The implementation of a Lagrangian Particle Dispersion Model in Large Eddy Simulations of the Atmospheric Boundary Layer

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Abstract

With the growing awareness of a possibly changing climate, more and more research is performed on the prediction of wheater systems. In order to make these predictions better, one has to understand, among many other things, the behaviour of small cumulus clouds. One of the ways to investigate shallow cumulus clouds, is by performing Large Eddy Simulations (LES). In an LES, the lowest few kilometers of the atmosphere are modelled.

A way to extend the possibilities of the research, is to develop a Lagrangian Particle Dispersion Model (LPDM), that has massless particles traveling through the domain. The LPDM, developed in this thesis, runs simultaneously with the LES and uses the intermediate output of the LES-velocities to calculate the new positions of the particles. Since these 3D-velocities are available only on a discrete grid, a 1st order linear interpolation scheme is used in space. With the interpolated velocities, a second order Adams-Bashfort scheme is used to calculate the new position of the particle. Simulations have been performed with over 10 million particles, where the LPDM-routine took about 30% of the total computation time. The LPDM has been validated by comparing Eulerian statistics obtained from the LES, to Lagrangian statistics obtained from the LPDM.

In the world of atmospheric researchers, there exists a controversy about, whether mixing of a cloud and the surrounding air can be described best by lateral mixing, or by vertical mixing. The main argument of people who defend the top-bottom mixing theory, is the conserved variable diagram, also called a Paluch diagram. In this thesis a simulation is performed using the LPDM where particles, that are present at the same height, at the same time, in the same cloud are tracked back in time. It is shown that the particles originate from all heights, with the majority originating from heights just below the observation height. This result gives good evidence for the lateral mixing concept to be the most appropriate for shallow cumulus clouds.
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Chapter 1

Introduction

Throughout history, mankind has always felt the need to predict the weather. Until the 20th century, the prediction of the weather was dominated by experience. People knew, by looking at the sky, whether to expect rain or sunshine. In the 18th and 19th century, meteorological research started to become more and more scientific. People tried to develop equations that describe the motion of a fluid. The first equation for an ideal fluid was already introduced in 1755, by Euler. This equation did not incorporate the effect of viscosity. The person who included the viscosity was Claude Navier, in 1822. The equations that are used nowadays were presented in 1845, by George Stokes. At that time, it was impossible to solve the so called Navier-Stokes equations. People who did research on the equations, could only work on the mathematics, in order to get towards a solution of the equations. With their work and with the invention of the computer it became possible to solve the discretized equations numerically. Performance was poor in the beginning, but, as computers became faster and faster, the accuracy of the meteorological models was increasing almost continuously.

1.1 The need for parameterization

In atmospheric modeling, the distinction can be made between global weather predictions and local weather predictions (usually called a General Circulation Model, GCM). The local predictions are conducted on a fine grid and have limited durability. On the opposite, the large scale models have a coarse grid and the simulation time is much larger than the few days of the local weather predictions. Depending on the goal, accuracy varies from moderate to poor. The grid of a global simulation has nowadays come to in the order of 10 km. With this grid size, it is impossible to account for any effect that has a scale that is smaller than 10 km.

1.2 Shallow cumulus clouds

Although there are numerous kinds of clouds, in this thesis only one kind of cloud is investigated. Shallow cumulus clouds are typically up to 1 km wide, while they can reach heights of 1-3 km. They have a cloud cover of under 20%, which means that the biggest part of the sky is clear blue sky. Shallow cumulus clouds are therefore also called ‘fair weather’ cumulus. Since these clouds are relatively small, they are not resolvable in a GCM. The incorporation of this type of clouds is very important, because these clouds tend to react
1.3 Large Eddy Simulations

There are two ways to increase knowledge of clouds. The first way is by performing measurements. These measurements can be performed by releasing balloons and by flying through clouds by aircraft, but in the last decades more and more measurements are performed by using satellite, radar, lidar, etcetera. The properties that are measured are temperature, density or moisture profiles; cloud droplet distributions, velocities and so on. These profiles can be used as initial conditions for numerical simulations or as a reference for the outcomes of simulations. This is the second method for the investigation of shallow cumulus clouds. In a Large Eddy Simulation (LES), the lowest few kilometers of the atmosphere are modelled. The grid size of the LES is in the order of $25 \times 25 \times 25$ m. This usually is enough to resolve most of the turbulence in the domain and it is good enough to resolve the largest clouds.

