface layer where no counter-gradient correction is applied. Note that the behaviour of HB2 is not satisfactory, as it shows an unrealistic decrease of $\langle \theta \rangle$ towards the inversion, consistent with the earlier discussion (Equation (4.50)).

In conclusion, the model of Holtslag and Boville reproduces the equilibrium LES velocity profiles at least as satisfactorily as the local mixing length model across a range of stabilities. As K_m and K_h are prescribed and are not sensitive to small local gradients it is potentially more robust than the local model, and can also include the counter-gradient term which improves the temperature profile. Nevertheless, it is not clear that the simple profiles used will be able to perform adequately in conditions when the geostrophic wind varies with height. Hence the performance of this model will be examined again in Chapter 5, when such cases are considered.

4.6.3 Transilient turbulence models

This section on non-local models would not be complete without mention of transilient turbulence models (see e.g. Stull and Driedonks, 1987). In a sense these appear to be more genuinely non-local than the modified exchange coefficient methods studied in this chapter, as they attempt to consider exchange of properties in turbulent flows between all levels in the boundary layer. This is done by constructing a mixing matrix of dimension $N \times N$ (where N is the number of levels). The element c_{ij} of the matrix then represents the amount of air from level i that arrives at level j during a timestep.

Unfortunately, there are two major problems with this approach. The first is that it is inevitably more expensive than traditional eddy coefficient based models, as the number of calculations required per timestep is proportional to N^2 (rather than N). Secondly, the most appropriate values of the matrix elements c_{ij} are not well known. Fiedler and Moeng (1985) derived a matrix for modelling the behaviour of passive scalars in the CBL using LES. A more general model for the coefficients was proposed by Stull and Driedonks (1987), based on a mixing potential derived using a non-local analogy of the TKE equation. Nevertheless, the assumptions that have to be made do restrict the potential performance. For example, the exchange hypothesis, $c_{ij} = c_{ji}$ excludes anisotropic mixing which prevents the model from producing counter-gradient heat fluxes. In fact, Chrobok *et al.* (1992) found that the model of Stull and Driedonks performed no better than a simple eddy viscosity model based on the dimensionless gradient functions of Moeng and Wyngaard (1984) for the case of a cold air outbreak. Similarly, Cuxart *et al.* (1994) found that the model of Bougeault and Lacarrère (1989), which is essentially a revision of that of Therpy and Lacarrère (1983), performed at least as well as the transilient model in clear-sky convective conditions. In fact, they diagnosed the transilient matrix implied by the Bougeault and Lacarrère (1989) model, and found it to be surprisingly similar to that used in the model of Stull and Driedonks (1987). Thus they argued that simple models like that of Bougeault and Lacarrère effectively provide an elegant and inexpensive way of parametrizing the transilient coefficients. Thus the conclusion is that

it seems unlikely that transilient turbulence models will be able to produce sufficient improvement over eddy coefficient based models to justify their increased computational cost in a boundary layer parametrization in a large-scale model.

4.7 Interaction of different parametrization schemes

The tests conducted so far have looked at the performance of various boundary layer parametrization schemes. However, such schemes do not act in isolation in practical large-scale models, and the ways in which they interact with other parametrization schemes may be very significant. For example, most large-scale models have separate schemes for boundary layer turbulence and for convection. This is done because the methods thought most appropriate for representing the effects of deep convection (e.g. mass flux schemes such as that of Gregory and Rowntree, 1990, or convective adjustment schemes such as that of Betts and Millar, 1986) are not the same as those favoured for boundary layer schemes (usually eddy coefficient based). However, this section will show that the ability of the Single Column version of the Meteorological Office Unified Model (the SCM) to reproduce the LES results can depend critically on the way in which the boundary layer and convection schemes interact.

4.7.1 Local boundary layer – convection scheme interaction

The equilibrium SCM boundary layer wind and temperature profiles are influenced primarily by the effects of the boundary layer scheme (Smith, 1993) and the convection scheme (Gregory and Rowntree, 1990). The boundary layer scheme uses local mixing for heat and momentum, with stability dependent viscosity and diffusivity as described in Section 4.4. The convection scheme is a mass flux scheme, primarily designed to deal with deep convection, but which also leads to non-local mixing of heat in the boundary layer. Note that it does not include momentum transports at present. Here, in order

CHAPTER 4: MEAN STRUCTURE

to assess the impact of the convection scheme on the equilibrium boundary layer structure, results obtained using the full model are compared with those obtained with the convection scheme switched off.

The model was set up to be driven by imposed geostrophic wind and surface heat flux, so that it could be run to equilibrium for comparison with LES. The tests performed used the vertical resolution of the mesoscale model, with initial conditions as follows. The wind components, $\langle u \rangle$ and $\langle v \rangle$, were set to their geostrophic values at all levels (10 ms^{-1} and 0 ms^{-1} respectively). Temperatures were initialized such that the potential temperature, $\langle \theta \rangle$, was approximately constant ($\simeq 288 \text{ K}$) from level 1 to level 8 and a strong inversion was set up between levels 8 and 9, giving a boundary layer depth, z_i , of around 860 m. This successfully prevented convection above the boundary layer which would have made the results less comparable with those from LES. However, it was found that entrainment tended to cause a slow increase in boundary layer depth so, to prevent this, the boundary layer fluxes of heat and momentum were set to zero above level 9. All boundary layer temperatures were adjusted downwards each timestep by the amount required to keep the near surface temperature constant – this procedure kept the temperatures realistic, without altering the profile shapes. This was not necessary in the LES and closure model runs in which only the profile shapes are relevant, but was necessary in the SCM tests as absolute temperature values are important for the radiation scheme. All moisture fields and fluxes were set to zero in all cases.

Figure 4.18 compares the equilibrium values of u_* predicted by the SCM, both with and without the convection scheme, with the LES results and the mixed layer model predictions. Note that although the SCM runs have boundary layer depths of around 860 m (compared with 1000 m for LES), the mixed layer model suggests that this difference should not have a significant effect on u_* (see Figure 4.21).

The results obtained using an SCM timestep of 60 s are considered first. The u_* predictions of the SCM without the convection scheme can be seen to be broadly consistent with the LES results, although not showing quite such a strong stability dependence. In

Figure 4.18: Variation of u_* with stability, for $G = 10 \text{ ms}^{-1}$ with $z_0 = 0.1 \text{ m}$. Results from the LES model (squares) and the mixed layer model (solid lines) are shown as before (for $z_i = 1000 \text{ m}$). Single Column Unified Model results, for $z_i \approx 860 \text{ m}$, are shown, both with and without the convection scheme (SCM CON and SCM NO CON). The plot on the left shows SCM results using a timestep of 60 s; that on the right shows results using a timestep of 1800 s.

fact, as expected, the results are very similar to those which were obtained using solely the local boundary layer scheme in Section 4.4. In convective conditions, the velocity profiles are not quite sufficiently well mixed, and $\langle \theta \rangle$ again decreases with height throughout the boundary layer in order to support the turbulent flux. Figure 4.19 shows the $\langle \theta \rangle$ profile for the most unstable SCM test without the convection scheme ($-z_i / L = 17$), and also the heating rate due to the boundary layer scheme. Note that, in the absence of heat transport by the convection scheme, the boundary layer scheme heating rate is almost constant throughout the CBL, although slightly reduced close to the surface where heating by the long wave radiation scheme is not negligible.

In contrast, the results obtained when using the convection scheme, are much less satisfactory, showing little or no increase in surface stress (see Figure 4.18) and little change in the velocity profiles with increasing instability. This behaviour can be explained by considering first the effects of the convection scheme on the boundary layer temperature profile. The $\langle \theta \rangle$ profile shown in Figure 4.19 is unconditionally unstable to parcel ascent. A profile of this shape would cause convection to be initiated, leading to a cooling of

Figure 4.19: Profiles from most unstable SCM test with no convection scheme using a timestep of 60 s. The first plot shows the potential temperature profile, and the second shows the rate of change of $\langle \theta \rangle$ due to increments from the boundary layer scheme, B, and the convection scheme, C (zero in this case).

the lower boundary layer, and a warming of the upper boundary layer. This would change the shape of the boundary layer heating profile, which in turn would affect the operation of the convection scheme. Eventually an equilibrium temperature profile shape would be reached. Figure 4.20 shows that temperature profile and the boundary layer and convection scheme heating rates for the most unstable test run. The heating from the boundary layer scheme is concentrated in the lowest few model levels (due to the stable profile in the upper boundary layer), while the convection scheme cools the lower boundary layer and warms aloft. The sum of the contributions from the two schemes (and the small amount of heating by the long wave scheme close to the surface) gives a well mixed heating profile as before.

It might be thought that, as the total heating profile remains well mixed, it matters little whether the boundary layer mixing is carried out by the boundary layer or convection scheme. Indeed, the slightly stable $\langle \theta \rangle$ profile of Figure 4.20 is possibly less unrealistic than the unstable profile of Figure 4.19. However, the relative size of the contributions from the two schemes is important for two main reasons:

Figure 4.20: Profiles from most unstable SCM test including the convection scheme, using a timestep of 60 s.

1. The rate of entrainment into the boundary layer may be affected, being relatively rapid when the convection scheme dominates, but relatively slow when mixing is predominantly by the boundary layer scheme.
2. The boundary layer scheme mixes momentum, while the convection scheme (at present) does not.

The present tests have not been designed to consider entrainment effects, and that area is left for a later study. However, the effects of the interactions of the two schemes on momentum mixing are both clear and significant. The stress depends on local shear and local temperature gradient. The interaction of the convection scheme with the boundary layer scheme leads to a more stable temperature profile than that obtained using the boundary layer scheme alone. This leads to reduced momentum mixing (due to the stability dependence of the viscosity), and hence less well mixed velocity profiles and significant underestimates of u_* .

The results discussed so far have been from SCM runs using a timestep of 60 s. This value of timestep was chosen as it is considerably smaller than the boundary layer turnover time, t_* , which is around 2000 s for the neutral runs, and about 500 s for the most unstable

CHAPTER 4: MEAN STRUCTURE

runs. However, it is not possible to use such a small timestep in large-scale models - the mesoscale model calls the 'physics' subroutines every 300 s, while the climate model does so only once every 1800 s. The second plot in Figure 4.18 shows the results obtained using a timestep of 1800 s. The results using only local mixing (SCM NO CON) are much as before. However there has been a significant change in performance when using the convection scheme in conjunction with the local boundary layer scheme (SCM CON). u_* values remain too low, but do tend to be significantly larger when using a timestep of 1800 s. This is because the equilibrium solution now has a slightly unstable temperature profile (although not as unstable as obtained using the boundary layer scheme alone). Consistent with this change, more of the mixing is now done by the boundary layer scheme, u_* is increased and the velocity profiles are more mixed. Thus the size of the error depends on the fraction of the mixing of heat performed by the convection scheme, and there is evidence that this may be rather sensitive to changes in the model numerics (numerical scheme, timestep, resolution etc.) and conceivably also to changes in external forcing (note the rather unsteady variation of u_* with stability when using the convection scheme with a timestep of 1800 s in Figure 4.18).

Essentially, the problem stems from the use of non-local mixing for heat, while using local mixing for momentum. Momentum mixing is not sufficiently enhanced, and near surface winds are underestimated. This is almost certainly the cause of a systematic underestimate of 10 m winds in convective conditions over land by the operational model.

One possible solution is to increase momentum mixing in unstable conditions by allowing non-local momentum transport by the convection scheme. Work is currently being performed to include such mixing in the scheme, based on the results of a cloud-resolving model for deep convection. The scheme of Tiedtke (1989), in use at ECMWF, already incorporates a simple parametrization of convective momentum transports. However, it is not clear that it is possible to tune such a scheme to give reasonable results in the boundary layer. It is suspected that the results might well be sensitive to the exact proportions of the mixing carried out by the local boundary layer scheme and the non-local convection scheme. Therefore, tuning of the schemes to give optimum results across a

CHAPTER 4: MEAN STRUCTURE

range of conditions, and for a variety of model timesteps, could prove difficult.

The sensitivity of the results to the way in which the boundary layer and convection schemes interact might be reduced by changing to a non-local boundary layer scheme in unstable conditions (so that viscosity was not related to local temperature gradients). Even in this case it is suspected that having two separate schemes performing vertical mixing in the boundary layer might lead to difficulties. Instead, the proposed solution is to attempt to ease the problem by preventing the convection scheme from mixing in the boundary layer. It must still be initialized close to the surface (for deep convection), and it has been suggested (R.N.B. Smith, private communication) that average boundary layer convective temperature and humidity increments could be applied at all levels in the boundary layer. Thus the convection scheme could not change the shape of the boundary layer profiles and, in cases where there was no significant convection above z_i , the convective increments would be close to zero everywhere. If desired, the local boundary layer scheme could then be used, as the temperature and humidity gradients would no longer be determined non-locally. Although very simplistic, as boundary layer turbulence in unstable conditions is undeniably non-local in nature, it has been shown that such schemes can perform reasonably (the SCM NOCON tests). This approach seems attractive, at least in the short term, as a way of increasing momentum mixing in unstable conditions.

In summary, this section has examined one case where the interaction of two parametrization schemes is of critical importance. The non-local convection scheme in conjunction with the local boundary layer scheme has been shown to produce results considerably poorer than those produced by any of the boundary layer schemes which have been looked at in isolation. A possible solution has been suggested, but the behaviour of the two schemes would still need to be studied carefully, as its implementation could affect the initialization of the convection scheme (Gregory and Rowntree, 1990), due to increased buoyancy gradients close to the surface, and the rate of boundary layer ventilation by deep convection could also be affected due to the changes in the convective heating profile brought about by averaging the increments in the boundary layer.

