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Organizers: H. van Dop, A.A.M. Holtslag and J. Vilà-Guerau de Arellano

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Tutorials by

Jordi Vilà-Guerau de Arellano\(^1\)
Harm Jonker\(^2\)
Bob Beare\(^3\)
Steve Derbyshire\(^4\)
Evgeni Fedorovich\(^5\)
Bernard Geurts\(^6\)

\(^1\)Wageningen University (The Netherlands)
\(^2\)Delft Technical University (The Netherlands)
\(^3\)University of Exeter (United Kingdom)
\(^4\)Met-Office (United Kingdom)
\(^5\)University of Oklahoma (USA)
\(^6\)University of Twente (The Netherlands)
Cover: Potential temperature profile of a dry smoke cloud conceptually modelled by Lilly (1968) using a mixed-layer model (left) and relative humidity field above heterogeneous surfaces simulated by van Heerwaarden and Vilà-Guerau de Arellano (2008) using a large-eddy simulations (right). Large-eddy simulation results and mixed-layer models will be used during the tutorials.
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1 Introduction

An important component of this International Summer School is to put in practice some of the theoretical concepts and research methodologies explained and discussed during the lectures. By so doing, the participant will get acquainted with modelling tools and data analysis techniques used currently in studies of the atmospheric boundary layer. This manual contains a brief explanation of the fundamental concepts and variable definitions, the user instructions and the exercises.

The following five practical exercises are designed and introduced in this booklet:

1. Flux profile calculations in the atmospheric surface layer based on multi-level measurement data

Atmospheric surface layer similarity concepts are applied to analyze field observations. By calculating dimensionless groups based of scaling variables and using the Monin-Obukhov similarity theory, one can calculate turbulent fluxes in the atmospheric surface layer from mean velocity, temperature, and humidity values measured at different elevations.

2. Clear and cloud-topped convective boundary layers: two analyses of LES data

The idea of this practicum is to get more insight into the dynamics of the dry convective boundary layer and shallow cumulus clouds and their role in the transport of heat, moisture and chemical species. To this end we will study two data bases containing the results of a clear and a cloud-topped boundary layer simulated by means of a Large-Eddy Simulation (LES). With the program MATLAB and some predefined procedures, one can easily visualize the 3D time-dependent cloud field and perform the usual statistical analyses on the data like calculating mean profiles, variances and fluxes (resolved and subgrid). Particular attention will be paid to determining the cloud mass-flux and cloud averages of various quantities, including that of chemically reacting species like $NO$, $NO_2$ and $O_3$. Finally we assess how well a mass-flux approach, normally used to model shallow cumulus in large scale models, is able to represent the fluxes observed in the LES.

3. Evolution of a convective boundary layer and its influence on ozone diurnal variability

We study the daily evolution of a convective boundary layer by means of a mixed-layer model. The temporal evolution of the boundary layer growth and thermodynamic variables are calculated under different surface, inversion and free tropospheric conditions. We carry out sensitivity analysis on the surface forcings and analyze the role of the exchange (entrainment) between the atmospheric boundary layer and the free troposphere. The results are discussed by analyzing the feedbacks between the different thermodynamic variables. Furthermore, we apply the mixed to study the role of the diurnal boundary layer growth on the ozone variability. We carry out sensitivity analysis on the strenght of the thermal inversion, emission of nitric oxide and hydrocarbons and chemical time scales.

4. Explicit and implicit filtering in large-eddy simulation
The basis for a large-eddy formulation of a turbulent flow is a partial filter. In this practical exercise we analyze the basic operation of a filter and quantify its effect on numerical solutions of a Navier-Stokes equation.

5. **Stable Boundary Layer**

This practical exercise is designed to study the dynamics of stable stratified boundary layers under steady and unsteady conditions. In both cases we will use a simple one-D model which uses a first-order turbulence closure with Richardson number dependence \((1 – Ri/Ri_c)^2\). A simple soil model is implemented to study the coupling between the surface and the atmosphere.
Chapter 1

Practicum 1: Flux profile calculations in the atmospheric surface layer based on multi-level measurement data

by Eugeni Fedorovich

1. Turbulence scales in the atmospheric surface layer

- Friction velocity, \( u_* = (-\overline{uw'})^{1/2} \), where \( u' \) and \( w' \) are, respectively, turbulent fluctuations of the horizontal and vertical velocities and the overbar signifies (Reynolds) averaging over the ensemble of turbulent fluctuations, is employed as turbulence velocity scale in the atmospheric surface layer (ASL) under the usual ASL assumption that wind is directed along the shear stress. The vertical variation of kinematic momentum flux \( \overline{uw'} \) (which is negative of shear stress divided by density) is relatively small within the surface layer. Thus, \( \overline{uw'} \) characterizes the whole near-surface portion of the boundary-layer flow and is usually regarded as surface kinematic momentum flux.

- Hereafter, the overbars will be omitted in the notation for mean (Reynolds-averaged) velocity, temperature, humidity and associated meteorological variables.

- Near-surface (vertical kinematic) turbulent fluxes of heat and humidity are given by \( \overline{w'\theta'} \) (where \( \theta' \) is the turbulent fluctuation of the potential temperature) and \( \overline{w'q'} \) (where \( q' \) is the turbulent fluctuation of the specific humidity), respectively. They are used together with the friction velocity to construct the surface-layer temperature and humidity turbulence scales: \( \theta_* = -\overline{w'\theta'}/u_* \) and \( q_* = -\overline{w'q'}/u_* \). Changes of \( \overline{w'\theta'} \) and \( \overline{w'q'} \) with height in the idealized (stationary and horizontally homogeneous) ASL flow are relatively small and near-surface values of both fluxes are considered representative of the whole atmospheric surface layer.

- In the ASL flow analyses, it is convenient to introduce also the buoyancy turbulence scale \( b_* = -\overline{w'b'}/u_* \), where buoyancy \( b \) is defined as \( b = -(g/\rho_\infty)(\rho - \rho_\infty) = (g/\theta_\infty)(\theta_v - \theta_\infty) \) and subscript \( c \) denotes reference values of density \( \rho \) and virtual potential temperature \( \theta_v \).
Taking into account that 
\[
\beta w' \theta' = \overline{w'b'} = -u \beta \varepsilon \theta_{w} = -\beta u \varepsilon \theta_{w}, \quad \text{where} \quad \beta = g / \theta_{w}
\]
is the buoyancy parameter, \(b_e\) can be expressed in terms of the virtual potential temperature scale \(\theta_v\) as 
\[
b_e = \beta \theta_v.
\]
By using
\[
-w \beta u \varepsilon \theta_{w} = \beta \overline{w'} \theta = \overline{w'q'} = \beta \overline{u'} - 0.61 g \overline{w'q'},
\]
it can further be expressed through the temperature and humidity scales as 
\[
b_e = \beta \theta_v + 0.61 g \theta_{q}. \quad \text{Since} \quad \beta = g / \theta_{w} \neq g / \theta_{v}, \quad \text{it also follows from the above relationships that} \quad \theta_v = \theta_v + 0.61 g \theta_{q}. \]

**Summary of surface-layer scales:** 
\[
u^* = \frac{2}{1} \overline{w'} - (\text{for velocity}), \quad \overline{w'} - \overline{\theta v} (\text{for virtual potential temperature}), \quad \overline{w'} - \overline{\theta u} (\text{for potential temperature}), \quad \overline{w'} - \overline{q} (\text{for humidity}), \quad \overline{w'} - \overline{b} (\text{for buoyancy}).
\]

**Note** that signs of temperature, humidity, and buoyancy scales are opposite to those of fluxes and therefore coincide with signs of the corresponding vertical gradients.

Under **unstable** (convective) conditions: 
\[
\overline{w'} > 0, \quad \partial \theta_v / \partial z < 0, \quad \text{and} \quad \theta_v < 0.
\]
\[
\overline{w'b'} > 0, \quad \partial b_z / \partial z < 0, \quad \text{and} \quad b_e < 0.
\]

In the **stable** surface layer: 
\[
\overline{w'} < 0, \quad \partial \theta_v / \partial z > 0, \quad \text{and} \quad \theta_v > 0.
\]
\[
\overline{w'b'} < 0, \quad \partial b_z / \partial z > 0, \quad \text{and} \quad b_e > 0.
\]

Under **neutral** conditions: 
\[
\overline{w'} = 0, \quad \partial \theta_v / \partial z = 0, \quad \text{and} \quad \theta_v = 0.
\]
\[
\overline{w'b'} = 0, \quad \partial b_z / \partial z = 0, \quad \text{and} \quad b_e = 0.
\]

**2. The Monin-Obukhov similarity hypothesis; Monin-Obukhov length**

Fundamental underlying assumption of the Monin-Obukhov hypothesis: at \(z \gg z_0\) in the atmospheric surface layer, the turbulence regime on all scales of motion except for the dissipation range depends only on distance \(z\) from the surface and kinematic fluxes of momentum \(\overline{u'w'} = -u^2\) and buoyancy \(\overline{w'b'} = \beta \overline{w' \theta'} = -\beta u \varepsilon \theta_{w} = -u \beta \varepsilon \theta_{w}\).

The **Monin-Obukhov hypothesis** states that in the surface layer flow at \(z \gg z_0\) the vertical gradients of (mean) meteorological variables \(u, \theta_v, \theta, q, b\) as well as turbulence statistics of these variables (turbulence moments) are universal functions of dimensionless height \(z / L\) when they are normalized by the corresponding surface-layer turbulence scales \((u_e, \theta_{w}, \theta_e, q_e, b_e\), see above the definitions of these scales) and length scale \(L\).

This length scale \(L\) is called the **Monin-Obukhov length**. It is introduced (according to fundamental assumption of the Monin-Obukhov theory, see above) as a combination of the surface momentum and buoyancy fluxes:

\[
L = -\frac{u^3}{\kappa \overline{w'b'}} = -\frac{u^3}{\kappa \beta \overline{w' \theta'}} = -\frac{(-u^2 w'^{1/2})^3}{\kappa \beta \overline{w' \theta'}}.
\]

The Monin-Obukhov length can also be expressed in terms of surface layer scales as

\[
L = \frac{u_e^2}{\kappa \beta \theta_{w}} = \frac{u_e^2}{\kappa (\beta \theta_{w} + 0.61 g \theta_{q})}.
\]

In the case of dry atmosphere:

\[
L = \frac{u_e^2}{\kappa \beta \theta_{w}}.
\]
3. Universality of dimensionless gradients of meteorological variables

- According to the Monin-Obukhov hypothesis,
  \[
  \frac{L \frac{\partial u}{u_* \partial z}}{L} = \frac{\partial (u/u_*)}{\partial (z/L)} = \varphi_m' (z/L),
  \]

Universal functions \( \varphi_m \) and \( \varphi_h \) of dimensionless height \( \zeta = z/L \)

\[
\frac{L \frac{\partial \theta}{\theta_* \partial z}}{L} = \frac{\partial (\theta/\theta_*)}{\partial (z/L)} = \varphi_h' (z/L),
\]
\[ \frac{L}{q_e} \frac{\partial q}{\partial z} = \frac{\partial (q / q_e)}{\partial (z / L)} = \varphi'_m (z / L), \]
\[ \frac{L}{\theta_{e_v}} \frac{\partial \theta}{\partial z} = \frac{\partial (\theta / \theta_{e_v})}{\partial (z / L)} = \varphi'_h (z / L), \]
\[ \frac{L}{b_{e_v}} \frac{\partial b}{\partial z} = \frac{\partial (b / b_{e_v})}{\partial (z / L)} = \varphi'_b (z / L), \]

where \( \varphi'_m, \varphi'_h, \varphi'_q, \varphi'_b \), and \( \varphi'_v \) are \textbf{universal functions} of dimensionless height \( \zeta \equiv z / L \).

- The above relationships can be rewritten in the following way:

\[ \frac{\kappa_z}{u_e} \frac{\partial u}{\partial z} = \kappa_z \frac{z}{L} \varphi'_m (z / L) \equiv \varphi'_m (\zeta), \]
\[ \frac{\kappa_z}{\theta_{e_v}} \frac{\partial \theta}{\partial z} = \kappa_z \frac{z}{L} \varphi'_h (z / L) \equiv \varphi'_h (\zeta), \]
\[ \frac{\kappa_z}{q_e} \frac{\partial q}{\partial z} = \kappa_z \frac{z}{L} \varphi'_q (z / L) \equiv \varphi'_q (\zeta), \]
\[ \frac{\kappa_z}{\theta_{e_v}} \frac{\partial \theta}{\partial z} = \kappa_z \frac{z}{L} \varphi'_v (z / L) \equiv \varphi'_v (\zeta), \]
\[ \frac{\kappa_z}{b_{e_v}} \frac{\partial b}{\partial z} = \kappa_z \frac{z}{L} \varphi'_b (z / L) \equiv \varphi'_b (\zeta), \]

where \( \varphi'_m, \varphi'_h, \varphi'_q, \varphi'_v, \) and \( \varphi'_b \) are some other universal functions of the dimensionless height \( \zeta \equiv z / L \).

- In the neutral surface layer (where \( L \to \infty \)), \( \zeta = z / L = 0 \) and \( \kappa_z \frac{\partial u}{\partial z} = 1 \), and we have \( \varphi'_m (0) = 1 \).

Heat and water vapor in this case are transported as passive scalars and this transport should be independent of \( L \). Therefore, corresponding universal functions \( \varphi'_h, \varphi'_q, \varphi'_v, \) and \( \varphi'_b \) should become constants. This yields logarithmic profiles of temperature, buoyancy, and humidity under (quasi-)neutral conditions in the ASL. For instance, \( \frac{\kappa_z}{u_e} \frac{\partial u}{\partial z} = 1 \) integrates to

\[ u = \frac{u}{\kappa} \ln z + C. \]

- Measurements of the vertical gradients of \( u, \theta, \) and \( q \) in the ASL generally support predictions of the Monin-Obukhov similarity theory. Experimental data suggest that \( \varphi'_h \) and \( \varphi'_q \). Examples of measured \( \varphi'_m \) and \( \varphi'_h \) functions are shown in the plot from Sorbjan (1989) reproduced above.

4. \textbf{Empirical approximations of Monin-Obukhov universal functions}

- A series of specialized surface-layer experiments have been conducted in the 1960s and 1970s in different countries to prove/refute the Monin-Obukhov theory (or to determine limits of its applicability) and to obtain analytical approximations for \( \varphi'_m (\zeta) \) and \( \varphi'_h (\zeta) \).