1.4 Motivation for Lagrangian statistics

In the investigation of clouds with LES, there are two problems that emerge. First the amount of data generated by the LES can be enormous, making research slow and (computationally) difficult. The second and for this thesis most important problem is that it is very difficult to see details in the movement of air. A way to overcome these problems and to extend the possibilities of the research, is to develop a Lagrangian Particle Dispersion Model (LPDM) that has massless particles traveling through the domain. With such a model one can, for example, look at a cloud and determine where the particles entered and exited the cloud. This could answer questions about the entrainment of dry air into a cloud. Another important field of research is the dispersion of pollutants in the atmosphere. An LPDM seems to be a natural way to investigate the dispersive properties of the atmosphere. Lamb [12] was the first to incorporate such a particle model into an LES in 1978. He compared his results to the experimental results of Willis and Deardorff [38]. Others have successfully followed this approach: e.g. Mason [21], Weil et al. [37], Gopalakrishnan and Avissar [10], Kim et al. [15] and Uliasz and Sorbjan [35].

1.5 The goal of the research

The goal of this thesis is to develop, implement, test and use an LPDM. The starting point is the resolved velocity field, as given by the LES. If there is a finite number of massless particles that is released into the domain, then these particles can be tracked in time, by moving the particles with the resolved velocities. To improve the results, a subgrid scheme is added, based on the results of Weil et al. [37] and Thomson [34]. The LPDM will be used to
look at the entrainment of dry air into a cloud, by means of an analysis presented by Paluch [22].

1.6 Structure of the report

The first chapter of this report gives a short introduction into the subject of research, along with the background of the research. In chapter 2 more details are given about the atmosphere and the LES. In this chapter the necessary variables and equations will also be treated. After this, chapter 3 will introduce the LPDM, as it is derived and implemented in the LES. After the implementation, in chapter 4 the performance and validity of the LPDM will be discussed. Chapter 5 will deal with an application of the LPDM to cumulus clouds. At the end, some conclusions will be presented, together with some recommendations for future research.
Chapter 2

The Atmospheric Boundary Layer

The atmosphere surrounding the earth can be divided into many layers (see figure 2.1). This research will focus on the lowest few kilometers of the atmosphere, called the Atmospheric Boundary Layer (ABL). Together with the free troposphere, the ABL makes up the troposphere. The ABL couples the effects of the surface to the upper regions and is therefore very important in weather prediction, pollution dispersion and many other topics. More information on the ABL can be found in e.g. Stull [33], Rogers and Yau [27] or Garratt [9].

![Figure 2.1: An overview of the layers of the atmosphere (Picture taken from kennislink.nl)](image)

From the surface upwards, the temperature is decreasing with height. The top of the ABL is determined by a strong increase in the temperature, called the inversion. Above the inversion is the free troposphere where the temperature is again slowly decreasing with height.
2.1 Definitions of meteorological quantities

The convective ABL is formed because the sun heats the surface. At places where the air is warmer than the surrounding air, the air will rise. If there is water vapor in the air, a turbulent updraft can cause the rising water vapor to condensate, thus forming clouds. A way to determine whether a buoyancy driven flow is turbulent or not, is to look at the Rayleigh number \( Ra \). This number is defined as:

\[
Ra = \frac{g \rho \alpha \Delta T d^3}{k \eta}.
\]  \hspace{1cm} (2.1)

Here \( g \) is the gravitational acceleration, \( \rho \) is the density of air, \( \alpha \) is the thermal conductivity, \( \Delta T \) is a temperature difference on a length scale \( d \), \( k \) is the thermal diffusivity and \( \eta \) is the dynamic viscosity. In the atmosphere, \( Ra \) is in the order of \( 10^{16} \), so flow will be turbulent. This can also be concluded by looking at the Reynolds number \( Re \):

\[
Re = \frac{\rho v d}{\eta}.
\]  \hspace{1cm} (2.2)

where \( v \) is a characteristic velocity. For atmospheric conditions, a Reynolds number of \( 10^7 \) can be expected. During the night there is a similar process going on, however with opposite result. Because of the radiative cooling of the surface, the air close to the surface is cooler than its surrounding, so the ABL is stabilized. This chapter will first introduce some quantities that are commonly used in meteorological science. When this is done, the formation of clouds can be explained. After this, the governing equations that are used in the LES will be given. Then the subgrid scheme, as implemented in the LES, will be treated. This is followed by two case descriptions and finally, there will be some extra information about the LES.