4.8 Summary

*Can you make
a general statement
or mixing in the b.l.
local/non local $\Rightarrow$
what is to be preferred?
is there some physical argument
to lead us*

In this chapter LES results for the mean fields and various similarity coefficients have been presented. Both velocity and temperature profiles rapidly become well mixed with increasing instability, and it has been shown that the similarity coefficients predicted by a simple mixed layer model are in good agreement with LES for $-z_i/L \gtrsim 2$.

The performance of a simple local mixing length parametrization has been shown to be highly satisfactory in neutral conditions. In convective conditions this model produces insufficiently well mixed velocity and temperature profiles, leading to an underestimate of the surface stress and an overestimate of the temperature difference between the surface and boundary layer top. Various other schemes which seek to alleviate these deficiencies have been tested. It has been argued that relating the eddy coefficients to TKE (for which a prognostic equation must be carried) is not cost effective except in very high resolution mesoscale modelling. However, relating the eddy coefficients to some non-local measure of stability (rather than local Richardson number) does appear to be potentially beneficial. This can be done either through the mixing length (e.g. Therry and Lacarrère, 1983), or by specifying eddy coefficient profiles directly (e.g. Holtslag and Boville, 1993). Once stability effects are incorporated in a non-local manner, it is possible to incorporate counter-gradient correction terms in the scalar flux parametrizations. It has been shown that these can lead to some improvements in the modelled temperature profiles.

Finally it has been shown that the way in which the boundary layer scheme interacts with other parametrizations can be of critical importance. Specifically, the way in which the local boundary layer scheme interacts with the mass flux convection scheme in the Meteorological Office Unified NWP and climate prediction model has been shown to lead to insufficient momentum mixing in unstable conditions. The proposed solution of averaging the convection scheme increments in the boundary layer is currently being tested.

z_0/m	u_*/ms^{-1}	$C_g^2 \times 10^3$	α_0
0.010	0.367	1.35	17.5
0.033	0.406	1.65	19.4
0.100	0.449	2.01	21.5
0.333	0.505	2.55	24.4
1.000	0.569	3.24	27.7

Table 4.2: Variation of u_* , C_g^2 and α_0 with z_0 for $G = 10 \text{ ms}^{-1}$. Values have been obtained using Rossby similarity coefficients $A = 2.42$ and $B = 3.27$ (Grant and Whiteford, 1987).

4.A Appendices to Chapter 4

4.A.1 Sensitivity of surface stress to roughness length

Most large-scale models use a roughness length to describe the properties of the surface with regard to momentum transfer. Although values have been measured over a large number of different surfaces, there are considerable uncertainties associated with the need to obtain a single value representative of an entire NWP model grid square in which the surface may be highly heterogeneous. Recently enhanced orographic roughness lengths have been introduced in some models. These attempt to allow for the enhanced drag in the boundary layer due to subgrid scale orography, and their introduction has led to improved performance of the Meteorological Office Unified Model. However the values used are subject to considerable uncertainty, both due to the parametrization of the orographic drag and to the limited resolution of the available orographic datasets.

Here Rossby similarity theory is used to obtain an approximate estimate of the sensitivity of the surface stress to the roughness length. Table 4.2 shows the values of u_* , $C_g^2 (= u_*^2/G^2)$ and α_0 obtained iteratively for a range of values of z_0 with $G = 10 \text{ ms}^{-1}$, using $A = 2.42$ and $B = 3.27$ (Grant and Whiteford, 1987). The range of values of z_0 has been chosen to cover typical vegetative values over land (effective roughness lengths due

CHAPTER 4: MEAN STRUCTURE

M_{Ch}	$z_0/10^{-4}\text{m}$	u_*/ms^{-1}	$C_g^2 \times 10^3$	α_0
0.012	0.85	0.263	0.694	12.4
0.020	1.5	0.273	0.745	12.9
0.032	2.6	0.282	0.798	13.3

Table 4.3: Variation of z_0 , u_* , C_g^2 and α_0 with z_0 with the Charnock constant, M_{Ch} , for $G = 10 \text{ ms}^{-1}$. Values have been obtained using coefficients $A = 2.42$ and $B = 3.27$ (Grant and Whiteford, 1987).

to orography are potentially much larger). The table shows that changing z_0 by a factor of 3.3 leads to roughly a 10% change in u_* , or, equivalently, a 20% change in C_g^2 . Note that the ageostrophic angle, α_0 , changes only slowly with z_0 , so that this gives approximately a 20% change in the spin-down time scale ($t_{sd} \propto 1/(C_g^2 \cos \alpha_0)$).

A similar sensitivity to z_0 is found using other values of G as the drag coefficient is only a weak function of the geostrophic windspeed ($G = 30 \text{ ms}^{-1}$ gives $C_g^2 = 1.65 \times 10^{-3}$ for $z_0 = 0.1 \text{ m}$). It is concluded that if it is assumed that the appropriate value of roughness to use for a large-scale model grid-box is known to within a factor of two or three, then the associated uncertainties in u_* are of order 10%.

Over the sea the situation is rather different. The roughness length is commonly related to the surface stress (due to changes in the state of the sea surface) through the formula of Charnock (1958)

$$z_0 = \frac{M_{Ch} u_*^2}{g} \quad (4.51)$$

Here M_{Ch} is the Charnock constant. Garratt (1992) tabulates some experimental values for M_{Ch} , and these range from 0.012 to 0.032. Table 4.3 shows the effects on z_0 , u_* , C_g^2 and α of changing the Charnock constant over this range (for $G = 10 \text{ ms}^{-1}$ and $A = 2.42$ and $B = 3.27$ as before). Note that there is only a factor of three change in z_0 over the entire range of M_{Ch} values used. The sensitivity of u_* to changes in z_0 is also slightly smaller than over land due to the the larger value of $u_*/(fz_0)$.

Figure 4.21: Variation of u_* with $-z_i/L$ from mixed layer model of Garratt *et al.* (1982) for varying z_i . All curves are for $G = 10 \text{ ms}^{-1}$, $z_0 = 0.1 \text{ m}$. The dotted curve, unlabelled for clarity, is for $z_i = 2000 \text{ m}$.

4.A.2 Sensitivity of surface stress to boundary layer depth

This annex assesses the sensitivity of the surface stress to the boundary layer depth using similarity theory. This is relevant as a large-scale model might have an inaccurate value of z_i , due, for instance, to poor representation of the surface and entrainment fluxes, or to poor vertical resolution which means that only a few discrete values of z_i are possible. Equations (4.11) and (4.12) are most suitable, as they retain the boundary layer depth, z_i , explicitly. Unfortunately, as discussed earlier, the coefficients A_i and B_i are not well determined experimentally and once again the predictions of the mixed layer model of Garratt *et al.* (1982) are used. As discussed earlier, this is not valid in neutral conditions, but it should be adequate for $-z_i/L \gtrsim 2$.

Figure 4.21 shows u_* as a function of $-z_i/L$ obtained by iterative solution of Equation (4.19) for $G = 10 \text{ ms}^{-1}$, $z_0 = 0.1 \text{ m}$ and a range of values of z_i . It can be seen that, for constant z_i/L , u_* increases with increasing z_i for small z_i , but reaches a maximum value after which it decreases slowly with further increases in z_i .

CHAPTER 4: MEAN STRUCTURE

This behaviour can be understood with reference to Equation (4.19). For 'shallow' boundary layers, the second term on the RHS dominates over the first, giving

$$u_* \simeq (fGz_i)^{\frac{1}{2}} \quad (4.52)$$

i.e. the surface stress increases linearly with increasing boundary layer depth. Note that the stability function, Ψ , does not appear in this expression, consistent with the curve for $z_i = 200\text{m}$ in Figure 4.21 showing only a weak stability dependence. A non-dimensional sensitivity parameter, s , which relates a fractional change in z_i to a fractional change in u_* can be defined as follows

$$s = \frac{z_i}{u_*} \frac{\partial u_*}{\partial z_i} \quad (4.53)$$

and in this limit it has a value of 0.5 i.e. a 20% error in z_i would lead to a 10% error in u_* .

For 'deep' boundary layers, the second term on the RHS of Equation (4.19) becomes small compared to the first, giving

$$u_* \simeq \frac{\kappa G}{\left[\ln \left(\frac{z_i}{z_0} \right) - \Psi \right]} \quad (4.54)$$

$$s = \frac{z_i}{u_*} \frac{\partial u_*}{\partial z_i} \simeq - \frac{1}{\left[\ln \left(\frac{z_i}{z_0} \right) - \Psi \right]} \quad (4.55)$$

For $z_i = 2000\text{m}$ and $z_i/L = -5$ this gives $s = -0.15$ i.e. u_* depends only weakly on z_i , decreasing slowly as the boundary layer depth increases.

Figure 4.22 shows the variation of s with z_i between these two limits for various values of G . All curves are for $z_i/L = -5$, $z_0 = 0.1\text{ m}$, and were obtained by differentiating (4.19) with respect to z_i , and using the iteratively obtained values of u_* . All curves show the similar behaviour, although the 'shallow' regime where u_* is relatively sensitive to z_i extends to greater depth with large values of G .

It is concluded that for 'deep' boundary layers, the surface stress is fairly insensitive to the exact depth – a 20% change in z_i for $z_i \gtrsim 700\text{ m}$ with $G = 10\text{ ms}^{-1}$ is predicted to give less than a 2% change in u_* . However, shallower boundary layers do show greater

CHAPTER 4: MEAN STRUCTURE

Figure 4.22: Sensitivity parameter, s , (defined as in text) as a function of z_i . The curves are for $G=5$, 10, 15 and 20 ms^{-1} and have been obtained using the mixed layer model of Garratt *et al.* (1982) with $z_i/L = -5$, $z_0 = 0.1$ m.

sensitivity. Note also that most large-scale models which use finite-difference methods have poor vertical resolution – typically of $O(100$ m). This means that fractional errors in z_i can be large, particularly for shallow boundary layers.

Chapter 5

The influence of baroclinicity on CBL turbulence

All the simulations that have been considered so far have used imposed geostrophic winds that did not vary with height. In fact, the author is not aware of any published LES studies of the boundary layer in which the geostrophic wind was a function of height. However, the thermal wind equations (Section 5.1) indicate that in practice there will commonly be significant shear in the geostrophic wind across the atmospheric boundary layer. Furthermore, there is some evidence (described in Section 5.2) that the simple parametrizations which can be used in NWP and climate prediction models may perform poorly in such conditions. This provides ample motivation for an LES study, and the results for the mean wind profiles are compared with the predictions of two simple closure models. The influence of shear in the geostrophic wind on scaled turbulence statistics is also discussed.

5.1 The thermal wind equations

The geostrophic wind (u_g, v_g) is defined through

$$u_g = -\frac{1}{f\rho} \frac{\partial P_0}{\partial y} \quad (5.1)$$

$$v_g = +\frac{1}{f\rho} \frac{\partial P_0}{\partial x} \quad (5.2)$$

(Equations (2.4) and (2.5), except using local rather than reference density). Differentiating with respect to z and using the hydrostatic approximation ($\partial P_0/\partial z = -\rho g$) and the ideal gas law ($P_0 = \rho RT$ where R is the gas constant and T is the absolute temperature), the thermal wind equations can be obtained

$$\frac{\partial u_g}{\partial z} = -\frac{g}{fT} \frac{\partial T}{\partial y} + \frac{u_g}{T} \frac{\partial T}{\partial z} \quad (5.3)$$

$$\frac{\partial v_g}{\partial z} = +\frac{g}{fT} \frac{\partial T}{\partial x} + \frac{v_g}{T} \frac{\partial T}{\partial z} \quad (5.4)$$

As discussed by Arya and Wyngaard (1975), the second terms on the right-hand side of Equations (5.3) and (5.4) are usually neglected - assuming that the temperature gradient is close to the dry adiabatic lapse rate, these terms lead to a fractional change in geostrophic windspeed of less than 4% per kilometre. The shear in the geostrophic wind in the atmosphere is therefore largely determined by the horizontal temperature gradients. These can be large in the vicinity of mesoscale systems such as fronts and orographically induced flows (of order 10 K per 100 km), but are also likely to be significant in situations which appear to be closer to idealized. For example, a temperature gradient of only 1.5 K per 100 km at 45° N, is consistent with a shear in the geostrophic wind of 0.005 s⁻¹ (i.e. a change of 5 ms⁻¹ over a boundary layer 1000 m deep). Temperature gradients of this order of magnitude are common place - assuming a surface temperature difference of 50 K between equator and pole, even the mean north-south temperature gradient must be around 0.5 K per 100 km. It is concluded that significant shear in the geostrophic wind in the lower atmosphere is common place, but its effects remain poorly understood.

5.2 Possible parametrization problems

Hollingsworth (1994) identified a systematic error in the performance of the ECMWF weather prediction model. Figure 5.1 shows a comparison of composited radiosonde observations and short-range forecasts of wind shear across the boundary layer (between the surface and 850 hPa), in cases where the observed wind backed (turned anticlockwise) with height. The North Atlantic composite was made using five radiosonde stations over three winter months. It can be seen that the forecast model did not reproduce the observed backing wind shear. Similar errors were found in the forecasts over the Great Plains of North America, and in the Pacific trade wind zones both north and south of the equator. In regimes in which the observed wind veered with height, the model performance was found to be much better.