- Numerous sets of analytical approximations for the Monin-Obukhov universal functions have been proposed. Two most commonly used sets are those of Businger \textit{et al.} (1971) and Dyer (Dyer and Hicks 1970, Dyer 1974), see corresponding references in Sorbjan (1989).

\textit{Convective (unstable) surface layer} (\( \zeta = z / L \leq 0 \)).
Businger et al.: \( \varphi_m(z/L) = \left(1-15\frac{z}{L}\right)^{-1/4}, \varphi_h(z/L) = 0.74\left(1-9\frac{z}{L}\right)^{-1/2}, \kappa = 0.35. \)

Dyer: \( \varphi_m(z/L) = \left(1-16\frac{z}{L}\right)^{-1/4}, \varphi_h(z/L) = \left(1-16\frac{z}{L}\right)^{-1/2}, \kappa = 0.4 \) (originally, 0.41).

**Stable surface layer** \( (\zeta = z/L \geq 0). \)

Businger et al.: \( \varphi_m(z/L) = 1+4.7\frac{z}{L}, \varphi_h(z/L) = 0.74+4.7\frac{z}{L}, \kappa = 0.35. \)

Dyer: \( \varphi_m(z/L) = 1+5\frac{z}{L}, \varphi_h(z/L) = 1+5\frac{z}{L}, \kappa = 0.4 \) (originally, 0.41).

Note that Dyer's set provides \( C_h = 1, \) while Businger's set provides \( C_h = 0.74. \)

5. **Turbulent exchange coefficients in terms of universal functions**
   - In the ASL flow, kinematic fluxes of momentum and heat are related to gradients of the corresponding mean fields through the turbulent exchange coefficients as \( k(\partial u/\partial z) = -\overline{u'w'} = u_*^2, \) where \( k \) is the turbulent exchange coefficient for momentum (it is often called *eddy viscosity*) and \( k_h(\partial \theta/\partial z) = -\overline{w'\theta'} = u_* \theta, \) where \( k_h \) is the turbulent exchange coefficient for momentum (it is often called *eddy diffusivity*).
   - Combining \( k(\partial u/\partial z) = -\overline{u'w'} = u_*^2 \) and \( \frac{k\zeta}{u_*} \frac{\partial u}{\partial z} = \varphi_m(\zeta), \) we have:
     \[
     k(z) = \frac{k\zeta}{\varphi_m(\zeta)} = k\zeta L \frac{\zeta}{\varphi_m(\zeta)},
     \]
     which for the neutral conditions \( (\zeta = z/L = 0) \) provides \( k(z) = k\zeta L. \)
   - Using Dyer's expressions of \( \varphi_m \) for unstable conditions and stable conditions (see above), we have
     \[
     k(z) = k\zeta L (1-16\frac{z}{L})^{-1/4} \quad \text{for unstable conditions, } \zeta = z/L \leq 0, \text{ and}
     \]
     \[
     k(z) = k\zeta L \frac{1}{1+5\frac{z}{L}} \quad \text{for stable conditions, } \zeta = z/L \geq 0.
     \]
   - Taking into account that \( k_h(\partial \theta/\partial z) = -\overline{w'\theta'} = u_* \theta, \) and \( \frac{k\zeta}{\theta} \frac{\partial \theta}{\partial z} = \varphi_h(\zeta), \) see sections 2 and 3, we obtain the following expression for the turbulent heat exchange coefficient
     \[
     k_h(z) = \frac{k\zeta}{\varphi_h(\zeta)} = k\zeta L \frac{\zeta}{\varphi_h(\zeta)}.
     \]
   - Note that because \( \varphi_q(\zeta) = \varphi_m(\zeta) \) the turbulent exchange coefficient for humidity \( k_q(z) \) is approximately equal to \( k_h(z). \)
   - In terms of Dyer's universal functions:
     \[
     k_h(z) = k\zeta L (1-16\frac{z}{L})^{-1/4} \quad \text{for unstable conditions, } \zeta = z/L \leq 0, \text{ and}
     \]
     \[
     k_h(z) = k\zeta L \frac{1}{1+5\frac{z}{L}} \quad \text{for stable conditions, } \zeta = z/L \geq 0.
     \]
   - Note that under stable conditions, the considered approximations of the universal functions provide equality of the exchange coefficients for momentum and heat \( k_h(z) = k(z). \) Under neutral conditions, when \( \zeta = z/L = 0: \) \( k_h(z) = k(z) = k\zeta L. \)
Based on the above relationships, the turbulent Prandtl number $Pr_t = k / k_h$ can be expressed in terms of universal functions $\varphi_m(\zeta)$ and $\varphi_h(\zeta)$ as $Pr_t(\zeta) = \varphi_h(\zeta) / \varphi_m(\zeta)$. With Dyer's functions, this provides $Pr_t(\zeta) = (1 - 16\zeta/L)^{1/4}$ in the unstable surface layer ($\zeta = \zeta/L \leq 0$), and $Pr_t(\zeta) = 1$ in the stable surface layer ($\zeta = \zeta/L \geq 0$).

Due to $\varphi_q(\zeta) \equiv \varphi_h(\zeta)$, the turbulent Schmidt number $Sc_t(\zeta) = k / k_q$ is approximately equal to the turbulent Prandtl number $Pr_t(\zeta)$.

**Note** that under neutral conditions: $Pr_t(0) = Sc_t(0) = \varphi_h(0) / \varphi_m(0) = C_h$.

### 6. Relationships between $\zeta/L$ and Richardson numbers

Richardson numbers, specified as

$$\text{Ri}_f = \frac{b w' \theta'}{u' w'(\partial u / \partial z)}$$

(flux Richardson number) and

$$\text{Ri} = \frac{\beta (\partial \theta / \partial z)}{(\partial u / \partial z)^2}$$

(gradient Richardson number),

where $\text{Ri}_f = \frac{k_h}{k} \text{Ri} = \frac{\text{Ri}}{Pr_t}$, characterize proportion between buoyancy and shear contributions to the turbulence kinetic energy production in a turbulent flow.

- The following sequence of relationships is worth of memorizing: $Pr_t \perp Sc_t = \varphi_h / \varphi_m = k / k_h = \text{Ri}/\text{Ri}_f$.

- In terms of Dyer's functions, under unstable conditions, when $\zeta = \zeta/L \leq 0$: $\text{Ri} = \frac{\zeta}{L} = \zeta \leq 0$ (because $\varphi_h = \varphi_m^2$) and $\text{Ri}_f = \zeta (1 - 16 \zeta)^{1/4} \leq 0$; under stable conditions, when ($\zeta = \zeta/L \geq 0$): $\text{Ri} = \text{Ri}_f = \zeta / (1 + 5 \zeta) \geq 0$.

- **Note** that in the latter case $\zeta = \text{Ri} / (1 - 5 \text{Ri})$ at $\text{Ri} = 0.2$ corresponds to the infinitely large positive $\zeta$ (or infinitesimal positive $L$) that is the case of extreme stability when turbulence cannot exist. In other words, Dyer's approximation yields the critical Richardson number value $\text{Ri}_c = 0.2$.

**Exercise 1**

1. Based on $\varphi_h = \varphi_q$, show that $\varphi_{hu} = \varphi_h = \varphi_h$.

2. Obtain expressions $\text{Ri} = \frac{\varphi_{hu}}{\varphi_m^2 L} \frac{\text{Pr}_t}{\varphi_h}$ and $\text{Ri}_f = \frac{\varphi_{hu}}{\varphi_m L} \frac{\text{Pr}_t}{\varphi_h}$ taking into account that $\varphi_h \perp \varphi_h$, and $Pr_t = \varphi_h / \varphi_m$.

3. Based on Dyer's universal functions, obtain the following expressions for $k$ and $k_h = k_q$ as functions of Ri:

   - $k(z) = \kappa u, z(1 - 16 \text{Ri})^{1/4}$, $k_h(z) = \kappa u, z(1 - 16 \text{Ri})^{1/2}$ for $\zeta = \zeta/L \leq 0$, $\text{Ri} \geq 0$,
   - $k(z) = k_h(z) = \kappa u, z(1 - 5 \text{Ri})^{1/2}$ for $\zeta = \zeta/L \geq 0$, $\text{Ri} \geq 0$.

4. Expanding Dyer’s $\varphi_m(\zeta)$ and $\varphi_h(\zeta)$ for $\zeta \leq 0$ in the Maclaurin series around $\zeta = 0$ and neglecting terms of the order higher than 1, obtain the following approximations of $\varphi_m(\zeta)$ and $\varphi_h(\zeta)$ for $\zeta \leq 0$ and $|\zeta| \ll 1$: $\varphi_m(\zeta) = 1 + 4\zeta$ and $\varphi_h(\zeta) = 1 + 8\zeta$. Find values of $\zeta < 0$, at
which differences between the above linear approximations $\phi_m(\zeta)$ and $\phi_h(\zeta)$ and regular Dyer's universal functions exceed 10%.

7. Integral forms of flux-profile relationships

- The dimensionless gradients of velocity, temperature, and humidity, which are universal functions of $\zeta \equiv z/L$, can be integrated over $z$ to obtain the explicit expressions of the corresponding profiles.

- Integration of $\phi_m(z / L) = \frac{k}{u_*} \frac{\partial u}{\partial z}$ between levels $z_i$ and $z > z_i$ in the surface layer leads to the following expression for the wind velocity profile: 
  
  \[ u(z) = u(z_i) + \frac{u_*}{\kappa} \left[ \ln \frac{z}{z_i} - \psi_m \left( \frac{z}{L}, \frac{z_i}{L} \right) \right], \]

  where $\psi_m(z, z_i) = \int_{z_i}^{z} (1 - \phi_m(z / L)) dz \ln z = \int_{z_i}^{z} (1 - \phi_m(\zeta)) dz \ln \zeta$.

- If the lower integration level is taken to be the surface roughness height (length) $z_0$, where the mean flow velocity is assumed to be zero, the wind profile appears as

  \[ u(z) = \frac{u_*}{\kappa} \left[ \ln \frac{z}{z_0} - \psi_m \left( \frac{z}{L}, \frac{z_0}{L} \right) \right]. \]

  The latter expression indicates that function $\psi_m(z, z_0) = \psi_m(\zeta, z_0)$ describes the deviation of the velocity profile from the logarithmic law due to the effect of atmospheric stability/instability. It is commonly called the stability correction function, or simply stability correction.

- In practical applications, $\zeta_0 = z_0 / L$. In $\psi_m(\zeta, z_0)$ is often replaced by zero and the stability correction is taken as $\Psi_m(\zeta) = -\psi_m(\zeta, 0)$, so that the velocity profile has the following approximate form:

  \[ u(z) = \frac{u_*}{\kappa} \left[ \ln \frac{z}{z_0} - \Psi_m \left( \frac{z}{L} \right) \right]. \]

- Dyer's universal functions $\phi_m(\zeta)$ provide (see Exercise 2)

  \[ \Psi_m(\zeta) = 2 \ln \frac{1 + x}{2} + \ln \frac{1 + x^2}{2} - 2 \tan^{-1} x + \frac{\pi}{2}, \quad \text{where} \quad x = (1 - 16 \zeta)^{1/4}, \quad \text{for} \quad \zeta \leq 0 \quad \text{(unstable flow)} \]

  \[ \Psi_m(\zeta) = -5 \zeta \quad \text{for} \quad \phi_m(\zeta) = 1 + 5 \zeta \quad \text{for} \quad \zeta \geq 0 \quad \text{(stable flow)}. \]

- Integration of the universal function $\phi_h(\zeta)$ between levels $z_i$ and $z > z_i$ leads to

  \[ \theta(z) = \theta(z_i) + \frac{\theta_*}{\kappa} \left[ \ln \frac{z}{z_i} - \psi_h \left( \frac{z}{L}, \frac{z_i}{L} \right) \right] \]

  and

  \[ q(z) = q(z_i) + \frac{q_*}{\kappa} \left[ \ln \frac{z}{z_i} - \psi_h \left( \frac{z}{L}, \frac{z_i}{L} \right) \right], \]

  where $\psi_h(z, z_i) = \int_{z_i}^{z} (1 - \phi_h(z / L)) dz \ln z = \int_{z_i}^{z} (1 - \phi_h(\zeta)) dz \ln \zeta$. 

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Using the concepts of roughness lengths for temperature and specific humidity (\(\theta = \theta_s\) at \(z = z_{0\theta}\), \(q = q_s\) at \(z = z_{0q}\)), we can express the temperature and humidity profiles as

\[
\theta(z) = \theta_s + \frac{\theta_s - \theta_f}{\kappa} \left[ \ln \frac{z}{z_{0\theta}} - \Psi_h \left( \frac{z}{L} \right) \frac{z_{0\theta}}{L} \right]
\]

and

\[
q(z) = q_s + \frac{q_s - q_f}{\kappa} \left[ \ln \frac{z}{z_{0q}} - \Psi_h \left( \frac{z}{L} \right) \frac{z_{0q}}{L} \right],
\]

Approximate forms of these profiles are

\[
\theta(z) = \theta_s + \frac{\theta_s - \theta_f}{\kappa} \left[ \ln \frac{z}{z_{0\theta}} - \Psi_h \left( \frac{z}{L} \right) \right]
\]

and

\[
q(z) = q_s + \frac{q_s - q_f}{\kappa} \left[ \ln \frac{z}{z_{0q}} - \Psi_h \left( \frac{z}{L} \right) \right],
\]

where \(\Psi_h(\zeta) \equiv \Psi_h(\zeta, 0)\).