2.1 Definitions of meteorological quantities

It makes sense to express the variables used in the model into quantities that are conserved for adiabatic processes. In the warm ABL, there is no ice present. The relative water content can thus be defined as the sum of the relative amount of liquid water and the relative amount of vapor, present in the air:

\[
q_t = q_l + q_v,
\]  \hspace{1cm} (2.3)

where the relative amount represents a mass fraction. In order to derive the equation of state of the atmosphere, first the equation of state of dry air is given:

\[
p = \rho R_d T,
\]  \hspace{1cm} (2.4)

where \( R_d \) is the specific gas constant for dry air. This equation is known as the ideal gas law. It states that only two out of the three variables \( (p, T, \rho) \) are independent. For adiabatic processes, the temperature is not a conserved variable. It needs to be compensated for pressure changes. This effect can be eliminated by introducing the new, conserved variable, called the potential temperature:

\[
\theta = T \left( \frac{p}{p_0} \right)^{\frac{R_d}{c_p}}.
\]  \hspace{1cm} (2.5)
In this equation \( c_p \) is the specific heat of dry air. The derivation of \( \theta \) can be found in appendix A. \( \theta \) can be seen as the temperature that a parcel of air would have if it was brought adiabatically to the reference pressure \( p_0 \), in this thesis taken to be \( 10^5 \) Pa. If the air contains water vapor, there is another correction necessary to include the effects of phase changes. The new variable is the liquid potential temperature \( \theta_l \).

\[
\theta_l \approx \theta - \frac{L}{c_p} \left( \frac{p}{p_0} \right) \frac{R_d}{c_v} q_l,
\]

where \( L \) is the latent heat of vaporization. Now both \( \theta_l \) and \( q_l \) are conserved variables for adiabatic processes. Since the equation of state of dry air is no longer valid if there is water present, an equation of state for moist air has to be given:

\[
p \equiv \rho R_d T_v,
\]

where \( T_v \) is the virtual temperature, defined as follows:

\[
T_v = \left[ 1 - \left( 1 - \frac{1}{\epsilon} \right) q_v - q_l \right] T.
\]

In this equation, \( \epsilon \) is the ratio of \( R_d \) and \( R_v \). By introducing the virtual temperature, it is possible to keep working with the dry gas constant, instead of a changing ‘constant’. Furthermore, the effects of moisture on density can be captured in the introduction of the virtual potential temperature:

\[
\theta_v = T_v \left( \frac{p}{p_0} \right) \frac{R_d}{c_v},
\]

Finally, the lapse rate is also of importance in order to determine whether a parcel of air will move upwards or downwards, if it were to be released at a certain height:

\[
\Gamma_{\theta_v} = -\frac{d\theta_v}{dz}.
\]

The overline denotes a horizontal average.

### 2.2 Formation of shallow cumulus clouds

In this section, the physics behind the formation of clouds is given. On a sunny day, the sun heats up the surface and water evaporates. The surface warms up the air at the bottom of the ABL, so the warmed up air will move upward. In figure 2.2 there is a layer where the lapse rate of the dry air is bigger than the lapse rate of the environment. This layer is unstable and is therefore called the Convective Boundary Layer (CBL). This layer is turbulent until the ‘level of neutral buoyancy’ is reached. Above this level, the parcel of air that was moving upwards has negative buoyancy and is thus forced back into the CBL. If the parcel has enough momentum, then the parcel may overshoot this level and the parcel might reach the lifting condensation level. At this level the water vapor starts to condensate, thus forming a cloud. This happens because, during the rise of the parcel, the environmental temperature \( T \) has been gradually decreasing with height. In a condensation process, heat is released. If there is enough water present, this process can give the parcel of air enough
buoyancy to become once again positively buoyant. The level at which the parcel starts to become positively buoyant is called the level of free convection. From this level on, if there is enough water, the parcel of air will rise all the way to the top of the ABL. Above the level of zero buoyancy the parcel of air will become negatively buoyant again.