It was shown in Chapter 4 that, with a constant geostrophic wind, the wind veers with height across the boundary layer, both in neutral and convective conditions. Hence, none of the closure model tests which were described in that chapter are directly relevant for the cases where Hollingsworth (1994) found the largest errors, namely those in which the observed wind backed with height. This backing with height is likely to be associated with a geostrophic wind which varies with height. Indeed, two of the baroclinic large-eddy simulations which are described in the next section do show a net backing of the wind across the boundary layer. Comparisons of the LES and closure model predictions for the wind profiles are made in Section 5.4, in order to assess the validity of the suggestion of Hollingsworth (1994) that the forecast errors noted above are caused by the failure of simple eddy viscosity based closure models in baroclinic conditions.

5.3 LES of the baroclinic boundary layer

The baroclinicity of the atmosphere is usually characterized (e.g. Arya and Wyngaard, 1975) using the parameters, M and β . For constant geostrophic shear, M is simply equal

Figure 5.1: From Hollingsworth (1994). Composites (based on a 3-month sampling period) of mean surface and 850 hPa winds as observed (labelled 1000R and 850R) and forecast (labelled 1000F and 850F) for four groups of selected radiosonde stations (a, North Atlantic; b, Great Plains of North America; c, the tropical Pacific north of the equator; d, the tropical Pacific south of the equator). The composites were made using cases when the observed surface wind exceeded 5 ms^{-1} and the observed backing of the wind (veering in the Southern Hemisphere) was between 12 and 27° . The errors in the surface wind direction are given in degrees ($\delta\phi$ in the notation of Hollingsworth, with positive values indicating surface ageostrophic angle too large).

CHAPTER 5: BAROCLINICITY

Run	$\langle w'b' \rangle_0 / \text{m}^2 \text{s}^{-3}$	u_{g0} / ms^{-1}	v_{g0} / ms^{-1}	$(\partial u_g / \partial z) / \text{s}^{-1}$	$(\partial v_g / \partial z) / \text{s}^{-1}$	$\gamma / (\text{deg.})$
N0	0	10	0	0.005	0.000	0.0
N90	0	10	0	0.000	0.005	90.0
N180	0	10	0	-0.005	0.000	180.0
N270	0	10	0	0.000	-0.005	270.0
N135	0	10	0	-0.010	0.010	135.0
C0	10^{-2}	10	0	0.005	0.000	0.0
C90	10^{-2}	10	0	0.000	0.005	90.0
C180	10^{-2}	10	0	-0.005	0.000	180.0
C270	10^{-2}	10	0	0.000	-0.005	270.0
C135	10^{-2}	10	0	-0.010	0.010	135.0

Table 5.1: Summary of baroclinic runs. External parameters.

to the magnitude of the geostrophic shear vector normalized by u_*/z_i , and β is the angle between that vector and the surface stress (positive for shear backed relative to surface stress).

The simulations described in this section have been designed to look at the effects of geostrophic shear as functions of its magnitude and direction, in both neutral and highly convective conditions. For simplicity, it was decided to use stress-free rigid lids to form the boundary layer tops at $z_i = 1000$ m. Therefore these simulations cannot be used to learn about the effects on the turbulence (and the entrainment rate in particular) of enhanced shear across the inversion. The simulations were run for 100000 s, using $40 \times 40 \times 32$ points and with domains of horizontal extent $3 \text{ km} \times 2 \text{ km}$ for the neutral simulations, and $4 \text{ km} \times 4 \text{ km}$ for the convective simulations. All were driven by a geostrophic wind of surface speed 10 ms^{-1} (at 45°N) and, in both neutral and convective conditions, geostrophic shears of 0.005 s^{-1} were imposed at angles (γ) of 0, 90, 180 and 270° to the surface geostrophic wind direction. Additionally, one further simulation was performed in each case, with larger shear at 135° , so that the geostrophic wind at z_i was backed 90° from that at the surface. A summary of the simulations performed can be found in Table 5.1.

CHAPTER 5: BAROCLINICITY

Equations (5.3) and (5.4) tell us that, in thermal wind balance, a shear in the geostrophic wind is associated with a horizontal temperature gradient. It could be argued that an extra term should have been incorporated in the equation for $\partial\theta/\partial t$, allowing for advection of this mean temperature gradient. Such a modification to the model is easily made, and would provide non-uniform heating or cooling as the mean wind speed is a function of height. However a test simulation confirmed that the effect of such a modification was not significant in convective conditions as the change in heat flux required to balance the non-uniform advective heating was negligible compared to the total flux i.e. the flux profile remained almost exactly linear. With zero surface flux (the 'neutral runs') the effect was not found to be negligible as buoyancy fluxes of maximum magnitude of around $10^{-4}\text{m}^2\text{s}^{-3}$ were set up to balance the non-uniform heating/cooling caused by the advection term. Nevertheless, it was decided to concentrate on runs without this term, in order to study the purely dynamical effects of a height dependent geostrophic wind, without the complicating stability effects. This seems to be a reasonable approach, as the LES simulations are undoubtedly highly idealized in any event. The closure models tested were set up in a consistent manner.

*chlochl
clater me
an shear
had parallel
wavy* γ, β and α_0 have already been introduced, and now two further angles, ϕ_- and ϕ_+ , are introduced. ϕ_- is the angle between the surface wind and the wind just below z_i , and ϕ_+ is that between the surface wind and the geostrophic wind at z_i . Note that it is assumed that the wind above z_i is geostrophic, so ϕ_+ gives the total turning across the boundary layer i.e. turning across boundary layer interior ($= \phi_-$) plus turning across inversion. For ease of reference, definitions of all these angles are given in Table 5.2.

Results of the baroclinic runs are shown in Table 5.3. Note that the values of non-dimensional baroclinicity, M , obtained in the simulations with geostrophic shears of 0.005 s^{-1} , are of order 10. Grant and Whiteford (1987) found that values of M in flights from the KONTUR experiment in near neutral conditions over the North Sea were between 2.9 and 13.7 with a mean of 7.5, so it can be concluded that the LES values are by no means excessive. Indeed, in none of these cases is the baroclinicity strong enough to cause a net backing of the wind with height, although ϕ_+ does become close to zero in

CHAPTER 5: BAROCLINICITY

γ	Angle between directions of geostrophic wind shear and surface geostrophic wind. Imposed in the present simulations.
α_0	Angle between directions of surface wind and surface geostrophic wind.
β	Angle between directions of geostrophic wind shear and surface wind (i.e. $\beta = \gamma - \alpha_0$)
ϕ_-	Angle between directions of surface wind and wind just below z_i .
ϕ_+	Angle between directions of surface wind and geostrophic wind at z_i .

Table 5.2: Definitions of angles. All are positive when the first direction is backed (rotated anticlockwise) relative to the second e.g a positive value of ϕ_+ indicates that the surface wind is backed relative to the geostrophic wind at z_i or, alternatively, that the wind veers with height across the boundary layer.

Run	u_*/ms^{-1}	$-z_i/L$	M	$\gamma/(\text{deg.})$	$\alpha_0/(\text{deg.})$	$\beta/(\text{deg.})$	$\phi_-/(\text{deg.})$	$\phi_+/(\text{deg.})$
BNLR	0.45	0.0	0.0	—	18.0	—	10.0	18.0
N0	0.55	0.0	9.2	0.0	15.0	345.0	1.2	15.0
N90	0.48	0.0	10.4	90.0	28.4	61.6	1.6	1.8
N180	0.36	0.0	13.7	180.0	24.8	155.2	25.9	24.8
N270	0.45	0.0	11.2	270.0	4.0	265.6	9.8	30.6
N135	0.41	0.0	34.9	135.0	52.9	82.1	−13.7	−37.1
M134	0.67	13.4	0.0	—	25.8	—	−0.4	25.8
C0	0.77	8.8	6.5	0.0	25.5	334.5	−4.5	25.5
C90	0.67	13.2	7.5	90.0	39.1	50.9	−0.6	12.5
C180	0.54	24.8	9.2	180.0	23.2	156.8	0.2	23.2
C270	0.68	12.9	7.4	270.0	11.4	258.6	−1.2	38.0
C135	0.54	26.1	26.4	135.0	68.2	66.8	−0.8	−21.8

Table 5.3: Results of baroclinic runs. Also shown, for comparison, are results from simulations BNLR and M134.

simulation N90. The two more strongly baroclinic runs, N135 and C135, were specifically designed to make the wind back with height, with the geostrophic wind backing by 90° across the boundary layer. The values of M in these simulations are around 30, which are comparable with those found in convective conditions over the East China Sea during the AMTEX experiment (Lenschow *et al.*, 1980).

5.4 Mean fields

In this section the effect of shear in the geostrophic wind on the mean wind profiles in neutral and convective conditions is examined. In each case the LES results are compared with the predictions of two simple closure models which were described in Chapter 4 – the local mixing length model and the non-local model of Holtslag and Boville (1993).

5.4.1 Neutral results

Figure 5.2 shows the mean wind profiles from simulations BNLR, N0, N90, N270, N180 and N270 (solid lines). As expected, the addition of a shear in the geostrophic wind has a significant effect on the wind shears in the boundary layer interior. Nevertheless, it is found that the stress remains closely parallel to the shear in all the neutral runs (not shown). Figure 5.3 shows profiles of λ_M/z_i , diagnosed from the five neutral baroclinic simulations, as was done in Chapter 4 for the non-baroclinic simulation BNLR. Below around $0.6z_i$, the length scales diagnosed from the different runs are in surprisingly good agreement, with the differences between them being only slightly larger than the statistical uncertainties associated with any one of them (estimated by comparing results from successive averaging periods). The differences in the upper boundary layer are more marked, but probably not particularly significant as both stress and shear become small. Therefore, although simulation N180 does show slightly low values in mid-boundary layer and the results from the highly baroclinic simulation, N135, differ somewhat close to the surface, it is

CHAPTER 5: BAROCLINICITY

Figure 5.2: LES mean wind profiles (solid lines) from the neutral runs. The geostrophic wind components, u_g and v_g are shown as dotted lines. Note that in N135, $\langle v \rangle > \langle u \rangle$. Also shown are attempts to reproduce the LES results using closure models. Dashed lines : mixing length model with $\beta = 0.15$; Dot-dash lines : non-local model of Holtslag and Boville (1993).

Figure 5.3: Length scale, λ_M/z_i , diagnosed from simulations N0, N90, N180, N270 and N135. The squares show profile implied by the parametrization $1/\lambda_M = 1/(\beta z_i) + 1/(\kappa z)$, with $\beta = 0.15$.

concluded that the parametrization $1/\lambda_M = 1/(0.15z_i) + 1/(\kappa z)$ (which was advocated in Chapter 4 on the basis of results from BNLR) remains reasonably successful even with considerable shear in the geostrophic wind.

In view of this finding, it is not surprising that runs of the mixing length model using this parametrization are highly successful in reproducing the LES wind profiles – the dashed lines in Figure 5.2 show the mixing length model predictions and in many cases are indistinguishable from the LES results. The dot-dash lines in this plot are the predictions of the non-local model of Holtslag and Boville (1993), and are also in excellent agreement with the large-eddy results. Initially this might seem surprising, as if λ_M diagnosed from LES is not affected by geostrophic shear, then diagnosed K_m profiles would be expected to be affected due to changes in wind shear (as $K_m = \lambda_M^2 |\partial \langle \mathbf{u} \rangle / \partial z|$). In fact, Figure 5.4, shows that the diagnosed profiles of $(K_m / (u_* z_i))^{1/2}$ are still fairly insensitive to the geostrophic shear, although the scatter is rather larger than in the λ_M/z_i profiles of Figure 5.3. Thus the K_m profile prescribed by Holtslag and Boville remains in reasonably good agreement with those diagnosed from simulations N0, N90, N180 and

Figure 5.4: Profiles of $(K_m / (u_* z_i))^{1/2}$ diagnosed from simulations N0, N90, N180, N270 and N135. The squares (HB) show the profile obtained using $K_M = u_* \kappa z (1 - z/z_i)^2$, as given in Holtslag and Boville (1993).

N270 in lower and mid-boundary layer and, while the discrepancy is more serious in N135, it has been shown that it does not lead to major errors in the wind profiles (Figure 5.2).

Table 5.4 confirms that u_* , α_0 , ϕ_- and ϕ_+ are all well predicted, both by the mixing length model and by the non-local model, even in the case where the geostrophic shear is strong enough to cause backing of the wind with height. The conclusion is that inclusion of shear in the geostrophic wind does not, on its own, lead to failure of these simple parametrizations of the boundary layer.

5.4.2 Convective results

The effect of geostrophic shear in convective conditions is rather different. Figure 5.5 shows the mean wind profiles from the convective simulations. It is clear that these simulations are all convective enough for the profiles to remain well mixed even in the

CHAPTER 5: BAROCLINICITY

Run	Model	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	$\phi_-/(\text{deg.})$	$\phi_+/(\text{deg.})$
BNLR	LES	0.45	18.0	10.0	18.0
	ML	0.44	17.3	9.1	17.3
	HB	0.45	17.3	8.4	17.3
N0	LES	0.55	15.0	1.2	15.0
	ML	0.54	15.1	1.7	15.1
	HB	0.55	15.5	1.5	15.5
N90	LES	0.48	28.4	1.6	1.8
	ML	0.47	29.4	3.4	2.8
	HB	0.49	29.6	2.4	3.0
N180	LES	0.36	24.8	25.9	24.8
	ML	0.36	23.4	21.8	23.4
	HB	0.37	22.6	20.2	22.6
N270	LES	0.45	4.0	9.8	30.6
	ML	0.43	2.8	8.9	29.4
	HB	0.44	2.9	8.8	29.4
N135	LES	0.41	52.9	-13.7	-37.1
	ML	0.41	54.2	-10.9	-35.8
	HB	0.43	56.1	-10.2	-33.9

Table 5.4: Mixing length (ML) and non-local (HB) model results for u_* , α_0 , ϕ_- and ϕ_+ given the same forcing as LES simulations BNLR, N0, N90, N180, N270 and N135. The LES results for these quantities are shown for ease of comparison.