If \(\varphi_h(\zeta)\) is taken after Dyer (see section 4), the corresponding integral function is

\[
\Psi_h(\zeta) = 2 \ln \frac{1 + \frac{y}{2}}{\zeta}, \quad \text{where} \quad y = (1 - 16 \zeta)^{1/2}, \quad \text{for} \quad \zeta \leq 0 \text{ (unstable conditions) and}
\]

\[
\Psi_h(\zeta) = -5 \zeta \quad \text{for} \quad \zeta \geq 0 \text{ (stable conditions)}, \quad \text{see Exercise 2.}
\]

**Exercise 2**

1. Show that Dyer’s universal functions \(\varphi_m(\zeta)\) provide

\[
\Psi_m(\zeta) = 2 \ln \frac{1 + \frac{x}{\zeta}}{2} + \ln \frac{1 + \frac{x^2}{\zeta}}{2} - 2 \tan^{-1} \frac{x}{2}, \quad \text{where} \quad x = (1 - 16 \zeta)^{1/4}, \quad \text{for} \quad \zeta \leq 0 \text{ (unstable flow) and}
\]

\[
\Psi_m(\zeta) = -5 \zeta \quad \text{for} \quad \varphi_m(\zeta) = 1 + 5 \zeta \quad \text{for} \quad \zeta \geq 0 \text{ (stable flow).}
\]

2. Show that \(\varphi_h(\zeta)\) after Dyer provides

\[
\Psi_h(\zeta) = 2 \ln \frac{1 + \frac{y}{2}}{\zeta}, \quad \text{where} \quad y = (1 - 16 \zeta)^{1/2}, \quad \text{for} \quad \zeta \leq 0 \text{ (unstable conditions) and}
\]

\[
\Psi_h(\zeta) = -5 \zeta \quad \text{for} \quad \varphi_h(\zeta) = 1 + 5 \zeta \quad \text{for} \quad \zeta \geq 0 \text{ (stable conditions).}
\]

**8. Calculation of surface fluxes from meteorological measurements at two levels**

- In sections 3 and 4 we obtained in following expressions, which relate the surface layer turbulence scales \(u_*, \theta_*, \text{ and } q_*\) (and therefore, surface layer vertical kinematic turbulent fluxes of momentum: \(w'\bar{u} = -u_*^2\), heat: \(w'\bar{\theta} = -u_*\theta_*\), and humidity: \(w'q_* = -u_*q_*\)) to gradients of corresponding meteorological variables:

\[
\frac{\kappa_*}{u_*} \frac{\partial \theta}{\partial z} = \varphi_m(\zeta), \quad \frac{\kappa_*}{q_*} \frac{\partial q}{\partial z} = \varphi_m(\zeta), \quad \text{where} \quad \varphi_m \text{ and } \varphi_h \text{ are universal functions of dimensionless height} \quad \zeta = z/L. \quad \text{After Dyer, these functions may be approximated as} \quad \varphi_m(\zeta) = (1 - 16 \zeta)^{-1/4}, \quad \varphi_h(\zeta) = (1 - 16 \zeta)^{-1/2} \quad \text{for} \quad \zeta \leq 0 \text{ and} \quad \varphi_m(\zeta) = \varphi_h(\zeta) = 1 + 5 \zeta \quad \text{for} \quad \zeta \geq 0.
\]

- Now imagine that we have mean (Reynolds-averaged) values of \(u, T\) (absolute temperature), and \(q\) measured at two heights in the surface layer: \(z_1\) and \(z_2\), with \(z_2 > z_1\). This gives us three pairs of quantities: \((u_1, u_2), (\theta_1, \theta_2), (q_1, q_2)\), where subscripts denote corresponding measurement levels. We can also calculate finite differences of these variables across the layer \(\Delta z = z_2 - z_1\): \(\Delta u = u_2 - u_1\), \(\Delta \theta = \theta_2 - \theta_1\), and \(\Delta q = q_2 - q_1\).
We have to define a level between $z_1$ and $z_2$, to which values of the finite gradients and $\frac{\Delta \theta}{\Delta z}$, where $\beta = \frac{g}{\theta_v}$ is the buoyancy parameter, can be referred to in this case. Based on the fact that gradients of meteorological variables in the surface layer decrease fast with distance from the surface (in the neutral case they decrease as $1/z$), the reference level for $R_i$ is usually specified as $z_s = \sqrt{z_1 z_2}$. It is also possible to take $z_s = (z_2 - z_1) / \ln(z_2 / z_1)$, which is the height where $\Delta u / \Delta z = \partial u / \partial z$ in the case of perfectly logarithmic profile (please demonstrate it yourself).

The reference value of virtual potential temperature $\theta_v$ in $\beta = \frac{g}{\theta_v}$ may be taken constant, for instance, $\theta_v = 300$ K.

For calculation of actual (dynamic) turbulent fluxes (which are expressed through their kinematic counterparts as $\rho w u, \rho c_p w^\prime \theta^\prime$, and $\rho w^\prime q^\prime$) we will also need the values of air density $\rho$ and specific heat at constant pressure $c_p = 1004$ J kg$^{-1}$ K$^{-1}$. Due to small vertical variations of air density in the surface layer, $\rho$ can be evaluated from $\rho$ (usually known) and $T$ at one of measurement levels. For instance $\rho = \rho / (RT_s)$, if we take temperature at the first measurement level.

**Flux calculation algorithm**

1. The Richardson number at the reference level $z_s$ is evaluated from the approximate relationship:

   $$R_i(z_s) = \frac{\beta(\Delta \theta / \Delta z) + 0.61 g(\Delta q / \Delta z)}{(\Delta u / \Delta z)^2},$$

   where $z_s = \sqrt{z_1 z_2}$.

2. If $R_i(z_s) \geq 0.2$, further derivations make no sense because the value of $R_i$ is beyond the critical limit.

3. If $R_i(z_s) < 0.2$, we proceed with calculation of dimensionless height $\xi_s = z_s / L$ that is related to Richardson number $R_i(z_s)$ as

   $$\xi_s = R_i(z_s) \quad \text{if } R_i(z_s) \leq 0 \quad \text{(unstable stratification)}$$

   $$\xi_s = R_i(z_s) / [1 - 5 R_i(z_s)] \quad \text{if } R_i(z_s) \geq 0 \quad \text{(stable stratification)}$$

4. From $\xi_s$, the value of Monin-Obukhov length scale $L$ can be calculated as $L = z_s / \xi_s$. In the present algorithm, $L$ is a supplementary parameter.

5. The calculated $\xi_s$ enters the expressions of the universal functions $\varphi_m$ and $\varphi_h$:

   $$\varphi_m(\xi_s) = (1 - 16 \xi_s)^{-1/4} \quad \text{if } R_i(z_s) \leq 0 \quad \text{(unstable), } \varphi_m(\xi_s) = 1 + 5 \xi_s$$

   if $R_i(z_s) \geq 0 \quad \text{(stable)}$;

   $$\varphi_h(\xi_s) = (1 - 16 \xi_s)^{-1/2} \quad \text{if } R_i(z_s) \leq 0 \quad \text{(unstable), } \varphi_h(\xi_s) = 1 + 5 \xi_s$$

   if $R_i(z_s) \geq 0 \quad \text{(stable)}$.

6. From the universal function, we calculate the surface layer turbulence velocity, temperature, and humidity scales from $u_c = \frac{\kappa z_s}{\varphi_m(\xi_s) \Delta z}, \theta_c = \frac{\kappa z_s}{\varphi_h(\xi_s) \Delta z}$, and $q_c = \frac{\kappa z_s}{\varphi_h(\xi_s) \Delta z}$, where $\kappa = 0.4$ is the von Kármán constant.
7. The kinematic surface turbulent fluxes are calculated from $u_*$, $\theta_*$, and $q_*$ as

$$\overline{w'u} = -u_*^2$$

(momentum), $w'\theta' = -u_*\theta_*$ (heat), and $w'q' = -u_*q_*$ (humidity).

8. Finally, we obtain the surface vertical turbulent fluxes of momentum, $\rho w'u'$, heat, $\rho c_p w'\theta'$, and humidity, $\rho w'q'$.

Exercise 3
You are given four datasets with mean velocity, temperature, and specific humidity values measured at two levels in the atmospheric surface layer.

Set 1. Measurement levels: $z_1=0.5$ m and $z_2=2$ m. Data: $u_1=3$ m/s, $u_2=4$ m/s, $T_1=36$ ºC, $T_2=29$ ºC, $q_1=0.008$, $q_2=0.003$, $p_1=1000$ hPa.

Set 2. Measurement levels: $z_1=2$ m and $z_2=8$ m. Data: $u_1=4$ m/s, $u_2=8$ m/s, $T_1=20$ ºC, $T_2=22$ ºC, $q_1=0.004$, $q_2=0.006$, $p_1=1000$ hPa.

Set 3. Measurement levels: $z_1=1$ m and $z_2=4$ m. Data: $u_1=3$ m/s, $u_2=6$ m/s, $T_1=15$ ºC, $T_2=15$ ºC, $q_1=0.009$, $q_2=0.009$, $p_1=1000$ hPa.

Set 4. Measurement levels: $z_1=4$ m and $z_2=9$ m. Data: $u_1=2$ m/s, $u_2=3$ m/s, $T_1=-2$ ºC, $T_2=8$ ºC, $q_1=0.001$, $q_2=0.005$, $p_1=1000$ hPa.

For each of the above datasets (as long as physical limitations allow):

a. Determine class of stability (unstable, stable, or neutral), and evaluate corresponding value of $L$;

b. Calculate the surface layer turbulence scales and turbulent fluxes of momentum, heat, humidity, and buoyancy;

c. Find values of turbulent exchange coefficients for momentum, $k$, and heat, $k_h$, and calculate turbulent Prandtl number at $z_s = \sqrt{z_1z_2}$;

d. Calculate mean wind velocity, temperature, and specific humidity at $z_s$ and $z=10$ m.

9. Calculation of surface turbulent fluxes in the case of non-coinciding measurement levels

- In this case, we have mean values of $u$, $T$ (absolute temperature), and $q$ measured at following levels: $u_1$, $u_2$ at $z_{q1}$, $z_{q2}$ ($z_{q2} > z_{q1}$), $T_1 \uparrow \theta_1$, $T_2 \uparrow \theta_2$ at $z_{\theta_q1}$, $z_{\theta_q2}$ ($z_{\theta_q2} > z_{\theta_q1}$), and $q_1$, $q_2$ at $z_{q1}$, $z_{q2}$ ($z_{q2} > z_{q1}$).

- Like in the previously considered case of two-level measurements (see section 8), $c_p=1004$ J·kg$^{-1}$·K$^{-1}$, atmospheric pressure is assumed to be known, and the buoyancy parameter is $\beta = g / \theta_w$ with $\theta_w = 300$ K. Note that, like in the previous case, this is only one of several possible ways of evaluating $\theta_w$ in this case. The air density can be calculated as $\rho = p / (RT_1)$.

Flux calculation algorithm
1. In a first approximation, the profiles of $u$, $\theta$, and $q$ in the surface layer may be taken logarithmic.

Thus, we may express the increments of variables as $u_2 - u_1 = \frac{u_*}{\kappa} \ln \frac{z_{2}}{z_{1}}$, $\theta_2 - \theta_1 = \frac{\theta_0}{\kappa} \ln \frac{z_{2}}{z_{1}}$, and $q_2 - q_1 = \frac{q_0}{\kappa} \ln \frac{z_{2}}{z_{1}}$. These expressions provide first approximations for the surface layer turbulence scales $u_*$, $\theta_*$, and $q_*$. 


2. Based on the calculated turbulence scales, the Monin-Obukhov length is evaluated as
\[ L = \frac{u_s^2}{\kappa(\beta \theta_s + 0.61gq_s)}. \]

3. If \( \frac{z_e}{|L|} \ll 1 \), where \( z_e \) is the highest measurement level of the three (\( z_{u2}, z_{\theta2}, z_{q2} \)), the stratification of the surface layer may be considered neutral. One may take, for instance, \( \frac{z_e}{|L|} = 0.01 \) as the lowest limit for the non-neutral case. After that, the kinematic fluxes can be directly evaluated from scales \( u_s, \theta_s, \) and \( q_s \) as \( \bar{w'u'} = -u_s^2 \) (momentum), \( \bar{w'\theta'} = -u_s\theta_s \) (heat), and \( \bar{w'q'} = -u_s q_s \) (humidity).

4. If \( \frac{z_e}{|L|} \geq 0.01 \), we have to calculate new approximations of \( u_s, \theta_s, \) and \( q_s \) from
\[
\ln \frac{z_{u2}}{z_{u1}} = -\Psi_m \left( \frac{z_{u2}}{L} \right) + \Psi_m \left( \frac{z_{u1}}{L} \right),
\]
\[
\ln \frac{z_{\theta2}}{z_{\theta1}} = -\Psi_h \left( \frac{z_{\theta2}}{L} \right) + \Psi_h \left( \frac{z_{\theta1}}{L} \right),
\]
\[
\ln \frac{z_{q2}}{z_{q1}} = -\Psi_h \left( \frac{z_{q2}}{L} \right) + \Psi_h \left( \frac{z_{q1}}{L} \right),
\]
taking into account the sign of \( L \) and using appropriate integral functions from section 7.

5. With new scales \( u_s, \theta_s, \) and \( q_s \) we calculate new approximation for \( L = \frac{u_s^2}{\kappa(\beta \theta_s + 0.61gq_s)}. \)

6. Steps 4 and 5 are repeated until the relative difference between new and old values of \( L \) becomes reasonably small (let say, of the order of 0.01)

7. Based on the resulting values of \( u_s, \theta_s, \) and \( q_s \), the turbulent fluxes are calculated using \( \bar{w'u'} = -u_s^2, \bar{w'\theta'} = -u_s\theta_s, \) and \( \bar{w'q'} = -u_s q_s, \) and then multiplying kinematic fluxes by \( c_p = 1004 \text{J} \cdot \text{kg}^{-1} \cdot \text{K}^{-1} \) and \( \rho \).

8. Finally, velocity, temperature, and humidity at any level \( z \) within the surface layer can be obtained from
\[
u(z) = u_i + \frac{u_s}{\kappa} \ln \frac{z}{z_{u1}} = -\Psi_m \left( \frac{z}{L} \right) + \Psi_m \left( \frac{z_{u1}}{L} \right),
\]
\[
\theta(z) = \theta_i + \frac{\theta_s}{\kappa} \ln \frac{z}{z_{\theta1}} = -\Psi_h \left( \frac{z}{L} \right) + \Psi_h \left( \frac{z_{\theta1}}{L} \right),
\]
\[
q(z) = q_i + \frac{q_s}{\kappa} \ln \frac{z}{z_{q1}} = -\Psi_h \left( \frac{z}{L} \right) + \Psi_h \left( \frac{z_{q1}}{L} \right).
\]

Note that for such evaluation one can use velocity, temperature, and humidity values from any measurement level (for instance, \( u_2, \theta_2, \) and \( q_2 \) along with corresponding measurement levels may be used instead of \( u_1, \theta_1, \) and \( q_1 \)).