2.3 The governing equations

The equations that need to be solved are: the Navier-Stokes equations for the conservation of momentum, the conservation laws for heat, moisture and mass and the equation of state. The variables that are involved are: the three components of the velocity $\vec{u} = (u, v, w)$, the liquid water potential temperature $\theta_l$ and the total specific humidity $q_t$. In the coordinate system used here, the $x$ and $y$-directions make up a horizontal plane, whereas the $z$-direction is the vertical direction. For a complete description of the following equations, see e.g. Stull [33] or Garratt [9]. First, the Navier-Stokes equations for incompressible Newtonian fluids are given:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = X_i - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 u_i}{\partial x_j^2}; i, j \in [1, 3].$$

(2.11)

In this equation it is assumed that the density is constant. On the right hand side $X_i$ is the $i$-component of the external forces acting on the system. The second term is the pressure gradient force and the last term accounts for the viscous stress, with $\nu$ the kinematic viscosity. Since the Reynolds number is very large ($\approx 10^7$), in the remainder of this research the viscous stress term is neglected. The external forces include gravity and coriolis forces:

$$X_i = -\delta_{i3} g + \epsilon_{i3j} f_\varepsilon u_j + F_i.$$  

(2.12)
Here $\delta_{ij}$ is the Kronecker delta, $g$ is the gravitational acceleration, $\epsilon_{ij3}$ is the alternating unit tensor, $f_c$ is the Coriolis parameter and $F_i$ stands for any remaining external forces. In the tensors Einstein’s summation notation is used.

**The Boussinesq approximation** A further assumption that has to be made is called the Boussinesq approximation. This means that density fluctuations from the reference state are neglected in all terms of (2.11) except the external buoyancy forcing. This gives for the vertical component:

$$\frac{\partial w}{\partial t} + u_j \frac{\partial w}{\partial x_j} = g \frac{\theta'_v}{\Theta^0_v} - \frac{1}{\rho_0} \frac{\partial p'}{\partial z} + F_z.$$  \hspace{1cm} (2.13)

Here the superscript $'$ stands for a perturbation from the reference state of hydrostatic equilibrium, $\Theta^0_v$ is a reference value of $\theta_v$. It is assumed that perturbations of the pressure are much smaller than temperature or density fluctuations. The equations for the conserved variables $q_t$ and $\theta_l$ are:

$$\frac{\partial q_t}{\partial t} + u_j \frac{\partial q_t}{\partial x_j} = F_{q_t},$$  \hspace{1cm} (2.14)

$$\frac{\partial \theta_l}{\partial t} + u_j \frac{\partial \theta_l}{\partial x_j} = F_{\theta_l}.$$  \hspace{1cm} (2.15)

In these equations, $F_{q_t}$ represents the sources and sinks of moisture that can be present in the domain. An example is precipitation. Remember that in phase changes $q_t$ is conserved, so they are not in this term. Similar to this, $F_{\theta_l}$ contains the heating and cooling forcings, such as results from radiative flux divergence. The equations that make the set of governing equations complete are the mass conservation law:

$$\frac{\partial u_i}{\partial x_i} = 0$$  \hspace{1cm} (2.16)

and the equation of state, (2.7).

### 2.4 Large Eddy Simulations of the ABL

This thesis uses the method of LES to solve the equations presented in section 2.3. Since these equations cannot be solved directly, because that would require too much computer power, further approximations have to be made. The equations described in the previous section, will be filtered. This means that all variables are divided in a filtered part and a fluctuating, subfilter part.

$$\phi = \tilde{\phi} + \phi'.$$  \hspace{1cm} (2.17)

The widetilde denotes a filtered variable and the accent denotes a deviation from this value. After this filtering operation, the variables are sampled, since the equations can only be solved for a finite number of grid points. The impact of the unresolved motions needs to be modelled. The names subgrid and subfilter lie close together in meaning and are often used interchangeably. In the remainder of this thesis the name subgrid will be used. The subgrid
2.5 Subgrid scale model

model used in the LES is the diffusive-type model of section 2.5. It is possible to transform equation 2.11 into an equation for the filtered variables:

\[
\frac{\partial \tilde{u}_i}{\partial t} + \tilde{u}_j \frac{\partial \tilde{u}_i}{\partial x_j} = -\delta_{i3} g \frac{\partial \tilde{\theta}'}{\partial x_3} + \epsilon_{ij3} f c \tilde{u}_j + \tilde{F}_i - \frac{1}{\rho_0} \frac{\partial \overline{\rho \tilde{u}_i'}}{\partial x_i} - \frac{\partial \tilde{u}_i' \tilde{u}_j'}{\partial x_j}. \tag{2.18}
\]