CHAPTER 5: BAROCLINICITY

Figure 5.5: LES mean wind profiles (solid lines) from the convective runs. The geostrophic wind components, u_g and v_g are shown as dotted lines. Note that in C135, $\langle v \rangle > \langle u \rangle$. Also shown are attempts to reproduce the LES results using closure models. Dashed lines : mixing length model with $\beta = 0.15$; Dot-dash lines : non-local model of Holtslag and Boville (1993).

CHAPTER 5: BAROCLINICITY

presence of considerable geostrophic shear. Table 5.3 confirms that the values of ϕ_- , the amount of wind turning within the boundary layer, stay close to zero in all cases, although the surface ageostrophic angle and geostrophic departure just below z_i are affected. In fact the similarity coefficients A_m and B_m (not shown) are still well predicted by the mixed layer model of Garratt *et al.* (1982) which was studied in Chapter 4.

The dashed lines on Figure 5.5 show the results obtained using the mixing length model discussed in Chapter 4 (with $\beta = 0.15$), and the dot-dash lines show the predictions of the non-local model of Holtslag and Boville (1993). Once again, both models tend to predict too much shear in the boundary layer interior. Nevertheless, it is not clear that the results are systematically poorer in the baroclinic cases than in the non-baroclinic convective case M134.

Figure 5.6 shows the variation of u_* , α_0 , ϕ_- and ϕ_+ with γ predicted by various models when given the same forcing as the convective LES simulations with shear in the geostrophic wind of 0.005 s^{-1} . The LES results can be seen to be in excellent agreement with those obtained iteratively using the mixed layer model of Garratt *et al.* (1982). The mixing length model systematically underestimates u_* , with values between 7% and 12% below the LES results, while the non-local model gives values between 4% and 9% below the LES. Note however, that in convective conditions without geostrophic shear, the mixing length model predicts a u_* value 12% below that in simulation M134, while the non-local model gives u_* 7% below the LES. The discrepancies of a few degrees between the closure model and LES predictions for α_0 (and ϕ_- , ϕ_+) also do not appear to be systematically larger than those found in non-baroclinic convective conditions.

Note however that Hollingsworth (1994) found the largest errors in NWP model performance in cases where there was a net backing with height across the boundary layer and that all the convective cases considered in Figure 5.6 showed veering (ϕ_+ positive). The velocity profiles in Figure 5.5 suggest that the performance of the closure models in reproducing the LES results in the case where the wind backs with height (C135) is not especially poor, and this is confirmed by listing LES, mixed layer model, mixing length

CHAPTER 5: BAROCLINICITY

Figure 5.6: u_* , α_0 , ϕ_- and ϕ_+ as a function of γ , for $\langle w'b' \rangle_0 = 10^{-2} \text{m}^2 \text{s}^{-3}$, $z_i = 1000 \text{ m}$, $z_0 = 0.1 \text{ m}$, with a surface geostrophic windspeed of 10 ms^{-1} and a shear in the geostrophic wind of 0.005 s^{-1} at angle γ to the surface geostrophic wind direction. Squares : LES; solid lines : mixed layer model of Garratt *et al.* (1982); plus signs : mixing length model; multiplication signs : non-local model of Holtslag and Boville (1993).

Run	Model	u_*/ms^{-1}	$\alpha_0/(\text{deg.})$	$\phi_-/(\text{deg.})$	$\phi_+/(\text{deg.})$
C135	LES	0.54	68.2	-0.8	-21.8
	MIX	0.51	66.5	0.0	-23.5
	ML	0.50	64.1	-3.7	-25.9
	HB	0.53	66.2	-7.3	-23.7

Table 5.5: Mixed layer (MIX), mixing length (ML) and non-local (HB) model results for u_* , α_0 , ϕ_- and ϕ_+ given the same forcing as LES simulation C135. The LES results for these quantities are shown for ease of comparison.

model and non-local model results for u_* , α_0 , ϕ_- and ϕ_+ in Table 5.5. All the predicted u_* values are within 7% of the LES result, and the discrepancies in the angles are also still small. In fact, the closure models predict slightly more backing across the boundary layer than LES.

5.4.3 Discussion

To summarize, it has been shown that both the local mixing length and Holtslag and Boville (1993) schemes both perform well in neutral conditions, even with considerable shear in the geostrophic wind. In convective conditions the performance is less good, but does not appear to be significantly worsened by the presence of a shear in the geostrophic wind.

These results do not explain the findings of Hollingsworth (1994), as they indicate that simple eddy viscosity based boundary layer parametrizations are capable of predicting backing of the wind with height. This is the case both in neutral conditions when there is significant turning within the boundary layer, and in convective conditions when the boundary layer flow is approximately unidirectional and most of the backing occurs across the capping inversion.

CHAPTER 5: BAROCLINICITY

These tests are idealized as they have considered only the steady state and the dry boundary layer. Clearly this means that they are not directly relevant for complex frontal situations. Nevertheless, it seems unlikely that the effects of non-stationarity and moisture alone could cause sufficient degradation of the boundary layer parametrization scheme performance to account for the large systematic error identified by Hollingsworth (1994). However, note that cases in which the wind backs with height will often be unstable to convective ascent (for example, a cold air outbreak where cold air is advected over a relatively warm sea). Thus the problem may be related to the action of the model convection scheme and the way in which it interacts with the boundary layer scheme. One possibility is that convective momentum transports in the Tiedtke (1989) scheme may tend to reduce velocity shear both in the boundary layer interior and across the inversion, making it difficult for the model to sustain a net backing with height across the boundary layer.

5.5 Turbulence statistics

This chapter has concentrated on the effects of geostrophic shear on the mean wind profiles, and the ability of simple closure models to reproduce the LES results. There follows a brief discussion of the effects on some scaled turbulence statistics.

The simpler convective case is considered first. Addition of geostrophic shear causes the stress profiles (not shown) to become curved, so that the wind profiles may remain well mixed (see Equations (4.16) and (4.17)). Therefore, buoyancy production of energy continues to dominate over shear production throughout most of the CBL and it is found that turbulence statistics continue to scale convectively. For example, Figure 5.7 shows profiles of the scaled vertical velocity variance and skewness from simulations C0, C90, C180, C270 and M134, and clearly demonstrates that these quantities are not sensitive to the presence of shear in the geostrophic wind. Note that this result was implicitly assumed in Chapter 3 when the non-baroclinic LES results were compared with the data

Figure 5.7: Profiles of total vertical velocity variance (scaled by w_*^2) and skewness from simulations C0, C90, C180 and C270. The profiles from non-baroclinic simulation M134 are also shown for comparison.

of Lenschow *et al.* (1980), which was obtained in convective, baroclinic conditions (M between 20 and 40). In such conditions the effects on the turbulence are only likely to be significant close to the surface and close to z_i , both regions where shear production may be significant.

The situation in neutral conditions is rather more complex. Figure 5.2 showed that addition of geostrophic shear leads to changes in the shapes of the mean wind profiles. In the limit of $(u_*/fz_i) \rightarrow \infty$, the shape of the stress profiles is expected to be linear, even with shear in the geostrophic wind. This is because the time scale of the Coriolis effect (f^{-1}) is large with respect to the time scale for momentum exchange z_i/u_* (Nieuwstadt, 1983). Approximately linear stress profiles have been observed in shallow boundary layers (e.g. Grant (1986) and Brost *et al.* (1982), both for cases where $u_*/(fz_i) \simeq 10$), and it was shown in Chapter 3 that the non-baroclinic simulation BNHR ($u_*/(fz_i) \simeq 4.5$) also has a roughly linear profile. However, the LES boundary layers are too deep to be able to sustain linear stress profiles when $M \simeq 10$, as is shown in Figure 5.8.

Finally the effect of baroclinicity on the velocity variance profiles is considered. Assuming that the turbulent transport terms are small in neutral conditions, various diagnostic relations can be deduced from the parametrized budget equation for the second order mo-

Figure 5.8: Profiles of non-dimensional total stress from simulations N0, N90, N180 and N270. The profile from non-baroclinic simulation BNLR is also shown for comparison.

ment, $\langle u'_i u'_k \rangle$ (Grant, 1992). These include the result that the stress-energy ratio should be constant with height within the neutral boundary layer. The TKE budget of simulation BNLR shows an almost exact balance between shear production and dissipation, and it is found that the introduction of moderate geostrophic shear in simulations N0, N90, N180 and N270 changes the shapes of shear production profiles, but that they are still closely in balance with the dissipation profiles i.e. the transport terms remain small. For example, the first plot in Figure 5.9 shows the TKE budget of simulation N0. Figure 5.10 confirms that the diagnosed stress-energy ratio profiles from the moderately baroclinic runs do indeed all give approximately the same constant value (around 0.22) in the boundary layer interior. Note that the slightly lower values in the upper part of the boundary layer of simulation N90 are not thought to be significant as both stress and turbulence energy are small in this region. The remaining plots in Figure 5.10 show the scaled variance profiles, with the x -axis aligned with the surface stress. It can be seen that the introduction of shear in the geostrophic wind causes changes of $O(u_*^2)$ in the magnitudes of the variances of in mid boundary layer. Grant (1992) also predicted that the fraction of TKE in each of

CHAPTER 5: BAROCLINICITY

Figure 5.9: Turbulence kinetic energy budgets for simulations N0 and N135. The shear production, dissipation and total transport terms are shown, all normalized by (u_*^3/z_i) .

*wat bekent
dit resultaat
dat de productie van
turbulentie niet veranderd
is in de geostrophische wind
omdat de productie van
turbulentie niet veranderd
is in de geostrophische wind*

$\langle u'u' \rangle$, $\langle v'v' \rangle$ and $\langle w'w' \rangle$ should be constant and independent of height, provided that the x -axis is aligned with the local stress. Equivalently, as stress-energy ratio has been shown to be constant, $\langle u'u' \rangle / \langle \tau \rangle$, $\langle v'v' \rangle / \langle \tau \rangle$ and $\langle w'w' \rangle / \langle \tau \rangle$ should all be constant. This is well supported by the LES results, with the constants equal to 4.2, 2.7 and 2.0 (with a scatter of roughly ± 0.02) in mid-boundary layer. It is concluded that the effects of geostrophic shear on the variance profiles in these moderately baroclinic neutral conditions can be explained with reference to the changes in the stress profiles.

With greater non-dimensional shear in the geostrophic wind (N135), the situation is rather different. The shear production goes to zero at around $0.25z_i$ and the transport terms are no longer negligible (see Figure 5.9). Thus the assumptions of Grant (1992) are no longer valid, at least around this height. In fact the diagnosed profile of stress-energy ratio from this simulation (not shown) is similar to those from the moderately baroclinic simulations for $z/z_i \lesssim 0.1$ and for $z/z_i \gtrsim 0.4$, but shows a minimum of around 0.1 at $0.25z_i$.

CHAPTER 5: BAROCLINICITY

Figure 5.10: Profiles of stress-energy ratio and velocity variances (x -axis aligned with surface stress) from simulations N0, N90, N180 and N270. The profiles from non-baroclinic simulation BNLr are also shown for comparison.

5.6 Summary

This chapter has described large-eddy simulations of the boundary layer driven by a height dependent geostrophic wind. The effect of shear in the geostrophic wind on various turbulence statistics has been discussed. However, the most important results have concerned the effects on the mean wind profiles and the ability of two simple closures (a local mixing length model and the specified viscosity profile scheme of Holtslag and Boville) to reproduce the LES results. The performance of these models has been shown not to be significantly degraded, in either neutral or convective conditions, by the presence of a shear in the geostrophic wind.

Chapter 6

Entrainment

6.1 Introduction

Entrainment is the mechanism whereby turbulent fluid mixes fluid into itself across an interface. Specifically this chapter considers the entrainment of air across the inversion at the top of the atmospheric boundary layer which leads to deepening of the boundary layer. Also, as the air which is incorporated into the boundary layer is almost invariably relatively warm and dry, it can have a significant effect on the boundary layer temperature and moisture budgets. In particular, its realistic representation in NWP and climate prediction models can be of vital importance in obtaining accurate forecasts of boundary layer clouds and surface evaporation rates. Some examples of deficiencies in forecast model performance ascribed to the modelled entrainment fluxes being insufficiently large can be found in Beljaars and Betts (1992).

Note that this study concentrates on entrainment into the cloud-free boundary layer. The cloudy case has additional complexities due to radiative transfer and latent heat effects, and, from a simulation point of view, can be more difficult when these processes lead to the formation of a sharper inversion. Nevertheless further study is desirable as there is evidence that entrainment may be an important mechanism in the break-up of

stratocumulus sheets (Deardorff, 1980; MacVean and Mason, 1990).

6.2 Mechanisms and models

A detailed review of possible entrainment mechanisms can be found in Fernando (1991). Essentially there appear to be two distinct types of mechanism. The first is a shear layer or Kelvin-Helmholtz instability which leads to wave breaking in the inversion layer. The second is associated with production of TKE away from the inversion, and the impinging of eddies on the inversion which distort the interface and cause 'splashing' or 'engulfment' of quiescent fluid into the turbulent fluid. These mechanisms are not mutually exclusive and in many cases the dominant entrainment mechanism is not clear. However, in cases with strong inversions or with only weak eddies impinging on the inversion, the local instability mechanism appears likely to dominate. This is likely to be the case for near neutral cloud-topped boundary layers where the inversions are often relatively strong. In contrast the second mechanism has been observed to be important in the surface heated convective boundary layer (Palmer *et al.*, 1979).