10. Retrieval of surface roughness length values from the gradient measurements
- In the case, when the lower measurement levels in the surface layer are taken as (or assumed to be) roughness heights (lengths) \( z_{u1} = z_0, z_{\theta1} = z_{0\theta}, z_{q1} = z_{0q} \), at which, according to the definitions of roughness lengths, the meteorological variables reach their surface values \( u=0, \theta=\theta_s, \) and \( q=q_s \), the flux-profile relationships can be written as
\[ u(z_u) = \frac{u_z}{K} \left( \ln \frac{z_u}{z_0} - \Psi_m(\zeta_u) + \Psi_m(\zeta_0) \right) \]

\[ \theta(z_\theta) = \theta_z + \frac{\theta_z}{K} \left( \ln \frac{z_\theta}{z_\theta} - \Psi_h(\zeta_\theta) + \Psi_h(\zeta_\theta) \right) \]

\[ q(z_q) = q_s + \frac{q_s}{K} \left( \ln \frac{z_q}{z_q} - \Psi_h(\zeta_q) + \Psi_h(\zeta_q) \right) \]

- These expressions can be used for calculation of surface-layer turbulence scales and turbulent fluxes from meteorological measurements at a single level in the surface layer. However, for such calculation we need values of \( z_0, z_{\theta 0}, z_{q0}, \theta_s, \) and \( q_s, \) which generally are not very easy to obtain.

- On the other hand, given the surface values of temperature \( \theta_s \) and humidity \( q_s, \) as well as velocity, temperature, and humidity turbulence scales (determined, for instance, from the two-level measurements in the surface layer), the above expressions can be used for evaluation of surface roughness lengths \( z_0, z_{\theta 0}, \) and \( z_{q0}. \)

**Exercise 4**

You are given two sets of meteorological variables measured at different levels in the atmospheric surface layer.

Set 1. Measurement levels: \( z_{u1} = z_{\theta 1} = z_{q1} = 0.5m \) and \( z_{u2} = z_{\theta 2} = z_{q2} = 2m. \) Data: \( u_1 = 3m/s, u_2 = 4m/s, \)
\( T_1 = 36^\circ C, T_2 = 29^\circ C, q_1 = 0.008, q_2 = 0.003, p_{g1} = 1000hPa. \) For this dataset:

a. Calculate the surface turbulent fluxes employing the algorithm described in section 9.

b. Estimate mean velocity, temperature, specific humidity, turbulent exchange coefficients, and Ri at \( z = 10m. \)

c. Compare results with your calculations for the Set 1 in Exercise 3.

Set 2. Measurement levels: \( z_{u1} = 1m, z_{\theta 1} = z_{q1} = 2m, z_{u2} = 8m, z_{\theta 2} = z_{q2} = 6m. \) Data: \( u_1 = 2m/s, \)
\( u_2 = 8m/s, T_1 = 8^\circ C, T_2 = 11^\circ C, q_1 = 0.004, q_2 = 0.006, p_{g1} = 1000hPa. \) For this dataset:

a. Calculate the surface turbulent fluxes employing the algorithm described in 9.

b. Estimate mean velocity, temperature, specific humidity, turbulent exchange coefficients, and Ri at \( z = 10m. \)

**References**


Chapter 2

Practicum 2: Clear and cloud-topped boundary layers: two analyses of LES data

by Harm Jonker

1 Practicum 2.1

The purpose of this practicum is to get more insight into the dynamics of dry convective boundary layers, the associated growth of the mixed-layer due to entrainment, and the flux-gradient relationship of temperature. To this end we will study a database containing the results from a Large Eddy Simulation (LES) of a dry convective boundary layer. This database contains 4-dimensional information on the (thermo)dynamic quantities (three spatial directions and time). Details on the present LES run and the database are provided in table 2.2. Briefly, for each variable $\phi$ there are 48 three-dimensional instantaneous fields (snapshots) at 300s intervals, so the (4D) structure is: $\phi(i,j,k;n)$, with $i \in [1,64], j \in [1,64], k \in [1,64], n \in [1,48]$, where $i, j, k$ correspond to the $x$-, $y$-, and $z$-direction respectively; $n$ represents the frame number, so the corresponding time is $t_n = 300n \ [s]$. In the practicum you can make use of the matlab files CblVis.m, CblMovie.m, CblStat.m to which you can add your own commands. Besides some general matlab commands, the Cbl.m-files make use of the following predefined procedures

- *readlescbl.m*: read LES data-files.
- *avslab.m*: calculates an average of a (4D) field over $i$ and $j$.
- *avinterval.m*: calculates a time average over a specified interval.
- *ddz.m*: calculates the vertical derivative of a mean profile.
<table>
<thead>
<tr>
<th>Domain size $L_x \times L_y \times L_z$</th>
<th>3072m×3072m×1536m</th>
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<tr>
<td>Grid $N_x \times N_y \times N_z$</td>
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<tr>
<td>Resolution $\Delta x \times \Delta y \times \Delta z$</td>
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<tr>
<td>nr of instantaneous 3D fields</td>
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</tr>
<tr>
<td>(thermo)dynamic variables</td>
<td>$u, v, w, \theta$</td>
</tr>
<tr>
<td>tracers</td>
<td>'top-down' &amp; 'bottom-up'</td>
</tr>
<tr>
<td>Surface heat flux</td>
<td>$\langle w'\theta' \rangle = 0.094\text{Km/s (113W/m}^2\rangle$</td>
</tr>
<tr>
<td>Lapse rate</td>
<td>$\Gamma = \frac{d\theta}{dz} = 5\text{K/km}$</td>
</tr>
<tr>
<td>Surface flux 'bottom-up' tracer</td>
<td>$\langle w'c'_{ba} \rangle = 0.094\text{Km/s}$</td>
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<tr>
<td>Lapse rate</td>
<td>$dc_{ba}/dz = 0\text{K/km}$</td>
</tr>
<tr>
<td>Surface flux 'top-down' tracer</td>
<td>$\langle w'c'_{td} \rangle = 0\text{Km/s}$</td>
</tr>
<tr>
<td>Lapse rate</td>
<td>$dc_{td}/dz = 5\text{K/km}$</td>
</tr>
</tbody>
</table>

Table 2.1: Information regarding the CBL case, and the LES database

### 1.1 Exercise I: data visualization

1. Start `matlab` and type `CblVis` at the prompt. Make changes in the file to visualize the other variables or to see the data in a different way.

2. Start `CblMovie`: this will generate an animation of the 48 frames.

### 1.2 Exercise II: Mean profiles and fluxes

1. Start `CblStat`. All data will be read. As an example the code will calculate the *slab average* of potential temperature:

   $\bar{\theta}(k;n) = \frac{1}{N_xN_y} \sum_{ij} \theta(i,j,k;n)$

   and plot the instantaneous profiles.

   Next it will additionally calculate a *time average* over a specified time interval (in this example 12 frames, which amounts to an interval of 1hr), and it will plot the resulting (four) profiles, i.e.

   $\langle \theta(k) \rangle = \frac{1}{n_2 - n_1 + 1} \sum_{n=n_1}^{n_2} \bar{\theta}(k;n)$

   Locate (by eye) the inversion height for each profile and identify the inversion strength $\Delta \theta$. 

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2. Plot also the velocities profiles $\langle u \rangle$, $\langle v \rangle$ and $\langle w \rangle$. Are they zero on average?

**Inversion height $z_i$ and the entrainment velocity $w_e$**

Remove in CblStat.m the comment symbols below 'Inversion'. Following Sullivan et al. (1998) the program determines the instantaneous inversion height $z_i$ by locating the maximum gradient in $\theta$. It does so for each $i$ and $j$, after which a mean inversion height is calculated.

3. Study the employed algorithm step by step. Next plot $z_i$ as a function of time.

4. Compare $z_i(t)$ to the height one would have for 'encroachment' instead of entrainment:

$$z_{enc}(t) = \sqrt{\frac{2\psi t}{\Gamma}}$$

where $\psi = \overline{w^* \theta^*}_{z=0}$ represents the surface temperature flux.

5. Differentiate $z_i(t)$ with respect to time to obtain the entrainment rate $w_e(t)$. Plot the result.

6. How does the entrainment rate $w_e$ compare to the encroachment rate $w_{enc}$?

**Fluctuations and variance profiles**

The (spatial) fluctuations of a variable $\phi$ are

$$\phi'(i, j, k; n) = \phi(i, j, k; n) - \overline{\phi}(k; n)$$

The instantaneous variance profile is

$$\overline{\phi'^2}(k; n) = \frac{1}{N_x N_y} \sum_{ij} \phi'^2(i, j, k; n)$$

7. Calculate the instantaneous variance profiles of the vertical velocity and average these over one hour. Plot and study the shape of the resulting four profiles of $\langle w'^2 \rangle$.

8. Repeat this for $\langle u'^2 \rangle$ and $\langle v'^2 \rangle$.

9. Repeat for $\langle \theta'^2 \rangle$.

**Fluxes**

The instantaneous vertical flux profile of a variable $\phi$ is

$$\overline{w^* \phi'}(k; n) = \frac{1}{N_x N_y} \sum_{ij} w(i, j, k; n) \phi'(i, j, k; n)$$

10. Calculate the hourly averaged flux of $\langle w' \theta' \rangle$. What is the value of the flux at the surface? What is wrong?

**Subgrid contribution**

An important ingredient of an LES is the contribution of the sub-grid processes to

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the flux. That is, the evolution of a variable does not only depend on the resolved flux, but also on the subgrid flux:

\[
\frac{\partial}{\partial t} \varphi = - \frac{\partial}{\partial z} \left\{ w' \varphi^{\text{resolved}} + w' \varphi^{\text{subgrid}} \right\}
\]

Usually the subgrid contributions are calculated in LES by using an eddy diffusivity closure

\[
\left[ w' \varphi' \right]^{\text{subgrid}} = - K_h \frac{\partial}{\partial z} \varphi \quad \text{for} \quad \varphi \in \{ \theta, q_t, \text{species} \}
\]

where the eddy-diffusivity \( K_h \) is location and time dependent. The way \( K_h \) is determined may vary a lot between different LES codes. To calculate the subgrid fluxes for the present simulation we have added to the database the LES-generated \( K_h \)-fields. Due to the staggered grid arrangement of the employed LES, you can numerically derive the (local) subgrid flux by:

\[
\left[ w' \varphi' \right]^{\text{subgrid}} = - \frac{K_h(i, j, k; n) + K_h(i, j, k-1; n)}{2} \cdot \frac{\phi(i, j, k; n) - \phi(i, j, k-1; n)}{\Delta z}
\]

11. Remove in `CblStat.m` the comment symbols below 'Subgrid'. Determine the slab- and time-averaged subgrid flux \( \langle w' \varphi' \rangle^{\text{subgrid}} \) and plot the profiles. Add them to the resolved fluxes to get the total fluxes. Are the surface fluxes correct?

12. Determine the entrainment flux (the minimum of \( \langle w' \varphi' \rangle \)).

13. How confident can we generally be about those parts of the simulation domain where the subgrid contributions are large?

**Flux-profile relationship: counter-gradient transport**

14. Plot in two figures the gradient(s) \( d\langle \theta \rangle/dz \) and the total (resolved + subgrid) flux \( \langle w' \varphi' \rangle \). Zoom in using the `axis([xmin xmax ymin ymax])` command to study the sign of the gradient and the flux at various heights. Can you identify a region where there is counter-gradient transport?

15. Suppose we want to model the heat flux by a gradient diffusion hypothesis

\[
\langle w' \theta' \rangle = - K \frac{d\langle \theta \rangle}{dz}
\]

then plot the profile of the eddy diffusivity \( K \) that satisfies the above relation, i.e. plot

\[
K(z) = - \frac{\langle w' \theta' \rangle}{d\langle \theta \rangle/dz}
\]

For approaches that account for counter-gradient transport, see e.g. Holtslag and Moeng (1991).

**Scaling: the dimensionless presentation of data**

The convective velocity scale is given by

\[
w_* = \left( \frac{g}{\Theta_0} \right)^{1/3} z_i \left( \frac{w' \theta'}{z=0} \right)^{1/3}
\]
and forms together with $z_i$, a set of scaling variables for the CBL. A time-scale can be derived from $t_* = z_i/w_*$, and is referred to as the large-eddy turnover time. A temperature scale follows from $\theta_* = w^0 \theta_0/z = 0/w_*$. 

16. Determine $w_*$ and $z_i$ for each hour.

17. Rescale the vertical velocity variance $\langle u'^2 \rangle$ and plot the four profiles in dimensionless form. Do they coincide? Where is the maximum located?

18. Repeat this for $\langle u'^2 \rangle$ and $\langle \theta'^2 \rangle$.

19. Plot the heat fluxes in a non-dimensional form.

1.3 Exercise III: Bottom-up and top-down processes

20. Add your commands to the file Cb1Stat.m to study the profiles of the passive scalars, i.e. the 'bottom-up' tracer (BU) and the 'top-down' tracer (TD). Plot the instantaneous profiles as well hourly averaged profiles.

21. Verify that the $\theta$-profile can also be obtained by adding the profiles of BU and TD (see e.g. Jonker et al. (1999)).

22. Calculate and plot the time-averaged fluxes of BU and TD. Include the sub-grid terms.

23. Verify that the $\theta$-flux can also be obtained by adding the fluxes of BU and TD.

24. How long is the bottom-up tracer really representative of a pure bottom-up process? What is the problem?

25. How can one create a ‘pure’ bottom-up tracer field, without redoing the LES run?

26. Can the variance of $\theta$ be expressed as the sum of the BU- and TD-variances? Why/why not?

27. Do you observe counter-gradient transport for the BU or TD tracer? What is the theoretical relation between the eddy-diffusivity of $\theta$, $K_\theta$ and to the eddy-diffusivities $K_{BU}$ and $K_{TD}$? More info, see De Roode et al. (2004).

2 Practicum 2.2

The idea of this practicum is to get more insight into the dynamics of shallow cumulus clouds and their role in the transport of heat, moisture and chemical species, and into how shallow cumulus can be modeled in large scale models with the so-called mass-flux approach. To this end we will study a shallow cumulus cloud database containing the results from a Large Eddy Simulation (LES).