This equation can be used in a model, describing the atmosphere. The last term in the equation represents the impact of subgrid fluctuations on the mean variables and needs to be modeled. The LES-equations for the conserved variables \( q_t \) and \( \theta_l \) are:

\[
\frac{\partial \tilde{q}_t}{\partial t} + \tilde{u}_j \frac{\partial \tilde{q}_t}{\partial x_j} = F_{q_t} - \frac{\partial \tilde{u}_j' q_t'}{\partial x_j}, \tag{2.19}
\]

\[
\frac{\partial \tilde{\theta}_l}{\partial t} + \tilde{u}_j \frac{\partial \tilde{\theta}_l}{\partial x_j} = F_{\theta_l} - \frac{\partial \tilde{u}_j' \theta_l'}{\partial x_j}. \tag{2.20}
\]

The last term of these equations also needs to be modeled. The mass conservation law in Boussinesq approximation becomes:

\[
\frac{\partial \tilde{u}_i}{\partial x_i} = 0. \tag{2.21}
\]

2.5 Subgrid scale model

Unfortunately, the complete set of equations, as described in the previous section, can not be solved yet. This is because of the higher order terms in equations 2.18, 2.19 and 2.20. These equations contain an average over the product of two perturbations. This (co)variance is called a second order moment. All equations that are to predict a certain moment, must contain higher order moments. This problem is known as the closure problem. The way to handle this problem is to parameterize the influences, that subgrid terms have on the resolved variables. For equation 2.18 the model of the turbulent flux looks like this:

\[
\tilde{u}_i' \tilde{u}_j' = -K_m \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right). \tag{2.22}
\]

The higher order moment is now replaced by the local gradient of the mean variable. The closure model acts as a diffusion process. The eddy viscosity \( K_m \) is unknown and has to be modelled:

\[
K_m = C_e \lambda \sqrt{\varepsilon}. \tag{2.23}
\]

In this equation, \( C_e \) is a function of the Kolmogorov constant. \( \lambda \) is a mixing length scale and is for now assumed to be proportional to the grid size of the domain:

\[
\Delta = (\Delta x \Delta y \Delta z)^{\frac{1}{3}}, \tag{2.24}
\]

where \( \varepsilon \) is the subgrid turbulent kinetic energy (TKE), defined as:

\[
\varepsilon = \frac{1}{2} \sum_i \tilde{u}_i'^2. \tag{2.25}
\]
2. The Atmospheric Boundary Layer

Since $u_i'$ is not known, an equation for the subgrid TKE must be solved:

$$\frac{\partial e^{1/2}}{\partial t} + \tilde{u}_j \frac{\partial e^{1/2}}{\partial x_j} = \frac{1}{2e^{1/2}} \left( -\tilde{u}_i' \tilde{u}_i' \frac{\partial \tilde{u}_i'}{\partial x_j} + \frac{g}{\Theta_0} w' \theta' v \right) - \frac{\partial}{\partial x_j} \left( 2K_m \frac{\partial e^{1/2}}{\partial x_j} \right) - \frac{\epsilon}{2e^{1/2}}. \tag{2.26}$$

Because in other equations $e^{1/2}$ is used instead of $e$, the equation is written in such a way that $e^{1/2}$ is solved. In equations 2.19 and 2.20 the eddy diffusivity $K_\phi$ is defined and modelled as follows:

$$\tilde{u}_i' \phi' = -K_\phi \frac{\partial \phi}{\partial x_i}. \tag{2.27}$$

In this equation, $\phi$ is either $\theta_l$ or $q_t$. The eddy diffusivities for the conserved variables are related to $K_m$ by the turbulence Prandtl number $Pr$:

$$K_{\theta_l} = K_{q_t} = Pr^{-1} K_m. \tag{2.28}$$

The Prandtl number is an approximation of the ratio of momentum diffusivity and thermal diffusivity. In the LES, a Prandtl number is used of $\frac{1}{3}$. Furthermore, the dissipation rate $\epsilon$ can be modelled by:

$$\epsilon = \frac{c_\epsilon e^{2/3}}{\lambda}, \tag{2.29}$$

where $c_\epsilon$ is given by:

$$c_\epsilon = c_{\epsilon,1} + c_{\epsilon,2} \frac{\lambda}{\Delta}. \tag{2.30}$$