The entrainment flux, $\langle w'\theta' \rangle_i$, is usually modelled with reference to the TKE budget (Equation (4.32), but repeated here for ease of reference)

$$\frac{\partial \langle E \rangle}{\partial t} = -\frac{\partial}{\partial z} \langle w'E' + w'p'/\rho_r \rangle - \langle u'w' \rangle \frac{\partial \langle u \rangle}{\partial z} - \langle v'w' \rangle \frac{\partial \langle v \rangle}{\partial z} - \frac{g}{\theta_r} \langle w'\theta' \rangle - \langle \epsilon \rangle \quad (6.1)$$

There are two possible approaches

1. Vertically integrate (6.1) over the boundary layer. It is common to split the integral of the buoyancy term into two parts – production and consumption (Stage and Businger, 1981), although no consensus has been reached on the most appropriate partitioning. The entrainment flux is assessed as the difference between bulk production and dissipation.
2. Parametrize the terms in the local energy budget at z_i to obtain $\langle w'\theta' \rangle_i$.

CHAPTER 6: ENTRAINMENT

As pointed out by Driedonks (1982b), these two approaches are very similar as the same bulk turbulent velocity and length scales are used in both. Therefore it was decided to concentrate solely on the second method. Driedonks (1982b) gives a summary of the hierarchy of models used. The simplest assume that the entrainment flux is balanced by the transport term, giving

$$-\frac{g}{\theta_r} \langle w' \theta' \rangle_i = c_F \frac{w_m^3}{z_i} \quad (6.2)$$

where w_m is a mixed layer velocity scale, and c_F is an empirical constant. In convective conditions, $w_m = w_*$ and this reduces to

$$\langle w' \theta' \rangle_i = -c_F \langle w' \theta' \rangle_0 \quad (6.3)$$

6.3 LES of entrainment

Chapter 3 examined the importance of the entrainment flux on turbulence statistics in the boundary layer by comparing results from lid and inversion runs. However, the entrainment flux in the inversion runs was regarded almost as being externally prescribed, and no consideration was given to the factors that control its magnitude. This section examines the variation of the LES entrainment flux with stability. More fundamentally, the issue of whether the LES fluxes can be realistic given the relatively coarse resolution of the inversion region is also discussed. The potential problem is that while turbulence in the interior of the CBL is dominated by large thermals which are easily resolved, the entrainment process may depend critically on small scale mixing across the stable inversion region. Table 6.1 shows that the resolution that can be used in the inversion region is considerably poorer than that used by Mason and Derbyshire (1990) in LES of the stable boundary layer, as a much larger domain is required to simulate the CBL thermals.

The performance of LES in convective conditions without a mean wind, and then cases which also include shear will be examined in turn.

CHAPTER 6: ENTRAINMENT

	$\Delta x/\text{m}$	$\Delta y/\text{m}$	$\Delta z/\text{m}$
IC, inversion region	100	100	$\simeq 30$
ICHR, inversion region	50	50	$\simeq 18$
IN, inversion region	75	50	$\simeq 27$
INHR, inversion region	38	25	$\simeq 18$
Mason and Derbyshire (1990), SBL	12	12	$\lesssim 12$

Table 6.1: Resolution of free convective simulations, IC and ICHR, and neutral simulations, IN and INHR, in the inversion region. Also shown for comparison is the resolution used by Mason and Derbyshire (1990) in LES of the stable boundary layer (SBL).

6.3.1 Convective

Figure 6.1 shows mean potential temperature and heat flux profiles from three separate averaging periods of free convective simulation IC. The profiles look realistic, with approximately constant potential temperature and linear flux profiles in the boundary layer interior. The inversion structure has been sharpened somewhat relative to the initial profile, but appears similar at the three times shown. Note that the region of cooling has significant depth ($\simeq 150$ m), indicating that the most energetic eddies are reaching four or five grid points above the mean inversion level even in this low resolution simulation.

Table 6.2 shows results for $c_F (= -\langle w'\theta' \rangle_i / \langle w'\theta' \rangle_0)$ from successive 1000s averaging periods of simulations IC and ICHR (c.f. eddy turnover time of around 800s). The average values are 0.14 for the low resolution simulation, and 0.13 for the high resolution simulation. These values are consistent with previously published LES results for the entrainment coefficient in convective conditions, some of which are shown in Table 6.3. There is clearly some scatter in the LES results, although considerably less than found in observational results (Stull, 1976). Also note that almost without exception, the previously published LES results have been obtained using relatively short averaging periods, typically of the order of one eddy turnover time. Reference to Table 6.2 shows that the present results from successive 1000s averages ($\simeq 1.3t_*$) do show some scatter, and sug-

CHAPTER 6: ENTRAINMENT

Figure 6.1: Mean temperature and heat flux profiles from simulation IC. Results are shown after 5000s, 8000s and 11000s (all 1000s averages). The dotted lines show the values of z_i for these three averaging periods. The initial temperature profile is shown as a dashed line.

Averaging period			c_F	
Start/s	–	End/s	IC	ICHR
10000	–	11000	0.139	0.110
9000	–	10000	0.155	0.129
8000	–	9000	0.152	0.122
7000	–	8000	0.129	0.142
6000	–	7000	0.129	0.122

Table 6.2: LES results for the entrainment flux in the dry convective boundary layer. Average values of c_F are 0.14 for simulation IC, and 0.13 for ICHR.

CHAPTER 6: ENTRAINMENT

Paper	c_F	Notes
Deardorff (1974)	0.13	
Moeng (1984)	0.17	
Mason (1989)	0.15	
Schmidt and Schumann (1989)	0.17	
Nieuwstadt <i>et al.</i> (1991)	0.15	Intercomparison of four large-eddy models
	0.11	
	0.12	
	0.19	
Moeng and Sullivan (1994)	0.17	Mean wind, $-z_i/L = 18$
Present simulations	0.14	Low resolution (IC)
	0.13	High resolution (ICHR)

Table 6.3: Past and present LES results for the entrainment flux in the dry convective boundary layer.

gests that some, although not all of the discrepancies between the LES results may be statistical in origin.

Given the concerns expressed earlier about the ability of LES to resolve the entrainment process, the reasonable agreement between the results of different large-eddy model studies might seem surprising, especially as they were obtained using a variety of different resolutions and subgrid models. Accordingly, a more detailed examination is now made of the way in which simulations IC and ICHR model the entrainment flux. Figure 6.2 shows the resolved and subgrid contributions to the heat flux in these two simulations. In both cases the subgrid contribution is large near the surface, but becomes negligible in the upper CBL and the entrainment flux is almost entirely resolved. This is consistent with the LES results of Mason (1989) and Schmidt and Schumann (1989). The latter study presented horizontal cospectra of vertical velocity and temperature fluctuations which demonstrated that the negative heat flux at the inversion was dominated by large-scale motions on scales of order z_i . Experimental studies (e.g. Palmer *et al.*, 1979; Mahrt and Paumier, 1984) also support the importance of the contribution of large-scale motions to the entrainment heat flux.

CHAPTER 6: ENTRAINMENT

Figure 6.2: Resolved and subgrid heat fluxes from simulations IC and ICHR. The dotted and dashed lines show the contributions from regions of updraught ($w > 0$) and downdraught ($w < 0$).

CHAPTER 6: ENTRAINMENT

More can be learnt about the way in which LES resolves the entrainment flux by analysis of conditional averages. Updraughts (regions where $w > 0$) are found to cover $\simeq 50\%$ of the total area close to the surface, decreasing to only 45% at $z/z_i = 0.1$ and a little under 40% at $z/z_i = 0.9$, before increasing again to cover $\simeq 50\%$ for $z/z_i \gtrsim 1$. This indicates that the updraughts must be relatively strong compared to the downdrafts in the mixed layer (for $\langle w \rangle$ to be equal to zero), consistent with the skewness profiles shown in Figure 3.19. Figure 6.2 shows that heat flux is dominated by the contribution from these regions of updraught. Thus the positive heat flux in the mixed layer is largely due to buoyant thermals, while the negative entrainment flux is dominated by updraughts which have passed their neutral buoyancy level and are 'overshooting' into the stable air aloft. A similar result was found by Schumann and Moeng (1991), although their LES study used threshold values of w in defining updraughts and downdrafts, regions with w close to zero being regarded as 'environmental' air. The level of confidence in the LES results is again increased by agreement with the observations of Palmer *et al.* (1979). They found that regions of ascending air in the inversion region were almost invariably associated with a negative heat flux, while regions of descending air carried a smaller flux which could be either positive or negative in sign.

While it has been shown that the entrainment flux is well resolved and largely associated by overshooting updraughts, it is not clear that the LES results should be insensitive to the subgrid model. This is because the entrainment process must involve irreversible mixing at some stage, as otherwise the downdrafts would carry a positive flux in the inversion region, equal and opposite to that carried by the updraughts. This mixing might be carried out on a pointwise basis by the subgrid model in the inversion region, or within the mixed layer after quiescent air has been forced down by the splashing or engulfment mechanism.

In order to assess the sensitivity of the modelled entrainment flux to the subgrid parametrization, various additional simulations were performed. The first of these (IC2) was identical in every way to IC except that the critical Richardson number in the subgrid model was arbitrarily increased from 0.25 to 0.5 (giving a slower fall-off of viscosity

CHAPTER 6: ENTRAINMENT

and diffusivity in stable conditions). This was found to have only a minor effect on the entrainment flux, the average value of c_F from this simulation being 0.15. However, it was realized that changes in the behaviour of the subgrid model might be partially compensated for by changes in the amount of numerical diffusion caused by the TVD scheme used for advection of temperature. Accordingly the remaining tests were performed using the standard scheme of Piacsek and Williams (1970). Although not positive definite, and hence prone to giving spurious fluxes above the inversion, this scheme has the advantage of not being diffusive. Simulation IC3 used the standard subgrid model so that the impact of the change of advection scheme could be assessed. This gave $c_F = 0.11$, rather low compared to the value obtained in IC, although it was noted that most of the difference was due to IC3 having a significant upward subgrid flux in the inversion region. Simulation IC4 used this advection scheme, but the subgrid Prandtl number was arbitrarily reduced by a factor of ten at all points. This large change in the subgrid parametrization was found to lead to a reduction of about 50% in the magnitude of the modelled entrainment flux ($c_F = 0.05$). Finally, simulation IC5 used the reduced Prandtl number above 800 m, but the standard value below 700 m (with linearly interpolated values in between). This gave $c_F = 0.08$, intermediate between the results of IC3 and IC4. The difference between the values obtained in simulations IC4 and IC5 suggests that at least some of the irreversible mixing occurs in the boundary layer interior, consistent with a representation of the engulfment or splashing entrainment mechanism observed by Palmer *et al.* (1979). However, a more detailed study, possibly involving the use of tracers or Lagrangian statistics would probably be required to ascertain whether this is the dominant entrainment mechanism in simulations such as these.

It is concluded that LES results for the entrainment flux in convective conditions without shear are sensitive to the amount of mixing carried out by the subgrid model (and the advection scheme if diffusive). However the sensitivity is weak, and the result that a factor of ten change in subgrid Prandtl number (to a clearly unrealistic value) led to only a 50% reduction in the modelled flux is certainly encouraging. Thus the scatter in published LES results for c_F , although larger than that in most quantities in the CBL

Figure 6.3: Turbulence kinetic energy for simulation ICHR. All terms are normalized by (w_*^3/z_i) . Solid line : shear production; dotted line : dissipation; dashed line : total transport; dot-dash lines : buoyancy production.

interior, remains smaller than in observational results. Finally, for completeness, the energy budget from simulation ICHR is shown in Figure 6.3 (that for IC is very similar). This shows that there is essentially a three way balance between the transport, dissipation and buoyancy terms at all levels. Hence the success of the simple parametrization (6.2) is because both the transport and dissipation terms scale with w_*^3/z_i , rather than because of an exact balance between the transport and buoyancy terms in the inversion region.

6.3.2 Effects of shear

Figure 6.4 shows time series of the entrainment flux from four of the inversion runs, obtained from the maximum downward heat flux using horizontal averages but without any time averaging. Recall that the naming convention is designed so that the approximate stability can be ascertained from the simulation name (e.g. I77 has $-z_i/L \simeq 7.7$). All the series are very spiky, but by eye it is possible to discern that there is a trend with

CHAPTER 6: ENTRAINMENT

Figure 6.4: Time series of entrainment flux from simulations I77, I27, I10 and IN. In the first three cases the fluxes are normalized by the surface heat flux. For simulation IN (zero surface heat flux), the results are shown in dimensional terms.

CHAPTER 6: ENTRAINMENT

stability – the average ratio of the magnitude of the entrainment flux to that the surface flux seems to be about 0.15 for I77, 0.20 for I27 and 0.30 for I10. Results for simulation IN are shown dimensionally as they cannot be normalized by the surface flux which is zero in this case.

In making a more systematic analysis of the results, it is clearly essential to use long averages (obtained by combining results of short averages as functions of z/z_i as described in Chapter 3), particularly for simulations I27 and I10 which show signs of variability on a time scale of order a few eddy turnover times as well as the higher frequency variability which is seen in the other simulations. This is presumably associated with wave activity in these simulations which causes the $\langle w'w' \rangle$ profiles to show small peaks at around $z/z_i = 1.1$ which are not present in the other runs.