The case studied with the LES is based on the trade wind cumulus convection as observed during the Barbados Oceanographic and Meteorological Experiment (BOMEX). For more info see Siebesma et al. (2003), who used this case for an intercomparison between ten different LES models.
<table>
<thead>
<tr>
<th>Domain size</th>
<th>6.4km×6.4km×3200m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid</td>
<td>64 × 64 × 80</td>
</tr>
<tr>
<td>Resolution</td>
<td>100m × 100m × 40m</td>
</tr>
<tr>
<td>time-step</td>
<td>2s</td>
</tr>
<tr>
<td>total simulation period</td>
<td>4hr</td>
</tr>
<tr>
<td>period in database</td>
<td>last 2hrs</td>
</tr>
<tr>
<td>nr of instantaneous 3D fields</td>
<td>12 (each 600s)</td>
</tr>
<tr>
<td>(thermo)dynamic variables</td>
<td>u, v, w, \theta_l, q_l, \theta_v, K_h</td>
</tr>
<tr>
<td>chemical species</td>
<td>NO, NO_2, O_3</td>
</tr>
<tr>
<td>Surface heat flux</td>
<td>\langle w^j \phi_i^t \rangle = 8 \cdot 10^{-3} K m/s</td>
</tr>
<tr>
<td>Surface humidity flux</td>
<td>\langle w^j q_i^t \rangle = 5.2 \cdot 10^{-5} kg/kg m/s</td>
</tr>
</tbody>
</table>

Table 2.2: Information regarding the LES case, and the database

Details on the present LES run and the database are provided in table 2.2. For each variable $\phi$ there are 12 three-dimensional fields, so the (4D) structure is: $\phi(i, j, k; n)$, with $i \in [1, 64], j \in [1, 64], k \in [1, 80], n \in [1, 12]$, where $i, j, k$ correspond to the x-, y-, and z-direction respectively; $n$ represents the frame number, i.e. the corresponding time is $t_n = 600n + 7200s$.

In the practicum you can make use of the matlab files CuVis.m, CuMovie.m, CuStat.m to which you can add your own commands. Besides some general matlab commands, the Cu.m-files make use of the following predefined procedures

- **readles.m**: read LES data-files
- **avslab.m**: calculates an average of a (4D) field over $i$ and $j$.
- **avtime.m**: calculates an additional time average of the slab-averaged fields.
- **ddz.m**: calculates the vertical derivative of a mean profile.

### 2.1 Exercise I: 3D visualization of clouds

1. Start **matlab** and type CuVis at the prompt. The liquid water data $q_l$ are now read, and a snapshot of a 3D cloud field becomes visible. You can rotate and zoom the image to have a better look at the data.

2. Increase the threshold in the isosurface routine. What effect does it have on small and big clouds?

3. Start **CuMovie**: this will generate an animation of the evolution of the cloud field over the last two hours (12 frames).
2.2 Exercise II: Mean profiles and fluxes

1. Start CuStat. All data will be read. As an example the code will calculate the slab average of liquid water:

$$
\bar{q}_l(k;n) = \frac{1}{N_x N_y} \sum_{ij} q_l(i,j,k;n)
$$

and plot the instantaneous profiles.

Next it will additionally average these profiles in time and plot the result, i.e.

$$
\langle q_l \rangle = \frac{1}{N_t} \sum_n \bar{q}_l(k;n)
$$

What is the typical value for the average liquid water content in the cloud layer?

2. Add your commands to the file CuStat.m to study the profiles of the thermodynamic variables $q_t$, $\theta_t$, and $\theta_v$. Identify the cloud-layer, the sub-cloud layer and the free troposphere.

3. Plot also the velocities profiles $\langle u \rangle$ and $\langle v \rangle$. Why not $\langle w \rangle$?

**Fluctuations and variance profiles**

The fluctuations of a variable $\phi$ are

$$
\phi'(i,j,k;n) = \phi(i,j,k;n) - \bar{\phi}(k;n)
$$

The instantaneous variance profile is

$$
\phi'^2(k;n) = \frac{1}{N_x N_y} \sum_{ij} \phi'^2(i,j,k;n)
$$

4. Calculate the instantaneous variance profiles of the vertical velocity and average these in time. Plot and interpret the profile of $\langle w'^2 \rangle$.

**Fluxes**

The instantaneous vertical flux profile of a variable $\phi$ is

$$
\overline{w'\phi'}(k;n) = \frac{1}{N_x N_y} \sum_{ij} w'(i,j,k;n) \phi'(i,j,k;n)
$$

The time-averaged flux is

$$
\langle w' \phi' \rangle = \frac{1}{N_t} \sum_n \overline{w'\phi'}(k;n)
$$

5. Calculate the time-averaged fluxes $\langle w' q'_t \rangle$, $\langle w' \theta'_t \rangle$. What are the values of the surface fluxes. Is that correct?
Subgrid contribution
An important ingredient of an LES is the contribution of the sub-grid processes to the flux. That is, the evolution of a variable does not only depend on the resolved flux, but also on the subgrid flux:

\[
\frac{\partial \phi}{\partial t} = -\frac{\partial}{\partial z} \left\{ \bar{w}' \phi^{\text{resolved}} + \bar{w}' \phi^{\text{subgrid}} \right\}
\]

Usually the subgrid contributions are calculated in LES by using an eddy diffusivity closure

\[
\left[ w' \phi' \right]^{\text{subgrid}} = -K_h \frac{\partial}{\partial z} \phi \quad \text{for} \quad \phi \in \{ \theta_l, q_l, \text{species} \}
\]

where the eddy-diffusivity \( K_h \) is location and time dependent. The way \( K_h \) is determined may vary a lot between different LES codes. To calculate the subgrid fluxes for the present simulation we have added to the database the LES-generated \( K_h \)-fields. Due to the staggered grid arrangement of the LES, you can numerically derive the (local) subgrid flux by:

\[
\left[ w' \phi' \right]^{\text{subgrid}} = - K_h (i, j, k; n) + K_h (i, j, k-1; n) \Delta z \frac{\phi(i, j, k, n) - \phi(i, j, k-1, n)}{2}
\]

6. Determine the slab- and time-averaged subgrid fluxes \( \left< w' q_l' \right>^{\text{subgrid}} \) and \( \left< w' \theta_l' \right>^{\text{subgrid}} \) and plot them. Add them to the resolved fluxes to get the total fluxes. Are the surface fluxes correct?

7. How confident can we be about those parts of the simulation where the subgrid contributions are large?

2.3 Exercise III: Conditional sampling and cloud averages

Here we will determine the cloud-averaged values of various quantities. In this way we also get the cloud mass-flux, and therefore insight into the vertical transport by cumulus clouds.

Conditional averages can be easily derived from the data by defining an 'indicator' field that mark the cloudy points

\[
c(i, j, k; n) = \begin{cases} 
0 & \text{if} \quad q_l(i, j, k; n) = 0 \\
1 & \text{if} \quad q_l(i, j, k; n) > 0 
\end{cases}
\]

Then the (average) cloud fraction is given by

\[
\sigma = \frac{1}{N_x N_y N_t} \sum_{ijn} c(i, j, k; n) = \left< c \right>
\]

The average cloud mass-flux is given by

\[
M = \frac{1}{N_x N_y N_t} \sum_{ijn} c(i, j, k; n) w(i, j, k; n) = \left< c \ w \right>
\]
The ‘cloud average’ value of an arbitrary variable $\phi$ can be determined by

$$
\phi^c = \frac{\sum_{ijn} c(i,j,k;n) \phi(i,j,k;n)}{\sum_{ijn} c(i,j,k;n)} = \frac{\langle c \phi \rangle}{\langle c \rangle}
$$

1. Calculate and plot the cloud fraction. Note, in \texttt{matlab} it is very easy to construct the indicator field by the command: $c = q1 > 0$. This directly generates the desired 4D field consisting of 0,1 entries.

2. Plot the mass-flux profile.

3. Plot profiles of the cloud averaged vertical velocity $w^c$.

4. Plot profiles of the cloud averaged liquid water $q^c_l$, total water $q^c_t$, and the cloud values $\theta_i^c$, $\theta_v^c$. Compare with the mean profiles. How big is the $\theta_v$-excess (difference between the cloud value and mean value, $\theta_v^c - \langle \theta_v \rangle$)? Compare to the $\theta_t$-excess.
Chapter 3

Practicum 3: Evolution of a convective boundary layer and its influence on ozone diurnal variability

by Jordi Vilà-Guerau de Arellano

1 Theoretical background: summary of governing equations and definitions

In this section, we briefly discuss the governing equations for turbulent flow in the atmospheric boundary layer and we define the thermodynamic variables used during the course. Previous knowledge on the derivation of these equations and variables is assumed from introductory courses of atmospheric boundary layer theory.

1.1 The governing equations for mean quantities in a turbulent flow

Physical laws (conservation equations) allow us to describe the distribution and evolution of the main characteristics of the atmospheric boundary layer (ABL). In short these equations are described below. Beside the equation of state (1) and the continuity equation (2), this set of equations includes the conservation of momentum ($\bar{u}$ and $\bar{v}$) (3, 4), heat ($\bar{\theta}$) (5), moisture ($\bar{q}$) (6) or any scalar ($\bar{s}$) (7) which can represent chemical compounds, for example.

The equations are derived by using the Reynolds decomposition and averaging technique. The mean state of the atmosphere is assumed to be in hydrostatic equilibrium and the Boussinesq approximation is applied. Note that these governing equations apply to a situation of shallow convection, i.e., vertical motion is limited.

\[
\frac{\bar{P}}{\bar{R}_d} = \bar{p}T_v
\]  

(3.1)
\[ \frac{\partial \theta}{\partial x_j} = 0 \]  
(3.2)

\[ \frac{\partial \mathbf{U}}{\partial t} + \mathbf{U}_j \frac{\partial \mathbf{U}}{\partial x_j} = f_c (\nabla - \nabla g) - \frac{\partial (w'_j w')}{\partial x_j} \]  
(3.3)

\[ \frac{\partial \nabla}{\partial t} + \mathbf{V}_j \frac{\partial \nabla}{\partial x_j} = -f_c (\mathbf{U} - \mathbf{U}_g) - \frac{\partial (\mathbf{V}_j \mathbf{V}_g)}{\partial x_j} \]  
(3.4)

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{U}_j \frac{\partial \mathbf{u}}{\partial x_j} = -\frac{1}{\rho C_p} L_v E - \frac{1}{\rho C_p} \frac{\partial E'_j}{\partial x_j} - \frac{\partial (u'_j \theta')}{\partial x_j} \]  
(3.5)

\[ \frac{\partial \mathbf{q}_t}{\partial t} + \mathbf{U}_j \frac{\partial \mathbf{q}_t}{\partial x_j} = S_{q_t} \frac{\rho}{\rho} - \frac{\partial (u'_j q'_t)}{\partial x_j} \]  
(3.6)

\[ \frac{\partial s}{\partial t} + \mathbf{U}_j \frac{\partial s}{\partial x_j} = S_s \frac{\rho}{\rho} - \frac{\partial (u'_j s'_t)}{\partial x_j} \]  
(3.7)

For equations (3-7) the first terms of the left hand side (l.h.s.) are all storage (or tendency) terms and the second terms describe advection by the mean flow. Also, all the last terms on the right hand side (r.h.s.) describe the turbulent flux divergence.

For the momentum equations (3,4), the first term (r.h.s.) represents a departure from the geostrophic wind speed. The first term (r.h.s.) of both the moisture equation (6) and the scalar equation (7) is a source term \( S \) for additional moisture processes (for example precipitation) or tracer processes (e.g., chemical reaction or direct emission.) Lastly the heat equation (5) has two extra source terms (r.h.s.) that represent the latent heat release and the radiation divergence respectively.

For the full derivation of these equations, please refer to Chapter 3 of the book 'An introduction to Boundary Layer Meteorology', by Stull (1988).

1.2 Definitions of heat and moisture quantities and fluxes

Conserved variables

The above equations for heat and moisture are written in terms of the potential temperature \( \theta \) in Kelvin and the total specific humidity \( q_t \) in kg water/kg air. The latter is defined as the total mass of water, in all phases, per unit mass of moist air, and can be written as the water vapor specific humidity \( q_v \) in case no liquid water is present:

\[ q_t = q_v \]  
(3.8)

when \( q_v < q_s \) (unsaturated air). Here \( q_s \) is the saturation specific humidity and \( q_v = \epsilon \frac{p}{e} \), with \( \epsilon = 0.622 \), \( e \) as the water vapor pressure and \( p \) as the pressure. \( q_s \) is calculated with the same formula as \( q_v \) but by using \( e_s \), the saturation vapor pressure, instead of \( e \).

In the case of saturated air \( (q_v = q_s) \) and the liquid water specific humidity \( q_l > 0 \):

\[ q_t = q_l + q_s \]  
(3.9)

\[ ^1 \text{When the specific humidity in any text is specified as } q, \text{ it means } q = q_v. \]
Because $q_t$ accounts for all water phases, it is a so-called conserved variable, i.e., it remains constant no matter what processes (condensation or evaporation) occur. Beside the potential temperature used in the conservation of heat equation, the virtual potential temperature is a frequently used variable and it is defined as:

$$\theta_v = \theta(1 + 0.61q_s - q_t)$$

(3.10)

The virtual temperature $\theta_v$ takes into account the effect of water vapor or liquid water on the density of air. This is important when studying the buoyancy of air parcels, and thus the density of an air parcel as compared to its surroundings. When an air parcel contains liquid water, its buoyancy will be reduced because the density of water is higher than dry air. On the other hand, a parcel containing water vapor is more buoyant compared to dry air, because water vapor has a density smaller than that of dry air.

Neither the potential temperature nor the virtual potential temperature account for the release or absorption in latent heat when condensation or evaporation takes place. Therefore they cannot be given the status of conserved variable if phase changes occur. Two variables that do take these processes into account, are the liquid water potential temperature $\theta_l$ and the equivalent potential temperature $\theta_e$, defined as:

$$\theta_l = \theta - \left(\frac{\theta}{T}\right) \frac{L_v}{C_p} q_l$$

(3.11)

$$\theta_e = \theta + \left(\frac{\theta}{T}\right) \frac{L_v}{C_p} q_v$$

(3.12)

in which $\frac{\theta}{T}$ is often approximately unity.

These conserved variables in combination with $q_t$ can therefore be used to study both clear (unsaturated) and cloudy (saturated) boundary layers.