The upper plot in Figure 6.5 shows the variation with stability of the long average results for the entrainment flux (in buoyancy units) scaled by w_*^3/z_i . Coming from the convective end, it can be seen that there is little increase in the magnitude of the flux non-dimensionalized in this way until $-z_i/L$ is around 5. Some increase above the convective value (0.13, shown solid) is then observed, and the scaling breaks down completely in neutral conditions. Clearly an alternative velocity scale is required. One possibility is to make w_m proportional to the boundary layer root mean square vertical velocity for which a parametrization was developed in Chapter 3 (for non-baroclinic conditions). Hence the lower plot shows the same LES results, but this time normalized using w_m^3/z_i where $w_m^3 = w_*^3 + 3.4u_*^3$. It can be seen that this scaling is very successful, both for the high and low resolution simulation results. This suggests that, to first order, the entrainment flux is insensitive to the detailed inversion structure as the parametrization does not involve any measure of inversion strength or the local shear. For $-z_i/L \gtrsim 1$ this seems plausible because, as in the convective case, the boundary layer dynamics are dominated by the large thermal motions which impinge on the inversion. The amount of energy available for entrainment is related to the energy of these thermals and so the root mean square boundary layer vertical velocity is a relevant velocity scale, and parametrization (6.2) is successful. In conditions more close to neutral it is not clear whether the success of the

ray screen
alt. solar
per
Scha's
root is

Figure 6.5: Entrainment flux as a function of stability. Upper plot: results non-dimensionalized using w_*^3 / z_i ; lower plot : results non-dimensionalized using $w_m^3 / z_i = (w_*^3 + 3.4w_*^3) / z_i$. In each case results from IC and ICHR are plotted at $-z_i / L = 16$ to show the convective limit.

scaling is fortuitous. Arguably much higher resolution is required to simulate credibly the effects of local instabilities in the inversion region which may be particularly important in these cases. Nevertheless, it is encouraging that the total entrainment fluxes are similar in the high and low resolution neutral simulations, even though the subgrid contributions are non-negligible ($\simeq 33\%$ of the total in IN).

In a sense the true value of the entrainment flux for deep neutral boundary layers as simulated in IN and INHR is of academic interest only, as the fluxes are too small to have a significant impact on boundary layer development. Much shallower boundary layers, as might be observed in the early morning, will typically have greater shear across the inversion and local shear layer instabilities will almost certainly be significant (Fernando, 1991). Entrainment fluxes can be large and inversion rise can be rapid, and the simple parametrizations such as the one described above cannot be expected to perform well. Nevertheless no attempt has been made to model such cases because of the difficulty in deciding whether detailed results are realistic or artefacts of LES. Note that it is also very difficult to calibrate entrainment parametrizations using observational data. Hence Driedonks (1982b) found that using (6.2) with $w_m^3 = w_*^3 + 25u_*^3$ was as successful in a boundary layer growth model as various more complicated parametrizations. However, note that this velocity scale has a much stronger dependence on mechanical mixing than that proposed in this study. It was calibrated to give good agreement with observed growth rates for shallow boundary layers, and it is suggested that Driedonks (1982b) found that the strong u_* dependence performed best as it implicitly allowed for enhanced mechanical production at the inversion.

6.4 Parametrization in a large-scale model

As mentioned in the introduction, a good parametrization of entrainment is potentially important because of its effects on boundary layer temperature, depth and humidity. However, many models do not have a separate entrainment parametrization and rely in-

CHAPTER 6: ENTRAINMENT

stead on the boundary layer scheme (although it should be noted that convection schemes, if initialized, can also have an impact).

Three tests were performed with the local mixing length model, given the same initial conditions and external forcing as LES run I77, and using comparable vertical resolution. Test A used the model described in Chapter 4, except that the stability functions F_m and F_h were set to zero in stable conditions. In B, these functions were made to have the same dependence on local stability as used in the large-eddy subgrid model i.e. a cut-off at $Ri = 0.25$, consistent with experimental data (e.g. Businger *et al.*, 1971). In C the functions given in Chapter 4 were used. These are used in the Meteorological Office Unified Model, the relatively slow fall-off with increasing stability being justified by arguing that inhomogeneities within an NWP grid square will cause enhanced mixing even when the average stability is large (Mahrt, 1987).

Figure 6.6 shows the time series of normalized entrainment flux from the LES run and these three tests. Test A showed zero entrainment flux, which was expected as any stable gradient (required for a downward flux in this model) resulted in the eddy coefficients being set to zero. Test B developed a flux about 50% smaller than I77, while C gave a flux around 80% larger than the LES. Clearly the flux is sensitive to the stability functions used in stable conditions. These are usually designed to give a reasonable representation of mixing in the surface layer and boundary layer interior. However, even if the modeller were free to choose the functions solely in order to obtain the best results for the entrainment flux, then it seems unlikely that further tuning would be particularly beneficial. This is because the parametrization must remain sensitive to local shear (and temperature gradient) in the inversion region, even though the entrainment flux appears to be largely determined by the surface heat flux in moderately and highly convective conditions. Hence even if the functions were tuned to give a flux ratio consistent with that found in I77, then they could not be expected to give the same result for different values of G . To illustrate this, a further test was performed with the same stability functions and surface heat flux as used in C, but with $G = 3 \text{ ms}^{-1}$ (instead of 6 ms^{-1}). This gave $-\langle w'\theta' \rangle_i / \langle w'\theta' \rangle_0 \simeq 0.1$ (instead of $\simeq 0.22$), while a run with $G = 0.1 \text{ ms}^{-1}$ gave almost no entrainment. There

Figure 6.6: Time series of entrainment flux from LES run I77 (solid line) and from the mixing length model tests, A, B and C, which are described in the text (dotted lines). Note that the entrainment flux from test A was zero at all times.

is also considerable sensitivity to resolution, as a repeat of test C with degraded vertical resolution ($\Delta z = 140$ m instead of 30 m) gave an average entrainment flux of only about half the size of that found in the original test. It is concluded that parametrizations of this type are always liable to give errors in the entrainment flux of up to $O(100\%)$, with underestimates particularly likely in operational large-scale models which can only use coarse resolution (Beljaars and Betts, 1992).

The effects of these errors are now considered. Figure 6.7 shows time series of boundary layer depth from I77 and the mixing length model runs A, B and C. It is immediately clear that the fractional differences in boundary layer depth after 30000 s are much smaller than those in the entrainment flux. Both tests B and C have reproduced the LES boundary layer growth rate to within 10%. Test A was deliberately set up to be representative of a 'worst case' in which the model fails to develop any entrainment flux at all. The boundary layer then grows by thermodynamic encroachment alone, and this can be seen to still be capable of accounting for $\simeq 80\%$ of the LES boundary layer growth rate.

Figure 6.7: Time series of inversion height from LES run I77 (solid line) and from the mixing length model tests, A, B and C, which are described in the text (dotted lines).

It is concluded that modelled boundary layer depths are relatively insensitive to the entrainment parametrization. This is consistent with the results obtained by Driedonks (1982a and b) using a jump model. Errors of up to $\simeq 20\%$ in modelled values of z_i may be significant for some applications (e.g. dispersion modelling), but their influence on the surface stress is unlikely to be significant compared with other uncertainties, except for shallow boundary layers (see Section 4.A.2).

Figure 6.8 shows mean temperature profiles after 30000 s from the LES run and two of the mixing length model tests. Although there are clearly differences in the structure of the inversion region, the three profiles are very similar in the boundary layer interior, with mean temperatures all within $\simeq 0.1$ K of one another. This lack of sensitivity of mixed layer temperature to entrainment is again consistent with the jump model results of Driedonks (1982a and b). Essentially a larger downward heat flux at the inversion is compensated for by an increased rate of inversion rise such that the flux convergence within the boundary layer remains almost unchanged. However, it is noted that even though the direct impacts of a poor entrainment parametrization on the boundary layer

Figure 6.8: Mean temperature profiles after 30000 s from LES run I77 and from the mixing length model tests, A and C (B is omitted for clarity). Inversion levels are indicated with dotted lines.

temperature do not appear to be significant, those on the humidity may well be. This is because air above the inversion is almost invariably relatively dry, and insufficiently large entrainment rates (as seem to be common in NWP models) are likely to lead to modelled boundary layers which are too moist. In turn this may lead to erroneous predictions of the formation of boundary layer clouds and it will also have implications for the parametrized surface evaporation rate.

The tests described in this section have used a simple mixing length model and it is worth considering whether any of the other schemes discussed in Chapter 4 could be expected to perform any better with regard to entrainment. The use of models which carry energy might conceivably be beneficial in cases where enhanced turbulence in the inversion region leads to enhanced entrainment rates (e.g. cloud-topped boundary layers). However, they seem unlikely to be able to alleviate the basic problem in convective conditions that the entrainment flux should not be strongly correlated with local gradients in the inversion region. Even the models considered which determine eddy coefficients non-locally in the mixed layer tend to revert to formulations dependent on local gradients in the inversion

region (e.g. Therrey and Lacarrère, 1983, and Holtslag and Boville, 1993). Furthermore they continue to relate the downward heat flux at the inversion to the local temperature gradient through Equation (4.40). (Note that the counter-gradient term in this equation, which might be expected to reduce the magnitude of the entrainment flux, will almost invariably be negligible compared to the temperature gradient in the inversion region). Therefore it seems unlikely that the use of these boundary layer schemes will lead to a significantly improved entrainment parametrization.

Beljaars and Betts (1992) proposed a scheme in which the entrainment flux is specified directly by setting the eddy coefficients at a diagnosed inversion height to give the desired flux. For dry convective conditions the coefficients are given by

$$K_h = K_m = \frac{-\langle w'\theta' \rangle_i}{\frac{\partial \langle \theta \rangle}{\partial z}} = \frac{c_F \langle w'\theta' \rangle_0}{\frac{\partial \langle \theta \rangle}{\partial z}} \quad (6.4)$$

and specified eddy coefficient profiles are used within the mixed layer, similar to those proposed by Troen and Mahrt (1986). Although this boundary layer scheme is used on a finite difference grid, it acts rather like a bulk or mixed layer model in that both mixing within the boundary layer and the entrainment fluxes are related to the surface fluxes. The method used in near neutral and stable conditions is not made clear, although presumably the model can revert to a local scheme in cases where fluxes predicted by a local mixing length formulation are larger than those given by this non-local scheme. Beljaars and Betts (1992) reported some improvement in NWP model performance when using this scheme, particularly with regard to boundary layer moisture profiles, and it has been implemented in the operational model of the European Centre for Medium Range Weather Forecasting (ECMWF).

6.5 Summary

This chapter has presented results relating to entrainment at the top of the cloud-free atmospheric boundary layer. The large-eddy simulations, IC and ICHR, indicate that the magnitude of the downward heat flux at the inversion in free convective conditions

CHAPTER 6: ENTRAINMENT

is around 0.13 times that of the upward surface flux. This result has been shown to be sensitive to the subgrid model (and to the advection scheme used), but the sensitivity is relatively weak, and it has been argued that this explains the reasonable agreement found between the results of a number of LES studies. Confidence in the results has also been increased by noting that the entrainment flux is well resolved and dominated by overshooting updraughts, as found experimentally by Palmer *et al.* (1979). Nevertheless it is suggested that it would be useful to perform a more detailed study of the way in which LES models the entrainment flux, both in order to examine the dominant mechanisms and to assess the extent to which the model results for entrainment fluxes can ever become independent of the subgrid model (which must always be required to perform irreversible mixing at some stage).

A simple parametrization of the entrainment fluxes in the large-eddy simulations involving mechanical as well as buoyancy production has been developed. This uses as a velocity scale the root mean square vertical velocity in the boundary layer, for which a parametrization was developed in Chapter 3. Further tests could be performed to cover a wider region of parameter space (e.g changing inversion strength or boundary layer depth) in order to test the range of validity of this parametrization.

Finally the importance of the entrainment parametrization in a large-scale model has been discussed. The mean boundary layer temperature has been shown to be insensitive to the modelled entrainment flux. The sensitivity of the boundary layer depth to the modelled flux is also relatively weak, and errors are unlikely to have a major impact on the surface stress (except for shallow boundary layers). However, insufficient entrainment is liable to make modelled boundary layers too moist.

Chapter 7

Conclusions

Our present understanding of turbulence in the atmospheric boundary layer is based on information from a number of sources, including field and laboratory observations, and theoretical, conceptual and numerical models. This has been primarily a numerical modelling study, using a large-eddy model which was described in detail in Chapter 2. Simulations have been made across a range of stabilities between neutral and free convective conditions, with boundary layers capped by rigid lids (non-penetrative convection) and by temperature inversions (penetrative convection). Additionally, simulations have been made of baroclinic conditions in which the imposed geostrophic wind was a function of height.

The variation of various scaled turbulence statistics with stability has been presented, and the agreement between LES and available observational results has generally been encouraging. The simulation results have also been shown to be relatively insensitive to resolution. Backscatter has been used as standard in the present study, and its use is generally advocated. However, in free convective simulations its effects have been shown to be minimal, and thus the extra computational cost of the stochastic parametrization does not seem to be justifiable.

Quasi-equilibrium large-eddy simulation results for various similarity coefficients (as

CHAPTER 7: CONCLUSIONS

functions of stability) have been presented and compared with observational results. As velocity and temperature profiles rapidly become well mixed with increasing instability, it was found that the LES results were well reproduced by a simple mixed layer model for $-z_i/L \gtrsim 2$. The large-eddy datasets have also been used to assess the equilibrium performance of various boundary layer parametrization schemes. The performance of local mixing length models has been discussed in some detail as, although undoubtedly simplistic, they are still commonly used in weather forecasting and climate prediction models. They have been shown to be capable of accurately reproducing the LES results in neutral conditions. In convective conditions they produce insufficiently well mixed profiles, and the potential significance of the resulting underestimates of surface stress and overestimates of the temperature difference across the boundary layer has been discussed. In assessing the possible benefits of using more complex closures which seek to alleviate these deficiencies, great care has to be taken to distinguish between behaviour which is generic to a particular type of model, and behaviour which is solely related to the particular choices made for the empirical constants in any one model. However tests have been performed which suggest that closure schemes which incorporate stability effects in a non-local manner and include a counter-gradient correction in the heat flux parametrization are capable of producing improved results in convective conditions without a significant increase in computational cost. In contrast, it has been argued that carrying a prognostic equation for TKE is unlikely to be cost effective except in very high resolution models. Clearly further boundary layer parametrization schemes could be tested, both against the present and future large-eddy datasets. For example, some of the schemes examined in this study use a counter-gradient correction in the heat flux parametrization, and one area for further research might be the question of whether a counter-gradient momentum flux should be incorporated, as suggested recently by Frech and Mahrt (1995).

The simulations involving shear in the imposed geostrophic wind are of particular interest, as the author is not aware of any published LES studies of the baroclinic boundary layer. In neutral conditions the geostrophic shears applied were large enough to cause significant changes in the shapes of the velocity and stress profiles. Nevertheless, the

CHAPTER 7: CONCLUSIONS

stresses remained closely parallel to the shears, and the diagnosed mixing lengths were almost unchanged. Hence the performance of a simple mixing length model in reproducing the LES results was found to be highly satisfactory. In the convective simulations the turbulent mixing was shown to be sufficiently strong to keep the velocity profiles well mixed even with considerable geostrophic shear. The mixing length model performance in these conditions was found to be less good than in neutral conditions (as expected), but not significantly worse than in convective conditions with constant geostrophic wind. The results refute the suggestion of Hollingsworth (1994) that simple eddy viscosity based boundary layer parametrization schemes are incapable of sustaining a backing of the wind with height, and it has been suggested that the systematic forecast model error identified by Hollingsworth may be related to the action of the model convection scheme. In fact, the potential for interaction between NWP and climate model boundary layer and convection schemes has been emphasized several times in the present work, and the ways in which the two interact may often be as significant as the performance of each in isolation.

Parametrization of entrainment in the cloud-topped boundary layer is a difficult issue which has not been addressed here. However, even the cloud-free case is far from straightforward. LES results are reasonably consistent in indicating a downward heat flux at the inversion of magnitude around 0.15 times the surface heat flux in convective conditions, although the results are rather more sensitive to the subgrid parametrization than those for many statistics in the CBL interior. The present results suggest that, when shear is present in addition to surface heating, the flux scales approximately with the boundary layer root mean square vertical velocity. However, further simulations could usefully be carried out to explore a larger region of parameter space, including conditions in which this scaling might be expected to break down. These might include cases with particularly strong shear across the inversion, which might occur if simulations were performed of shallower boundary layers or with shear in the geostrophic wind across the inversion region. In these cases local TKE production could be highly significant and not well represented by a bulk boundary layer scaling. More fundamentally, it has been argued that a more detailed study of the way in which LES models the entrainment process would be of

CHAPTER 7: CONCLUSIONS

use, particularly in assessing the potential of the technique to produce realistic results in cases which seem likely to be more difficult to model (e.g. cloud-topped boundary layers with strong inversions).

Finally it is noted that with the ever increasing power of computers, and the difficulties and costs involved in carrying out field and laboratory experiments, numerical modelling studies seem likely to become progressively more dominant as a means of obtaining data. Clearly care has to be taken as the procedure of comparing model with model could potentially become rather incestuous. However as long as care is taken to assess the robustness of the results (e.g. examine the sensitivity to resolution and subgrid parametrization), and appropriate recourse is made to available observational datasets, then there is good reason to believe that further LES studies of this type should lead to an improved understanding and parametrization of the atmospheric boundary layer.

Plus we syn
wel te vrede
eye's slaad
natisthe vl parameteren
p15 is reached

References

- Adrian, R.J., Ferreira, R.T.D.S. and Boberg, T. (1986): Turbulent thermal convection in wide horizontal fluid layers. *Experiments in Fluids*, **4**, 121-141.
- Andrn, A., Brown, A.R., Graf, J., Mason, P.J., Moeng, C.-H., Nieuwstadt, F.T.M., and Schumann, U. (1994): Large-eddy simulation of a neutrally stratified boundary layer: a comparison of four computer codes. *Quart. J. Roy. Meteor. Soc.*, **120**, 1457-1484.
- Andrn, A. and Moeng, C.-H. (1993): Single-point closures in a neutrally stratified boundary layer. *J. Atmos. Sci.*, **50**, 3366-3379.
- Arya, S.P.S. (1975): Geostrophic drag and heat transfer relations for the atmospheric boundary layer. *Quart. J. Roy. Meteor. Soc.*, **101**, 147-161.
- Arya, S.P.S. and Wyngaard, J.C. (1975): Effect of baroclinicity on wind profiles and the geostrophic drag law for the convective planetary boundary layer. *J. Atmos. Sci.*, **32**, 767-778.
- Beljaars, A.C.M. and Betts, A.K. (1992): Validation of the boundary layer representation in the ECMWF model. Validation of models over Europe, Volume II, 7-11 September 1992, ECMWF, Shinfield Park, Reading.
- Betts, A.K. and Miller, M.J. (1986): A new convective adjustment scheme. Part II: Single column tests using GATE wave, BOMEX, ATEX and Arctic air-mass data sets. *Quart. J. Roy. Meteor. Soc.*, **112**, 693-709.

REFERENCES

- Bougeault, P. and Lacarrère, P. (1989): Parametrization of orography-induced turbulence in a meso-beta-scale model. *Mon. Wea. Rev.*, **117**, 1872-1890.
- Brost, R.A., Wyngaard, J.C. and Lenschow, D.H. (1982): Marine stratocumulus layers. Part II: turbulence budgets. *J. Atmos. Sci.*, **39**, 818-836.
- Brown, A.R., Derbyshire, S.H. and Mason, P.J. (1994): Large-eddy simulation of stable atmospheric boundary layers with a revised stochastic subgrid model. *Quart. J. Roy. Meteor. Soc.*, **120**, 1485-1512.
- Brown, R.A. (1970): A secondary flow model for the planetary boundary layer. *J. Atmos. Sci.*, **27**, 742-757.
- Brown, R.A. (1980): Longitudinal instabilities and secondary flows in the planetary boundary layer. *Rev. Geophys. Space Phys.*, **18**, 683-697.
- Brummer, B. (1985): Structure, dynamics and energetics of boundary layer rolls from KonTur aircraft observations. *Contrib. Atmos. Phys.*, **58**, 237-254.
- Businger, J.A., Wyngaard, J.C., Izumi, Y. and Bradley, E.F. (1971): Flux-profile relationships in the atmospheric surface layer. *J. Atmos. Sci.*, **28**, 181-189.
- Caughey, S.J. and Palmer, S.G. (1979): Some aspects of turbulence structure through the depth of the convective boundary layer. *Quart. J. Roy. Meteor. Soc.*, **105**, 811-827.
- Charnock, H. (1958): A note on empirical wind-wave formulae. *Quart. J. Roy. Meteor. Soc.*, **84**, 443-447.
- Chasnov, J.R. (1991): Simulation of the Kolmogorov inertial subrange using an improved subgrid model. *Phys. Fluids A* **3**, 188-200.
- Chlond, A. (1992): Three-dimensional simulation of cloud street development during a cold air outbreak. *Bound. Layer Meteor.*, **58**, 161-200.
- Christian, T.W. and Wakimoto, R.M. (1989): The relationship between radar reflectivities and clouds associated with horizontal roll convection on 8 August 1982. *Mon. Wea. Rev.* **117** 1530-1544.

REFERENCES

- Chrobok, G. Raasch, S. and Etling, G. (1992): A comparison of local and non-local turbulence closure methods for the case of a cold air outbreak. *Bound. Layer Meteor.*, **58**, 69–90. *Quart. J. Roy. Meteor. Soc.*, **96**, 91–114.
- Clarke, R.H. Dyer, A.J. Brook, R.R. Reid, D.G. and Troup, A.J. (1971): The Wangara experiment: Boundary layer data. Technical Paper No. 19, CSIRO, Div. Met. Phys., 362pp.
- Coleman, G.N., Ferziger, J.H. and Spalart, P.R. (1990): A numerical study of the turbulent Ekman layer. *J. Fluid Mech.*, **213**, 313–348.
- Cuxart, J. Bougeault, P. Lacarrère, P. Noilhan, J. and Soler, M.R. (1994): A comparison between transilient turbulence theory and the exchange coefficient model approaches. *Bound. Layer Meteor.*, **67**, 251–276.
- Deardorff, J.W. (1972a): Numerical investigation of neutral and unstable planetary boundary layers. *J. Atmos. Sci.*, **29**, 91–115.
- Deardorff, J.W. (1972b): Theoretical expression for the countergradient vertical heat flux.
- Deardorff, J.W. (1974): Three-dimensional numerical study of the height and mean structure of a heated planetary boundary layer. *Bound. Layer Meteor.*, **7**, 81–106.
- Deardorff, J.W. (1976): Discussion of 'Thermals over the sea and gull flight behaviour'. *Bound. Layer Meteor.*, **10**, 241–246.
- Deardorff, J.W. (1980): Cloud-top entrainment instability. *J. Atmos. Sci.*, **37**, 131–147.
- Deardorff, J.W. and Willis, G.E. (1985): Further results from a laboratory model of the convective planetary boundary layer. *Bound. Layer Meteor.*, **32**, 205–236.
- Driedonks, A.G.M. (1982a): Sensitivity analysis of the equations for a convective mixed layer. *Bound. Layer Meteor.*, **22**, 475–480.
- Driedonks, A.G.M. (1982b): Models and observations of the growth of the atmospheric boundary layer. *Bound. Layer Meteor.*, **23**, 283–306.

REFERENCES

- Dyer, A.J. and Bradley, E.F. (1982): An alternative analysis of flux-gradient relationships at the 1976 ITCE. *Bound. Layer Meteor.*, **22**, 3-19.
- Etling, D. and Brown, R.A. (1993): Roll vortices in the planetary boundary layer: a review. *Bound. Layer Meteor.*, **65**, 215-248.
- Etling, D. and Raasch, S. (1987): Numerical simulation of vortex roll development during a cold air outbreak. *Dyn. Atmos. Oceans*, **10**, 277-290.
- Faller, A.J. (1963): An experimental study of the instability of the laminar Ekman boundary layer. *J. Fluid Mech.*, **15**, 560-576.
- Fernando, H.J.S. (1991): Turbulent mixing in stratified fluids. *Annu. Rev. Fluid Mech.*, **23**, 435-493.
- Fiedler, B.H. and Moeng, C.-H. (1985): A practical integral closure for mean vertical transport of a scalar in a convective boundary layer. *J. Atmos. Sci.*, **42**, 359-363.
- Frech, M. and Mahrt, L. (1995): A two-scale mixing formulation for the atmospheric boundary layer. *Bound. Layer Meteor.*, **73**, 91-104.
- Garratt, J.R. (1992): The atmospheric boundary layer. Cambridge University Press, Cambridge. 316 pp.
- Garratt, J.R. Wyngaard, J.C. and Francey, R.J. (1982): Winds in the atmospheric boundary layer - prediction and observation. *J. Atmos. Sci.*, **39**, 1307-1316.
- Grant, A.L.M. (1986): Observations of boundary layer structure made during the KONTUR experiment. *Quart. J. Roy. Meteor. Soc.*, **112**, 825-841.
- Grant, A.L.M. (1992): The structure of turbulence in the near-neutral atmospheric boundary layer. *J. Atmos. Sci.*, **49**, 226-239.
- Grant, A.L.M. and Whiteford, R. (1987): Aircraft estimates of the geostrophic drag coefficient and the Rossby similarity functions A and B over the sea. *Bound. Layer Meteor.*, **39**, 219-231.

REFERENCES

- Gregory, D. and Rowntree, P.R. (1990): A mass flux convection scheme with representation of cloud ensemble characteristics and stability-dependent closure. *Mon. Wea. Rev.*, **118**, 1483–1505.
- Grossman, R.L. (1982): An analysis of vertical velocity spectra obtained in the BOMEX fair-weather, trade-wind boundary layer. *Bound. Layer Meteor.*, **23**, 323–337.
- Hibberd, M.F. and Sawford, B.L. (1994): A saline laboratory model of the planetary convective boundary layer. *Bound. Layer Meteor.*, **67**, 229–250.
- Hicks, B.B. (1981): An examination of turbulence statistics in the surface boundary layer. *Bound. Layer Meteor.*, **21**, 389–402.
- Hobson, J.M. Wood, N. and Mason, P.J. (1995): A new finite-difference diffusion scheme. *Accepted for publication in J. Comput. Phys.*
- Högström, U. (1988): Non-dimensional wind and temperature profiles in the atmospheric surface-layer: a re-evaluation. *Bound. Layer Meteor.*, **42**, 55–78.
- Højstrup, J. (1982): Velocity spectra in the unstable planetary boundary layer. *J. Atmos. Sci.*, **39**, 2239–2248.
- Hollingsworth, A. (1994): Validation and diagnosis of atmospheric models. *Dynamics of Atmospheres and Oceans*, **20**, 227–246.
- Holtslag, A.A.M. and Moeng, C.-H. (1991): Eddy diffusivity and counter-gradient transport in the convective atmospheric boundary layer. *J. Atmos. Sci.*, **48**, 1690–1698.
- Holtslag, A.A.M. and Boville, B.A. (1993): Local versus non-local diffusion in a global climate model. *J. Climate*, **6**, 1825–1842.
- Hunt, J.C.R. (1984): Turbulence structure in thermal convection and shear-free boundary layers. *J. Fluid Mech.*, **138**, 161–184.
- Hunt, J.C.R., Kaimal, J.C. and Gaynor, J.E. (1988): Eddy structure in the convective boundary layer – new measurements and new concepts. *Quart. J. Roy. Meteor. Soc.*, **114**, 827–858.