**Fluxes**

If the clear and cloudy boundary layers are mainly driven by convection (typical conditions on a sunny day), buoyancy is the most important term in the prognostic equation for turbulent kinetic energy TKE (see Chapter 5. of Stull (1988)). In the TKE equation the buoyancy term is written as:

$$\frac{g}{\theta_v} \left(\overline{w'\theta'_v}\right)$$

(3.13)

in which $\left(\overline{w'\theta'_v}\right)$ is the virtual potential temperature flux, or buoyancy flux. This flux is defined as:

$$\left(\overline{w'\theta'_v}\right) \simeq \left(\overline{w'\theta}\right) + 0.61 \overline{\theta} \cdot \left(\overline{w'q'}\right)$$

(3.14)

and derived by using the fluctuating part $\theta'_v$ of Equation 3.10, multiplying it by $w'$ and averaging. It is assumed that $q_l << q_v$. This equation states that a parcel can gain buoyancy by having a temperature excess or water vapor excess compared to the surrounding air. The temperature excess can also be due to the release of latent heat when condensation takes place (Garratt, 1992; Stull, 1988, 2000).
Lastly, the turbulent moisture flux $w'q'_t$ is defined as:

\[
\left( w'q'_t \right) = \left( w'q'_c \right) \quad q_t = 0
\]  
\[ (3.15) \]

\[
\left( w'q'_t \right) = \left( w'q'_a \right) + \left( w'q'_l \right) \quad q_t > 0
\]  
\[ (3.16) \]
2 The clear convective boundary layer

2.1 Introduction

In a convective boundary layer (CBL) the turbulent flow is mainly driven by buoyancy. In a CBL, warm rising air from the surface organizes itself into thermal plumes or eddies, that can occupy substantial areas (diameters of up to 1 km) and reach the top of the boundary layer. These plumes mix air from the surface to the top of the boundary layer very effectively, and thereby create a very well mixed layer. As a result quantities like heat and moisture remain almost constant with height and the vertical gradient is approximately constant in time (i.e., a pseudostationary condition). Under these conditions, three distinct regions can be recognized: (1) a surface layer, (2) a well-mixed layer and (3) an inversion layer. The inversion layer is a region of increasing temperature with height, also called the capping inversion or entrainment zone. Thermal plumes reaching the inversion layer are often unable to penetrate through this stable layer. Above the entrainment zone, a fourth layer can be distinguished, namely the free atmosphere (see Figure 3.1).

In the following sections the most important thermodynamic principals, the vertical structure and evolution and the modeling of the clear CBL by means of a bulk mixed-layer model are discussed. It is explicitly called a clear (cloud-free) CBL, because it is assumed the atmosphere is dry and no saturation takes place. Theoretical background information on a cloudy CBL is given in the next section (reference number).

Figure 3.1: A scheme representing the clear convective boundary layer, with turbulent plumes and a well-mixed layer. Also shown are typical profiles of the virtual potential temperature $\theta_v$, the total specific humidity $q_t$ and the buoyancy flux $\left(\overline{w'\theta'_v}\right)$. 

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2.2 Vertical structure and evolution of a clear CBL

In a clear CBL the profiles of various variables correlates strongly with the typical layer structure in a CBL, see Figure 3.1. During daytime the surface layer is unstable and characterized by a rapid decrease in temperature (superadiabatic gradient) and moisture with height and a strong wind shear. Sensible and latent heat fluxes, conducted by eddy motions, transport heat and moisture from this region into the well-mixed layer above and thereby heat and moisten the boundary layer from below. In this mixed-layer, the eddies grow into more vigorous thermal plumes with vertical velocities ranging from 1-2 ms$^{-1}$. As a result strong mixing is created throughout this whole layer. Air is not only being mixed upwards, but reciprocal downward moving plumes (so-called downdrafts or subsidence motions) are present as well. As a result, variables as temperature and humidity, and even the winds, are nearly constant with height in the well-mixed layer. In a clear CBL, we can use the conserved variables $q_t$ and $\theta_l$, but since there is no liquid water present ($q_l = 0$), $\theta_l$ can be written as $\theta$.

In the inversion layer, marking the transition from boundary layer air to the relatively dry and warm free atmosphere, the temperature increases and specific humidity decreases. When penetrating into this inversion layer, the eddies gain a negative buoyancy and sink back into the mixed-layer. When doing so, they transport warm and dry free atmospheric air into the mixed-layer (the process called entrainment).

The top of the mixed-layer, $z_i$, can be defined in various ways, but often it is defined as the location at which the heat flux has the minimum (negative) value. This occurs at some place in the inversion layer, where rising plumes become negatively buoyant ($w'\theta < 0$) due to the increase in surrounding potential temperature.

2.3 Modeling the CBL as a bulk mixed-layer

Evolution of quantities in a bulk mixed-layer

If we consider a horizontally homogeneous CBL, without latent heating and precipitation processes, the governing equations for wind, temperature, humidity and any scalar are simplified to:

\[
\frac{\partial U}{\partial t} = f_c (V - \bar{V}) - \frac{\partial (w'w')}{\partial z} \tag{3.17}
\]

\[
\frac{\partial V}{\partial t} = -f_c (U - \bar{U}) - \frac{\partial (v'w')}{\partial z} \tag{3.18}
\]

\[
\frac{\partial \bar{\theta}}{\partial t} = -\frac{1}{\rho C_p} \frac{\partial F_z}{\partial z} - \frac{\partial (w'\theta)}{\partial z} \tag{3.19}
\]

\[
\frac{\partial q_t}{\partial t} = -\frac{\partial (w'q_t)}{\partial z} \tag{3.20}
\]

\[
\frac{\partial s}{\partial t} = -\frac{\partial (w's)}{\partial z} \tag{3.21}
\]

The terms on the left hand side are called the tendency terms, the terms on the right hand side (aside from the ageostrophic terms in the momentum equations (17 and 18)) are called the flux divergence terms.
Using the property that the thermodynamic variables are well-mixed in the CBL, one can describe the CBL as a bulk layer, in which quantities are nearly constant with height. The structure of the CBL is therefore often represented by just two layers instead of the aforementioned four layers: (1) a bulk layer that incorporates the surface layer and (2) the free atmosphere. The aforementioned third layer, the inversion layer, is here simply a sharp discontinuity representing the difference between values in the bulk layer and the free atmosphere. This is called the zero-order jump approach of the CBL (see Figure 3.2).

The generic bulk mean values of any quantity are defined with the following formula (here for a quantity $s$):

$$s_m = \frac{1}{h} \int_{z_0}^{h} s \, dz$$  \hspace{1cm} (3.22)

with $h$ as the height of the bulk layer, which in our CBL case would be the boundary layer (or mixed-layer) height $z_i$, and $z_0$ the beginning of the CBL, which usually corresponds to 0 m.

Because a quantity at any height in the boundary layer can be expressed as a single slab value, the vertical profiles (i.e., the change of a quantity with height) do not change with time ($\frac{\partial}{\partial z} = \frac{\partial}{\partial t}$). The bulk mixed-layer is therefore in a quasi-steady state. To obtain an expression for the evolution of any quantity in the bulk layer, the simplified equations are integrated over the boundary layer depth (from $z_0$ to $z_i$):

$$\int_{z_0}^{z_i} \frac{\partial s}{\partial t} \, dz = \int_{z_0}^{z_i} \frac{-\partial w'^2}{\partial z} \, dz$$  \hspace{1cm} (3.23)

Leibniz’ rule of integration states that the integral of the tendency of any quantity $\int_{z_0}^{z_i} \frac{\partial s}{\partial t} \, dz$ is:

$$\int_{z_0}^{z_i} \frac{\partial s}{\partial t} \, dz = \frac{\partial s}{\partial t} \bigg|_{z_i} - \left[ s(z_i) - s_m \right] \frac{\partial z_i}{\partial t}$$  \hspace{1cm} (3.24)

Because in our case of the bulk mixed-layer $s(z_i) = s_m$, we obtain the following expression after integrating Equation 3.23 (here with temperature and humidity as an example):

$$\frac{\partial \theta_m}{\partial t} = \frac{(w'^\theta)_s - (w'^\theta)_e}{z_i}$$  \hspace{1cm} (3.25)

$$\frac{\partial q_m}{\partial t} = \frac{(w'^q)_s - (w'^q)_e}{z_i}$$  \hspace{1cm} (3.26)

and so on for the other quantities. The mean values $\bar{\theta}$ and $\bar{q}$ have been replaced by their slab mean values $\theta_m$ and $q_m$.

These equations state that the tendency of a quantity in a bulk mixed-layer, i.e., the evolution, is determined by the surface flux $(w'^\theta)_s$ and the flux at the top of the layer.
\( (\overline{w'\theta'})_e \), also called the entrainment flux. Again temperature is here taken as an example, but surface and entrainment fluxes occur in a similar way for the other quantities, such as CO\(_2\) or O\(_3\) or aerosols, etc.

**Entrainment fluxes and mixed-layer growth**

![Figure 3.2: The zero-order jump approach of the mixed-layer. The inversion layer is assumed to have zero thickness. Vertical profiles of temperature and the buoyancy flux are shown, with their respective jumps at the inversion layer. Notice the simplification of the inversion layer as compared to Figure 3.1.](image)

The entrainment process was defined as the process whereby air with properties from the free atmosphere is mixed into the mixed layer, and it is therefore related to the jump in a given quantity at the inversion. The zero-order closure defines this jump as \( \Delta s_{z_i} = s_{z_i+} - s_m \) over an infinitesimal inversion layer, in which \( s_{z_i+} \) is defined as the value at \( z_i + \epsilon \) with \( \epsilon \to 0 \) (see Figure 3.2). In this zero-order jump approach, the entrainment flux can be represented as the product of the entrainment velocity \( w_e \) (defined positive in the upward direction) and the jump of any quantity \( \Delta s_{z_i} \) at the inversion in the following way (for temperature):

\[
(\overline{w'\theta'})_e = -w_e \cdot \Delta \theta_{z_i}
\]

(3.27)

At this infinitesimally thin inversion layer, not only entrainment influences the mixed-layer properties, but also vertical subsidence motions from the free atmosphere, associated with the presence of, for example, synoptic high pressure systems, play a role. If we keep the vertical advection term, \( \left( \frac{\partial \rho}{\partial z} \right) \), when simplifying the conservation of heat equation from (5) to (19), and we integrate over the infinitesimal inversion (in a similar way as in Equation 3.23) the following expression for the entrainment flux is obtained:

\[
(\overline{w'\theta'})_e = -\Delta \theta_{z_i} \left( \frac{\partial z_i}{\partial t} - w_s \right)
\]

(3.28)

in which \( w \) has been replaced with \( w_s \), the subsidence velocity, which has a negative value \( (w_s < 0) \) in most fair-weather (shallow convection) situations. In our model, we have prescribe the subsidence velocity as:
\[ w_s = -C \, z_i \]  
\[ (3.29) \]

where \( C \) is a function of the wind divergence in \( s^{-1} \).

Rewriting the above equation and using Equation (3.27) gives an expression for the growth of the mixed-layer:

\[ \frac{\partial z_i}{\partial t} = \frac{(-w^0 \theta^0)}{\Delta \theta_{z_i}} + w_s = w_e + w_s \]  
\[ (3.30) \]

This equation states that the mixed-layer grows by entrainment of warm air from the free atmosphere \((w_e > 0)\), in the absence of subsidence \((w_s = 0)\). However, the temperature jump at the inversion \( \Delta \theta_{z_i} = \theta_{z_i +} - \theta_m \) changes during the growth and evolution of the mixed-layer. For example, while the mixed-layer warms up, as defined earlier in Equation 3.25, the jump will decrease as \( \theta_m \) increases. Or when the mixed-layer grows or subsidence plays a role, the jump will increase as \( \theta_{z_i +} \) increases. The latter two processes can be combined in an expression for the tendency of this temperature jump \( \Delta \theta_{z_i} \):

\[ \frac{\partial \Delta \theta_{z_i}}{\partial t} = \frac{\partial \theta_{z_i +}}{\partial t} - \frac{\partial \theta_m}{\partial t} = \gamma_\theta \left( \frac{\partial z_i}{\partial t} - w_s \right) - \frac{\partial \theta_m}{\partial t} \]  
\[ (3.31) \]

in which \( \frac{\partial \theta_{z_i +}}{\partial t} \) is written as \( \gamma_\theta \left( \frac{\partial z_i}{\partial t} \right) \), and \( \gamma_\theta \) is the temperature lapse rate in the free atmosphere. Consequently, the growth of the mixed-layer is governed by the heating of the mixed-layer. And to study this growth, one needs to study both the tendency of the jump across the inversion layer and the heating inside the mixed-layer (see Garratt (1992) for a more elaborate explanation).

The mixed-layer model

The mixed-layer model is a model that considers the CBL as a single bulk layer and thereby uses the Eulerian approach. In this approach the CBL is considered as a box in which quantities are influenced by all the in- and outgoing fluxes at all sides of the box. The box is closed, which implies that all sources and sinks have to be compensated and no energy is lost. As an example one can consider heat: if there is more heat coming into the box than is going out, the temperature in the box has to increase.

The mixed layer model assumes a quasi steady state and horizontal homogeneity, no radiative or latent heating effects or any other sources earlier denoted by \( S \) in the governing equations in section 3.1. Only the bottom and top of the box are considered as a possible source or sink of quantities, thus only surface fluxes and entrainment fluxes play a role. However, where the surface fluxes in the mixed-layer model are explicitly specified for the entire model simulation, the entrainment fluxes are not. These fluxes need to be resolved in the actual model simulation and they are only specified as an initial value at the start of the simulation.

Considering these assumptions, the mixed-layer model can be studied with the equations mentioned before. More specifically, in the model the equations for the tendency of the inversion potential temperature jump (3.31), the heating rate (3.25) and the entrainment flux (3.28) need to be solved numerically. However, combining these three equations, in
which $\overline{w'\theta'}_s$ and $w_s$ are explicitly specified as boundary conditions and $\gamma_\theta$ is known, we are left with the following four unknowns:

- $\overline{w'\theta'}_e$
- $\Delta \theta_{z_i}$
- $\theta_m$
- $z_i$

An additional closure equation is needed. An often used closure specifies the entrainment flux as a certain fraction, $\beta$, of the surface flux, that is often given the value of 0.2:

$$\overline{w'\theta'}_e = -\beta \overline{w'\theta'}_s$$  \hspace{1cm} (3.32)

With this closure all the equations in the mixed-layer, and not only the ones for temperature, are solved. In order to solve them numerically, we need to include them as discrete values.

3 Diurnal variation of ozone in a clear convective boundary layer

- Jacob (1999): Chapter 11

The mixed layer model allow us to investigate the role of boundary layer dynamics during the diurnal evolution of ozone and its related atmospheric compounds. Our aim is to show that in order to explain ozone formation and transformation, it is also necessary to understand the evolution of the boundary layer growth and its diurnal evolution.

In consequence, in addition to the main governing equations for the slab temperature, the potential temperature jump and the boundary layer growth, we add a chemical system which evolves on time and it is depending on the emissions at the surface and the exchange (entrainment) between the convective boundary layer and the free troposphere.

For the sake of a better understanding of the exercise, we have divided the chemical mechanism for ozone formation in two parts: simple and complex. The simple mechanism is composed by the following chemical reactions:

(R1) $NO + O_3 \rightarrow NO_2$ \hspace{1cm} $k_1 = 4.75 \times 10^{-4} \text{ ppb}^{-1} \text{s}^{-1}$

(R2) $NO_2 + h\nu + (O_2) \rightarrow NO + O_3$ \hspace{1cm} $j_1 \text{ varies on time,}$

where $NO$ is nitric oxide, $O_3$ is ozone and $NO_2$ is nitrogen dioxide. The photodissociaation of $NO_2$ ($j_1$) by photon in the ultraviolet spectrum range is represented by $h\nu$. For this simple chemical mechanism, it is very convenient to define a photostationary state $\Phi$ which represents the rate of production and destruction of reactions (1) and (2). It reads:

$$\Phi = \frac{k_1 \overline{NO} \overline{O_3}}{j_1 \overline{NO_2}}$$

If the value of $\Phi$ is equal to 1, the chemical system is in equilibrium.
In order to complete this simple scheme, we can add the following reactions to define a complex chemical mechanisms which contains the essential reactions in ozone formation during diurnal conditions. Thus, in addition to \( R_1 \) and \( R_2 \), the complex system is composed by:

\[
\begin{align*}
(R3) & \quad O_3 + h\nu + (H_2O) \to 2OH + O_2 & j_2 \text{ varies on time} \\
(R4) & \quad OH + CO + (O_2) \to HO_2 + CO_2 & k_2 = 6.0 \times 10^{-3} \text{ ppb}^{-1}\text{s}^{-1} \\
(R5) & \quad OH + RH \to HO_2 + \text{products} & k_3 = f \times 6.0 \times 10^{-3} \text{ ppb}^{-1}\text{s}^{-1} \\
(R6) & \quad HO_2 + NO \to OH + NO_2 & k_4 = 2.1 \times 10^{1} \text{ ppb}^{-1}\text{s}^{-1} \\
(R7) & \quad HO_2 + O_3 \to OH + 2O_2 & k_5 = 5.0 \times 10^{-5} \text{ ppb}^{-1}\text{s}^{-1} \\
(R8) & \quad 2HO_2 \to H_2O_2 + O_2 & k_6 = 7.25 \times 10^{-2} \text{ ppb}^{-1}\text{s}^{-1} \\
(R9) & \quad OH + NO_2 \to HNO_3 & k_7 = 2.75 \times 10^{-1} \text{ ppb}^{-1}\text{s}^{-1} \\
(R10) & \quad OH + O_3 \to HO_2 + O_2 & k_8 = 1.75 \times 10^{-3} \text{ ppb}^{-1}\text{s}^{-1} \\
(R11) & \quad OH + HO_2 \to H_2O + O_2 & k_9 = 2.75 \times 10^{-0} \text{ ppb}^{-1}\text{s}^{-1}. 
\end{align*}
\]

In short, ozone is photolized by ultraviolet radiation \( R_3 \). The presence of volatile organic compounds (represented by \( RH \)) and \( CO \) yield the formation of \( HO_2 \) (reactions \( R_4 \) and \( R_5 \)). \( HO_2 \) favours ozone formation by producing \( NO_2 \) (reaction \( R_6 \)), which is the only compound able to produce \( O_3 \) in reaction \( R_2 \). Moreover, by consuming \( NO \) in reaction \( R_6 \), less \( NO \) will be available to react with \( O_3 \) at reaction \( R_1 \). in the same reaction. As a result, the concentration of \( OH \) is characterized by a very short time scale. Production and destruction of \( OH \) is therefore determined by the longer-lived species and, consequently its concentration is calculated from:

\[
OH = \frac{2j_1O_3 + k_3HO_2NO + k_4HO_2O_3}{k_2(CO + fRH) + k_6NO_2 + k_7O_3 + k_8HO_2}.
\]

Although this is a simplified version compared to the more complete chemical system currently implemented in air quality models, it still retains the more important components which yield to ozone formation: (a) the presence of hydrocarbons represented by a generic component \( RH \) and (b) the formation of the cleansing radical component \( OH \).

4 User instructions for the mixed-layer model

In this course the mixed-layer model, presented in section 4.3, is applied to study the main characteristics and development of a clear convective boundary layer. The model is based on the mixed-layer theory and equations in section 4.3. A more detailed description of the model and the mixed-layer theory can be found in Garratt (1992) and Tennekes and...
4.1 Model input

The default conditions shown in Figure 3.3 are the ones of the control run. The following conditions need to be specified:

- **Characteristics of the model run:**
  The total simulation time and the timestep determine the duration and time resolution of the run. If one wants to study the evolution of the boundary layer characteristics in time, it is important to specify the frequency of results that will be printed in the graphical output. However, one has to bear in mind that it is compulsory to prescribe a value for the frequency that results in an integer value for the ratio between the total time and the frequency. The vertical prof freq determines the frequency of the vertical profiles. For instance, the default value prescribes that a profile is calculated each 1800 s. The max height vert prof specifies the maximum height at which the variables are calculated and plotted in a graph with vertical profiles. The default value will be sufficient in most cases.

- **Boundary layer depth and entrainment flux ratio:**
  The initial boundary layer depth $z_i$ is 750 m. This value corresponds to a typical mixed-layer depth at 0800 UTC, approximately three hours after sunrise. The entrainment flux ratio, introduced before as $\beta = -\overline{w' \theta'}_{z_i} / \overline{w' \theta'}_s = A_R$, is here specified as a constant. The default value of + 0.2 is often used as an average value that represents a turbulent boundary layer mainly driven by free convection. In the case of a shear-driven boundary layer, the constant $A_R$ can be expected to have a larger value (Stull, 1988; Pino et al., 2003). Also given as an input variable is the subsidence velocity in ms$^{-1}$, that is in the default case specified to 0.

- **Temperature initial and boundary conditions:**
  The surface sensible heat flux $\overline{w' \theta'}_s$ is the lower boundary condition of the mixed-layer model. It is specified either as a constant surface flux or as a diurnal cycle, by specifying 'Yes' or 'No' respectively. If you specify 'Yes' all the fluxes (for heat,
moisture and scalars) are automatically prescribed as constant fluxes in time. The temperature lapse rate $\gamma_\theta$ is the lapse rate of the free atmosphere located above the boundary layer. The surface temperature $\theta_s$ and temperature jump $\Delta \theta$ at the inversion height are specified as initial conditions for the model.

- **Humidity, scalar and wind initial and boundary conditions:**
  The input variables for these three are treated similarly as the temperature input variables. The surface fluxes are the lower boundary conditions. The gradients are the tropospheric humidity, scalar and wind gradients. The surface values and jumps at the inversion are initial conditions. Be aware of the units of specific humidity in gkg\(^{-1}\). The initial and boundary conditions of the scalar correspond to typical values of carbon dioxide. The units of a CO\(_2\) are given in ppm. The two components of the geostrophic wind speed are wind speeds in the free atmosphere.

![Figure 3.3: In this window the initial and boundary conditions for the mixed-layer model are specified. The default values are the ones of the control run.](image)

### 4.2 The model run

After specifying your initial and boundary conditions, a model run starts by simply clicking the 'Launch simulation' button. In the mixed-layer model, the partial differential equations in Part I Theory that represent the growth and evolution of a horizontally homogeneous
mixed-layer are solved numerically. This implies that the partial derivatives, $\partial$, are discretized by using finite differences, $\Delta$. For example, the equation for the evolution of the mixed-layer potential temperature (reference), earlier derived in Part I, is approximated with the finite difference method as follows:

$$\frac{\partial \theta_m}{\partial t} = \frac{\overline{w' \theta_s} - \overline{w' \theta'_e}}{z_i} = \frac{(1 + \beta)\overline{w' \theta'_s}}{z_i}$$

(3.33)

By discretizing (1) one obtains:

$$\frac{\Delta \theta_m}{\Delta t} = \frac{(1 + \beta)\overline{w' \theta'_s}}{z_i}$$

(3.34)

And after expanding the time difference, the equation reads:

$$\theta_m(t + \Delta t) = \theta_m(t) + \frac{(1 + \beta)\overline{w' \theta'_s}}{z_i(t)} \cdot \Delta t$$

(3.35)

The time step $\Delta t$ is prescribed by the value of $timestep$ in the initial conditions and for the above equations it is assumed that the surface fluxes are kept constant.

The mixed-layer model is written in the FORTRAN programming language. During each run, several files are generated containing the output results. The files are generated and saved in the same directory on your computer as where the model mxl_gui.exe is placed. For example the time evolution of the boundary layer and the relevant variables are studied from the result files output_dyn and output_sca. The vertical profiles of the relevant variables are studied from the file x_prof, where x is either t, q, c, u or v corresponding to temperature, humidity, a scalar quantity and the x-and y components of the wind field respectively. Another output file named saturation contains information on the vertical profiles of variables that are important when studying saturation processes in the boundary layer. What the specific variables in each file are exactly, is explained in the next section.

4.3 Model output

The following notations are used for the variables in the output files.
**output_dyn**: time evolution

- $z_i$ boundary layer height (m)
- $w_e$ entrainment velocity (ms$^{-1}$)
- $\theta_m$ mixed-layer potential temperature (K)
- $\Delta \theta$ potential temperature jump at inversion (K)
- $w'\theta' e$ entrainment heat flux (Kms$^{-1}$)
- $\beta$ ratio of the entrainment flux to surface heat flux (-)
- $u_m$ horizontal wind speed x-direction (ms$^{-1}$)
- $v_m$ horizontal wind speed y-direction (ms$^{-1}$)

**output_sca**: time evolution

- $z_i$ boundary layer height (m)
- $q_m$ mixed-layer specific humidity (gkg$^{-1}$)
- $\Delta q$ specific humidity jump at inversion (gkg$^{-1}$)
- $w'q' e$ entrainment humidity flux (ms$^{-1}$)
- $\beta_q$ ratio of entrainment humidity flux to surface humidity flux (-)
- $c_m$ mixed-layer scalar concentration (ppm)
- $\Delta c$ scalar concentration jump at inversion (ppm)
- $w'CO_2 e$ entrainment scalar flux (ppm ms$^{-1}$)

**saturation**: vertical profiles

- $p$ pressure (kPa)
- $T_m$ mixed-layer temperature (K)
- $T_p$ dry or wet adiabat (K)
- $q_t$ total specific humidity (g/g)
- $q_s$ saturation specific humidity (g/g)

The four files (**output_dyn**, **output_sca**, **saturation** and **x_prof**) can be loaded in the second window in which the variables are either plotted as a temporal evolution or as a vertical profile. If you plot a temporal evolution, a message will be printed on top of each graph indicating whether the saturation level is reached or not. Additional information is given in the third part: Practical Exercises. Depending on the **vert prof frequency** described in the model input section, one or more vertical profiles will appear in the same graph. On top of the graph, the time between each profile is printed as a reminder.

For example in Figure 3.4 the boundary layer height $z_i$ (Y-axis) is plotted as a function
**x_prof**: vertical profiles

\[ x = t \]

\( \theta_m \) mixed-layer potential temperature (K)

\( \frac{w' \theta'}{w \theta} \) turbulent potential temperature flux (Kms\(^{-1}\))

\[ x = q \]

\( q_m \) mixed-layer specific humidity (gkg\(^{-1}\))

\( \frac{w q}{w' q} \) turbulent specific humidity flux (gkg\(^{-1}\)ms\(^{-1}\))

\[ x = c \]

\( c_m \) mixed-layer scalar (ppm)

\( \frac{w' c}{w c} \) turbulent scalar flux (ppm ms\(^{-1}\))

\[ x = u \]

\( u_m \) mixed-layer horizontal wind speed x-dir (ms\(^{-1}\))

\( \frac{w' u'}{w u} \) turbulent momentum flux ((ms\(^{-1}\))^2)

\[ x = v \]

\( v_m \) mixed-layer horizontal wind speed y-dir (ms\(^{-1}\))

\( \frac{v' w}{v w} \) turbulent momentum flux ((ms\(^{-1}\))^2)

of time in seconds since the start of the simulation (X-axis). The graphs are saved as bmp files, and then used in the Practical exercises to support the answers and discussion for several questions. For further calculations, the data output files can also be read with Wordpad or Notepad applications.
Figure 3.4: In this window the result files of the mixed-layer model output are loaded and the variables are plotted. For instance, in this figure the boundary layer height $z_i$ is shown as a function of time. In this run saturation processes were not taking place, because the saturation level was located above the boundary layer height $z_i$. This is marked by the sentence 'Saturation level NOT reached'.

QUICK SUMMARY OF INSTRUCTIONS

How to run the mixed-layer model and produce graphical output?

1. Save the zip file mxl_gui.zip available on the website (Course material) to your workstation.

2. Unzip this file. A folder named mxl_gui is placed in the directory where you have saved the zip file. This folder contains the model itself and all the input and output files.

3. Open the model mxl_gui.exe by double clicking on it.

4. Specify the initial and boundary conditions in the first window.

5. Press 'Launch a simulation'.

6. Load one of the result files: output_dyn, output_sca, x_prof or saturation in the second window.
7. Select the variable you want to plot.

8. Save the graph as a bmp file or the output files if necessary.

**Please note** that any new run will replace the results obtained during the previous run, in other words: the 'old' results are substituted with the new results. It is therefore important to save your important results after each run, to prevent that you need to go back to a previous exercise and re-run an old simulation.
5 Exercise I: Temporal evolution of the clear convective boundary layer

Suggested literature:

- Garratt (1992): *Chapters 2, 6.1*
- Stull (1988): *Chapter 11*

1. Perform a control run of the mixed-layer model for a total time of 30000 seconds. Keep the default values for all the initial and boundary conditions. Assume a constant surface heat flux, i.e., no diurnal cycle. Refer to Figure 3.3 for the control run conditions. Load the file *output dyn* and plot the temporal evolution of the variables that best represent the development of a convective boundary layer.

2. A sensitivity analysis can be used to explore the influence of several variables on the warming of the boundary layer. Perform a sensitivity analysis on (1) the surface sensible heat flux $w \theta_s$, as a surface boundary condition and (2) the entrainment ratio $\beta$, as a top boundary condition. Discuss the results. Specify for instance:
   - The default value;
   - Double of the default value;
   - A very small value, etc.
   