REFERENCES

- Kaimal, J.C. Wyngaard, J.C. Haugen, D.A. Coté, O.R. Izumi, Y. Caughey, S.J. and Readings, C.J. (1976): Turbulence structure in the convective boundary layer. *J. Atmos. Sci.*, **33**, 2152-2169.
- Kato, H. and Phillips, O.M. (1969): On the penetration of a turbulent layer into stratified fluid. *J. Fluid Mech.*, **37**, 643-655.
- Kelly, R.D. (1984): Horizontal roll and boundary layer interrelationships observed over Lake Michigan. *J. Atmos. Sci.*, **41**, 1816-1826.
- Klinker, E. and Sardeshmukh, P.D. (1987): The diagnosis of systematic errors in numerical weather prediction models. ECMWF workshop on diabatic forcing. November 30 - December 2, 1987.
- Krettenauer, K. and Schumann, U. (1992): Numerical simulation of turbulent convection over wavy terrain. *J. Fluid Mech.*, **237**, 261-300.
- Krishnamurti, R. (1975): On cellular cloud patterns, 3, Applicability of the mathematical and laboratory models. *J. Atmos. Sci.*, **32**, 1373-1383.
- Kuettner, J.P. (1959): The band structure of the atmosphere. *Tellus*, **11**, 267-294.
- Kuettner, J.P. (1971): Cloud bands in the Earth's atmosphere. *Tellus*, **23**, 404-425.
- Kuo, H. (1963): Perturbations of plane Couette flow in stratified fluid and origin of cloud streets. *Phys. Fluids*, **6**, 195-211.
- van Leer, B. (1974): Towards the ultimate conservative difference scheme. II. Monotonicity and conservation combined in a second order scheme. *J. Comput. Phys.* **14**, 361-370.
- LeMone, M.A. (1973): The structure and dynamics of horizontal roll vortices in the planetary boundary layer. *J. Atmos. Sci.*, **30**, 1077-1091.
- LeMone, M.A. (1990): Some observations of vertical velocity skewness in the convective planetary boundary layer. *J. Atmos. Sci.*, **47**, 1163-1169.

REFERENCES

- Lenschow, D.H. Wyngaard, J.C. and Pennel, W.T. (1980): Mean-field and second moment budgets in a baroclinic, convective boundary layer. *J. Atmos. Sci.*, **37**, 1313–1326.
- Leonard, B.P. (1991): The ULTIMATE conservative difference scheme applied to unsteady one-dimensional advection. *Comput. Methods Appl. Mech. Eng.*, **19**, 17–74.
- Lilly, D.K. (1966): On the stability of Ekman boundary flow. *J. Atmos. Sci.*, **23**, 481–494.
- Louis, J.-F. (1979): A parametric model of vertical eddy fluxes in the atmosphere. *Bound. Layer Meteor.*, **17**, 187–202.
- MacVean, M.K. and Mason, P.J. (1990): Cloud-top entrainment instability through small-scale mixing and its parametrization in numerical models. *J. Atmos. Sci.*, **47**, 1012–1030.
- Mahrt, L. (1987): Grid-averaged surface fluxes. *Mon. Wea. Rev.*, **115**, 1550–1560.
- Mahrt, L. and Paumier, J. (1984): Heat transport in the atmospheric boundary layer. *J. Atmos. Sci.*, **41**, 3061–3075.
- Mason, P.J. (1985): A numerical study of cloud streets in the planetary boundary layer. *Bound. Layer Meteor.*, **32**, 281–304.
- Mason, P.J. (1989): Large-Eddy Simulation of the Convective Atmospheric Boundary Layer. *J. Atmos. Sci.*, **46**, 1492–1516.
- Mason, P.J. (1992): Large-eddy simulation of dispersion in convective boundary layers with wind shear. *Atm. Env.* **26A**, 1561–1571.
- Mason, P.J. (1994): Large-eddy simulation: A critical review of the technique. *Quart. J. Roy. Meteor. Soc.*, **120**, 1–26.
- Mason, P.J. and Brown, A.R. (1994): The sensitivity of large-eddy simulations of turbulent shear flow to subgrid models. *Bound. Layer Meteor.*, **70**, 133–150.

REFERENCES

- Mason, P.J. and Callen, N.S. (1986): On the magnitude of the subgrid-scale eddy coefficient in large-eddy simulations of turbulent channel flow. *J. Fluid Mech.*, **162**, 439-462.
- Mason, P.J. and Derbyshire, S.H. (1990): Large-eddy Simulation of the Stably-Stratified Atmospheric Boundary Layer. *Bound. Layer Meteor.*, **53**, 117-162.
- Mason, P.J. and Sykes, R.I. (1980): A two-dimensional numerical study of horizontal roll vortices in the neutral atmospheric boundary layer. *Quart. J. Roy. Meteor. Soc.*, **106**, 351-367.
- Mason, P.J. and Sykes, R.I. (1982): A two-dimensional numerical study of horizontal roll vortices in an inversion capped planetary boundary layer. *Quart. J. Roy. Meteor. Soc.*, **108**, 801-823.
- Mason, P.J. and Thomson, D.J. (1987): Large Eddy Simulation of the neutral-static-stability planetary boundary layer. *Quart. J. Roy. Met. Soc.* **113** 413-443
- Mason, P.J. and Thomson, D.J. (1992): Stochastic backscatter in large-eddy simulations of boundary layers. *J. Fluid Mech.*, **242**, 51-78.
- Moeng, C.-H. (1984): A large-eddy simulation model for the study of planetary boundary-layer turbulence. *J. Atmos. Sci.*, **41**, 2052-2062.
- Moeng, C.-H. and Rotunno, R. (1990): Vertical velocity skewness in the buoyancy driven boundary layer. *J. Atmos. Sci.*, **47**, 1149-1162.
- Moeng, C.-H. and Sullivan, P.P. (1994): A comparison of shear and buoyancy driven planetary boundary layer flows. *J. Atmos. Sci.*, **51**, 999-1022.
- Moeng, C.-H. and Wyngaard, J.C. (1984): Statistics of conservative scalars in the convective boundary layer. *J. Atmos. Sci.*, **41**, 3161-3169.
- Moeng, C.-H. and Wyngaard, J.C. (1986): An analysis of closures for pressure-scalar covariances in the convective boundary layer. *J. Atmos. Sci.*, **43**, 2499-2513.

REFERENCES

- Miyakoda, K. and Sirutis, J.P. (1977): Comparative integrations of global models with various parametrized process of subgrid-scale vertical transport: description of the parametrizations. *Beitr. Phys. Atmos.*, **50**, 445-487.
- Moin, P. and Kim, J. (1982): Numerical investigations of turbulent channel flow. *J. Fluid Mech.*, **118**, 341-377.
- Nicholls, S. and Readings, C.J. (1979): Aircraft observations of the structure of the lower boundary layer over the sea. *Quart. J. Roy. Meteor. Soc.*, **105**, 785-803.
- Nieuwstadt, F.T.M. (1983): On the solution of the stationary baroclinic Ekman-layer equations with a finite boundary layer height. *Bound. Layer Meteor.*, **26**, 377-390.
- Nieuwstadt, F.T.M., Mason, P.J., Moeng, C.-H., and Schumann, U. (1991): Large-eddy simulation of the convective boundary layer: a comparison of four computer codes. *Turbulent Shear Flows Vol. 8*, Springer Verlag, Berlin.
- Ohtaki, E. (1985): On the similarity in atmospheric fluctuations. *Bound. Layer Meteor.*, **32**, 25-38.
- Panofsky, H.A. and Dutton, J.A. (1984): *Atmospheric turbulence*. Wiley.
- Panofsky, H. A., Tennekes, H., Lenschow, D. H. and Wyngaard, J. C. (1977): The characteristics of turbulent velocity components in the surface layer under convective conditions. *Bound. Layer Meteor.*, **11**, 355-361.
- Palmer, S.G. Caughey, S.J. and Whyte, K.W. (1979): An observational study of entraining convection using balloon-borne turbulence probes and high-power doppler radar. *Bound. Layer Meteor.*, **16**, 261-278.
- Paulson, C.A. (1970): The mathematical representation of wind speed and temperature profiles in the unstable atmospheric surface layer. *J. Appl. Meteor.*, **9**, 857-861.
- Pennell, W.T. and LeMone, M.A. (1974): An experimental study of turbulence structure in the fair-weather trade wind boundary layer. *J. Atmos. Sci.*, **31**, 1308-1323.

REFERENCES

- Piacsek, S.A. and Williams, G.P. (1970): Conservation properties of convection difference schemes. *J. Comp. Phys.* **6** 392-405.
- Priestley, C.H.B. (1957): Convection from the Earth's surface. *Proc. Roy. Soc.* , **A238**, 287-304.
- Rayleigh, Lord. (1916): On convection currents in a horizontal layer of fluid, when the higher temperature is on the underside. *Phil. Mag. (Series 6)* **32** 520-546.
- Saunders, P.M. (1964): Sea smoke and steam fog. *Quart. J. Roy. Meteor. Soc.*, **90**, 156-165.
- Schilling, V.K. (1991): A parametrization for modelling the meteorological effects of tall forests – a case study of a large clearing. *Bound. Layer Meteor.*, **55**, 283-304.
- Schmidt, H. and Schumann, U. (1989): Coherent structure of the convective boundary layer derived from Large-Eddy Simulation. *J. Fluid Mech.*, **200**, 511-562.
- Schumann, U. and Moeng, C.-H. (1991): Plume fluxes in clear and cloudy convective boundary layers. *J. Atmos. Sci.*, **48**, 1746-1757.
- Smagorinsky, J. (1963): General circulation experiments with the primitive equations: 1. The basic experiment. *Mon. Wea. Rev.* **91** 99-164.
- Smith, R.N.B. (1993): Unified Model Documentation Paper No. 24. Subsurface, surface and boundary layer processes.
- Stage, S.A. and Businger, J.A. (1981): A model for entrainment into a cloud-topped marine boundary layer. Part I: Model description and application to a cold-air outbreak episode. *J. Atmos. Sci.*, **38**, 2213-2229.
- Stull, R.B. (1976): The energetics of entrainment across a density interface. *J. Atmos. Sci.*, **33**, 1260-1267.
- Stull, R.B. (1988): An Introduction to Boundary Layer Meteorology. Kluwer Academic Publishers.

REFERENCES

- Stull, R.B. and Driedonks, A.G.M. (1987): Application of the transilient turbulence parametrization to atmospheric boundary layer simulations. *Bound. Layer Meteor.*, **40**, 209-239.
- Sykes, R.I. and Henn, D.S. (1989): Large-eddy simulation of turbulent sheared convection. *J. Atmos. Sci.*, **46**, 1106-1118.
- Sykes, R.I., Lewellen, W.S. and Henn, D.S. (1988): A numerical study of the development of cloud-street spacing. *J. Atmos. Sci.*, **45**, 2556-2569.
- Teunissen, H.W, Shokr, M.E., Bowen, A.J., Wood, C.J. and Green, D.W.R (1987): The Askervein hill project: wind-tunnel simulations at three length scales. *Bound. Layer Meteor.*, **40**, 1-30.
- Therry, G. and Lacarrère, P. (1983): Improving the eddy kinetic energy model for planetary boundary layer description. *Bound. Layer Meteor.*, **25**, 63-88.
- Tiedtke, M., (1989): A comprehensive mass flux scheme for cumulus parametrization in large-scale models. *Mon. Wea. Rev.*, **117**, 1779-1800.
- Troen, I.W. and Mahrt, L. (1986): A simple model of the atmospheric boundary layer; sensitivity to surface evaporation. *Bound. Layer Meteor.*, **37**, 129-148.
- Walter, B.A. and Overland, J.E. (1984): Observations of longitudinal rolls in a near neutral atmosphere. *Mon. Wea. Rev.*, **112**, 200-208.
- Wayland, R.J. and Raman, S. (1994): Structure of the marine atmospheric boundary layer during two cold air outbreaks of varying intensities: Gale 86. *Bound. Layer Meteor.*, **71**, 43-66.
- Weston, K.J. (1980): An observational study of convective cloud streets. *Tellus*, **32**, 433-438.
- Willis, G.E. and Deardorff, J.W. (1985): A laboratory model of the unstable planetary boundary layer. *J. Atmos. Sci.*, **31**, 1297-1307.
- Woodcock, A.H. (1940): Soaring over the open sea. *Sci. Mon.* , **55**, 226-232.

REFERENCES

- Wyngaard, J.C., Coté, O.R. and Rao, K.S. (1974): Modelling the atmospheric boundary layer. *Advances in Geophys.* , 18A, 193-211.
- Young, G.S. (1988): Turbulence structure of the convective boundary layer. Part 1: variability of normalized turbulence statistics. *J. Atmos. Sci.*, 45, 719-735.
- Zeman, O. and Tennekes, H. (1977): Parametrization of the turbulent kinetic energy budget at the top of the daytime boundary layer. *J. Atmos. Sci.*, 34, 111-123.