   Remember to change only one variable at a time!

3. Study both the temporal evolution and the vertical profiles of the mixed-layer potential temperature $\theta_m$ (from *t prof*).
   
   a) Do the vertical profiles of any scalar quantity in the mixed-layer $\left( \frac{\partial \theta_m}{\partial z}, \frac{\partial q}{\partial z}, \frac{\partial s}{\partial z} \right)$ change with time?
   
   b) In a quasi-steady state situation $\frac{\partial}{\partial z} \left( \frac{\partial \theta_m}{\partial t} \right) \equiv 0$. In this case, can you speak of such a situation according to the answer given at 2a? What are the implications of the quasi-steady state of the potential temperature profile for the form of the vertical profile of the heat flux?
   
   c) Considering the temporal evolution of $\theta_m$, can you state the boundary layer is warming up at a constant rate, i.e., $\frac{\partial \theta_m}{\partial t} =$ constant?
   
   d) Discuss the main variables that influence the warming rate $\frac{\partial \theta_m}{\partial t}$.

   *Hint*: to answer this question use the heat conservation equation and assume horizontal homogeneity, neglect subsidence, radiation and latent heating. Integrate over height to derive an expression for the warming rate $\frac{\partial \theta_m}{\partial t}$.

   e) Can you give a physical explanation for the answer to 2c in terms of the supplied energy (or warmth) after observing the vertical profiles of $\theta_m$?
*Hint:* Use the equation derived in 2d and recall that the fluxes in this run are defined as constants.
6 Exercise II: The role of entrainment on the development of the CBL

Suggested literature:
- Garratt (1992): *Chapters 2, 6.1*
- Stull (1988): *Chapter 11*
- Tennekes and Driedonks (1981)
- Pino et al. (2003, 2006)

The following equations describe the growth of the boundary layer:

\[
\frac{\partial z_i}{\partial t} \approx w_e + w_s \tag{3.36}
\]

\[
\frac{\partial z_i}{\partial t} = \frac{w' \theta'_s - w' \theta'_e}{\gamma_\theta z_i} \tag{3.37}
\]

See also section 2.3. In this exercise we assume that subsidence \( w_s \) is negligible and the potential temperature lapse rate \( \gamma_\theta \) is constant.

We define *entrainment* as the intrusion and mixing of dry warm air from the free atmosphere into the mixed-layer, either by convective penetration of turbulent eddies or by the presence of shear stress at the inversion zone. The process whereby the boundary layer warms by surface heating alone, is called **encroachment**. In that case the ratio of the entrainment flux to the surface flux \( \beta \) is equal to 0 and the entrainment flux \( w' \theta'_e \approx 0 \). Notice that under this situation, the jump of the potential temperature at the entrainment zone is equal to zero.

1. What is the growth rate of the boundary layer for a value of the entrainment rate equal to 0.2, after a total run time of 10000 s?
2. What would be the growth rate after 10000 s in case only encroachment takes place?
3. Using the results in (2) and (3), how much does entrainment contribute to the total growth of the boundary layer?
   
   **Hint:** It is recommended to repeat exercise (2), but now prescribing a very small value for the jump of the potential temperature at the inversion, for instance \( \Delta \theta \approx 0.01 K \) (see also equation 3.30)
4. What is the influence of the initial *temperature inversion jump* \( \Delta \theta \) and the *potential temperature lapse rate* \( \gamma_\theta \) on the initial growth rate and the change of the growth rate during the model run? Perform a sensitivity analysis by:
• Using the default value;
• Doubling the default value;
• Specifying a very small value, etc.

*Hint:* Support your explanation with this expression for the entrainment flux that is used in the mixed-layer model:

\[ \overline{w' \theta'} = -w_e \cdot \Delta \theta \]  \hspace{1cm} (3.38)

and by keeping in mind that the surface fluxes are specified as constants in the model input. Include the relevant graphs in your discussion.

5. Show by integrating equation 3.37 given above that a convectively driven boundary layer grows with time according to \( z \sim t^{1/2} \). Does the mixed-layer model confirm the results?

6. Sensitivity of the boundary layer growth to large scale vertical subsidence. Find a value for the divergence (expression 3.29) where the boundary layer growth is approximately 0.
7 Exercise III: Influence of CBL dynamics on ozone formation

Suggested literature:

- Vilà-Guerau de Arellano et al. (2004)
- Jacob (1999): *Chapters 11 and 12*

All the results are visualized in the screen and the figures can be saved as a bmp file. You will find the output in the following files:

- *output_dyn*: time evolution of boundary layer dynamic variables: $h$, $\theta$ and $\Delta \theta$.
- *chem_conc*: time evolution of the reactants in the boundary layer
- *chem_photo*: time evolution of the photostationary state and photolysis rate

1. Boundary layer dynamics.

Let’s first analyze the time evolution of the main characteristics on the development of the atmospheric boundary layer. We will study first without the atmospheric compounds. We maintain all the variables fixed except the strength of the temperature inversion. Two cases are done: weak inversion (WI) with a potential temperature jump equal to 0.5 K and strong inversion (SI) with a potential temperature jump equal to 5 K.

Run the mixed-layer model for these two cases and answer the following questions:

a) Discuss the time evolution of $h$, $\theta$ and $\Delta \theta$.

b) For the case of strong inversion, explain the behaviour of the boundary layer variables between 6 local time (LT) and 10 LT. Discuss it in relation to the time evolution of $\Delta \theta$.

c) Discuss the implications of obtaining higher boundary layer height with respect to the concentration of the reactants.

2. Simple chemistry.

Simple chemistry system. Prescribe the following conditions:

- Constant photolysis rate.
- No emission of reactant compounds.
- Absence of entrainment.
- Only initial concentrations for $NO$, $O_3$ and $NO_2$. 

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Run the model for the two cases: (a) weak inversion and (b) strong inversion.

a) Plot the time evolution of the inert atmospheric compound, $NO$, $O_3$ and $NO_2$. Discuss the time evolution.

b) Why the ozone concentration evolution is constant on time? And the other species?

c) Explain the behaviour of the photostationary state.

3. The role of entrainment in the evolution of the inert tracer and ozone

Same conditions as at exercise 2, but now prescribing a mixing ratio difference for the inert and ozone between the free troposphere and the boundary layer.

a) Set up a case where the inert tracer is diluted by low mixing ratios transported from the free troposphere (positive entrainment flux) and $O_3$ is entrained (negative entrainment flux) into the boundary layer.

b) Analyze the main differences with respect the previous case: time evolution, difference weak and strong inversion, photostationary state.

c) What is the effect of strong temperature inversion on the entrainment of ozone at the early morning hours?

4. Emission of NO.

a) Maintaining the same case as in exercise 3, add now prescribing an emission of NO (for instance a rural value equal to 0.1 ppb (m/s)).

b) Discuss the main features with respect the previous case in terms of the boundary layer dynamics. Why ozone is decreasing in the early hours in the case of strong inversion?

c) Repeat the exercise by increasing the NO emission by a factor of 10. Discuss the main differences with the results of (a) and (b).

5. Daily variation of the photodissociation rate.

a) Same as exercise 4 (low NO emission), but now prescribing a diurnal variation of the photodissociation.

b) Discuss the main differences with respect the exercise 4. Under which case is the ozone production higher? Which is the chemical reaction most sensitive to the variation of the photodissociation rate?

c) By analyzing the tendencies of the mixing ratio at the end of the evolution, especluate which species will be formed and depleted during night conditions? What is the role of $NO_2$ during the night?

6. Complex chemistry. Standard case (same chemical conditions as exercise 4 with low NO emission). Run the model with the standard conditions of complex chemistry and constant photolysis rate under the conditions: (a) weak inversion and (b) strong inversion. Prescribe the following values for the emissions of NO and $RH$. 52
\[ E_{NO} = 0.1 \text{ ppb} (m/s) \]
\[ E_{RH} = 1.0 \text{ ppb} (m/s) \]

a) Is ozone produced in both cases? Compare the ozone production with the run done at exercise 4. Give an explanation from the point of view of the chemical mechanism.

b) What is the role of the reactants \( RH \), \( CO \) and \( OH \)?

c) What is the value of the photostationary state? Discuss your result.

d) Compare the evolution of ozone for the cases with weak and strong inversion. Does the boundary layer evolution influence the \( O_3 \)-diurnal variability?

7. Complex chemistry. High emission hydrocarbons.

Run the model with similar conditions as in the previous case, but now doubling the emissions of the hydrocarbons (\( RH \)).
a) Compare the results with the previous case and provide an explanation of the differences.

b) Why the nitrogen dioxide (\( NO_2 \)) is enhanced?

c) What happens with the time evolution of the \( NO \) concentration?


Run the case but now with the following emissions:

\[ E_{NO} = 1.0 \text{ ppb} (m/s) \]
\[ E_{RH} = 5. \text{ ppb} (m/s) \]

a) Describe the evolution of \( NO \), \( O_3 \) and \( NO_2 \). Give an explanation using the chemical mechanism.

b) Increase the emission of \( NO \) by 5. Compare the ozone evolution with case (a). Do we expect high values of ozone near very polluted areas?

9. Complex chemistry. Sensitivity to the reaction rate of hydrocarbons (reaction R5).

Run case 6, but now decreasing the chemical reaction rate of reaction R5 by a factor 10. You can do it by modifying the factor \( f \) on the screen.
a) Discuss the evolution of \( O_3 \), \( NO \), \( NO_2 \) and \( RH \). Do the slow reaction rate play a role on the ozone formation? What about the other species like \( RH \), \( OH \)?
Chapter 4

Practicum 4: Explicit and implicit filtering in large-eddy simulation

by Bernard Geurts

1 Exercises

The basis for a large-eddy formulation of a turbulent flow is a partial filter. In this exercise we analyze the basic operation of a filter and quantify its effect on numerical solutions of a Navier-Stokes equation.

1. Pen and paper consider the top-hat filter and express its operation in spectral space by focusing on the effect of filtering a Fourier mode. This will give you the Fourier-transform of the filter-kernel.

2. Pen and paper derive an expansion for the turbulent stress in terms of the filterwidth $\Delta$ of the filter. Under what conditions would you expect the second order truncation to be an accurate model for the turbulent stress tensor?

3. Pen and paper express an approximate inversion of the filter in terms of a geometric series. Analyze the lower order truncations of this inversion through its action on a Fourier mode. What generalized similarity model would you build from this? How does that relate to the truncation model of exercise b)?

4. Matlab use the matlab-script filter.m to visualize the effect of spatial filtering of a turbulent signal. What happens to the spectrum of the solution when the filterwidth $\Delta$ is increased? What would you consider a maximal filterwidth acceptable for accurately representing the turbulent flow? How does that relate to the spectrum?

In a large-eddy simulation the numerical method includes a spatial discretization. Often the spatial resolution is rather marginal and the spatial discretization method will contribute to the filtering of the solution. This is called implicit filtering.

5. Pen and paper. In one spatial dimension, consider second order central differencing and first order upwind discretization on a uniform grid with mesh-spacing $h$. Derive the numerical derivative of $\sin(kx)$ with either of these methods.
6. Pen and paper. What is the Fourier-transform of the filter-kernel, implied by these spatial discretizations?

7. Pen and paper. When would you consider the spatial discretizations to be accurate? Express your result in terms of \(kh\).

8. Pen and paper. When would you consider the implicit filtering irrelevant compared to the explicit filtering of a top-hat filter? Express your result in terms of \(?/h\).

9. Matlab. Use the matlab-script Qburgers.m R. Compare the numerical solution obtained with central differencing and upwind discretization. Vary the spatial resolution.

10. Matlab. Use the matlab-script Qburgers.m R. Adopt an eddy-viscosity model for the large-eddy simulation of the Burgers equation, in combination with central differencing. Is there a general similarity between this model and a low-resolution upwind discretization? How would you characterize that resemblance? What does it tell you about filterwidth and gridspacing that yield acceptable accuracy? What is the relevance of the subgrid model? And what of the spatial discretization?
Chapter 5

Practicum 5: Stable Boundary Layers

*Steve Derbyshire and Bob Beare*

1 Exercises

The stable BL exercises are designed to look at both steady and unsteady conditions. In both cases we will use a simple one-D model coded by Bob Beare, using a first-order turbulence closure with Richardson number dependence \((1 - Ri/Ri_c)^2\).

a) Steady stable BL

Run the one-D model based on a choice of geostrophic wind \(G = 10\text{ms}^{-1}\), Coriolis parameter \(f = 10^{-4}\text{s}^{-1}\). In subroutine bottom_boundary specify your choice of prescribed surface cooling rate (e.g. 0.5K/hour, 1, 2, ...)

How long does the model take to approach equilibrium? Plot the "equilibrium" surface heat-flux and \(u_\ast\) against cooling rate. What happens as the cooling-rate gets large?

b) Unsteady stable BL with surface coupling

In reality the surface may not cool steadily, but instead interacts with turbulence and other components of the surface energy balance. We now use a very simple soil model, treating it as a single layer with a heat capacity equivalent to a certain thickness of atmosphere: the ‘soil equivalent depth’.

In this exercise the student will vary the parameters IR (infra-red cooling) and SED (soil equivalent depth) via the namelist nml_1d_bl, and see under what circumstances the friction velocity falls to zero via e.g the following mechanism. Larger surface cooling leads to higher stability and then reduced surface heat flux, permitting larger surface cooling...

With the same \(G\) and \(f\) as before, try values such as SED=10m, IR=20Wm\(^{-2}\). Which parameter values allow the system to go into a low-turbulence regime?

c) Pen and paper exercise related to the equilibrium case

Nieuswstadt’s (1984) theory of a quasi-steady stable BL can be viewed as an asymptotic limit for the high-stability case. He derives relations in this limit of the form

\[
G/\upsilon_\ast \sim (1/kR_f)h/L
\]  

(5.1)
where $G$ is the geostrophic wind, $k$ the Karman constant, $h$ the BL depth and $L$ the Obukhov length. The theory assumes the flux Richardson number $R_f$ to be constant in this limiting regime.

Do Nieuwstadt’s equations remind you of any other standard BL formulae? Show that together they imply a relation between the surface buoyancy-flux $F_0$ and the geostrophic wind. How does this relate to your model results? What does it mean physically?

Hint: eliminate $h$ between the equations, and then use the definition of $L$. 
Bibliography