For the $\lambda$ in these equations the grid size $\Delta$ is used in case of turbulence. For the stable flow ($\frac{\partial \theta_v}{\partial z} > 0$) a correction must be made, so $\lambda$ is taken to be:

$$\lambda = \min \left( \Delta, c_N \frac{e^{1/2}}{N} \right), \tag{2.31}$$

$$N^2 = \frac{g}{\Theta_0} \frac{\partial \theta_v}{\partial z}.$$

The $N^2$ mentioned above is called the Brunt-Väisälä frequency. This frequency is a measure for the strength of the stratification. In the LES used in this thesis, $c_{\epsilon,1} = 0.19$, $c_{\epsilon,2} = 0.51$ and $c_N = 0.76$.

2.6 Case description

In this thesis two cases are used. One is the cloudy BOMEX-case, the other is a clear CBL-case. The cases differ, amongst others, in the initial and boundary conditions of the LES and in the large scale forcing that is applied. Now more details will be given about the cases.
BOMEX  The Barbados Oceanographic and Meteorological EXperiment was conducted in 1969 in the ABL above the ocean, east of Barbados. In this experiment, a fleet of 5 ships measured the surface fluxes, while every 90 minutes a sonde was released to measure the vertical profiles of temperature, moisture and wind. The results of these measurements are used as an initial condition for the LES, see Siebesma et al. [29]. Here the domain size was $6.4 \times 6.4 \times 3.2$ km. The grid resolution varied from $64 \times 64 \times 80$ points, with a timestep of 2 seconds in test cases, to $256 \times 256 \times 160$, with a timestep of 1 second in detailed simulations. A dry well-mixed layer of about 500 m height is topped by a conditionally unstable cloud layer, which in turn is capped by a stable inversion at 2000 m. A central differencing scheme is used to calculate the advection of the scalar quantities. Because the BOMEX case has a dominating wind in one direction, a Galilei transformation is performed. This means that the mean wind is subtracted from the local wind velocities.

CBL  The domain size of the simulations of a Convective Boundary Layer were somewhat smaller. The size was $3.2 \times 3.2 \times 1.2$ km, with a resolution of $32 \times 32 \times 48$. The timestep is taken to be 1 s. In this case no clouds can be formed, since there is not enough water in the air, so only the dry, well-mixed layer is present. This layer is about 775 m high and is confined by an inversion with a strength of about 5 K. In this case the so called κ-scheme is used to calculate the advection of the scalars. More information on this scheme can be found in Hundsdorfer et al. [11]. The relative simplicity of the CBL should make it a good candidate for test applications.

2.7 Boundary and initial conditions

The boundary and initial conditions of the LES are as follows:

at the bottom  At the bottom of the LES, no-slip conditions for velocities are applied. This means that $\tilde{u} = \tilde{v} = \tilde{w} = 0$. The total specific humidity flux and the liquid water potential temperature flux are set to a ground level value: $\phi_{q_t,\text{surface}}$ and $\phi_{\theta_l,\text{surface}}$. Values that are defined at the cell centers need to be extrapolated towards the bottom of the domain.

At the top  At the top of the LES, a free surface boundary condition is applied. The vertical derivatives of the horizontal velocities are set to zero, together with the vertical velocity and the sgs-TKE. This gives $\frac{\partial \tilde{u}}{\partial z} = 0$, $\frac{\partial \tilde{v}}{\partial z} = 0$, $\tilde{w} = 0$ and $\tilde{e} = 0$. For the total specific humidity and the liquid water potential temperature, the vertical derivative is set to a constant: $\frac{\partial \phi_{q_t}}{\partial z} = c_1$, $\frac{\partial \phi_{\theta_l}}{\partial z} = c_2$. Values that are defined at the cell centers need to be extrapolated towards the top of the domain.

At the sides  At the sides of the LES, periodic boundary conditions are applied, for all variables.

At the start  The begin conditions are as mentioned in the previous section. All variables are set planewise with values derived from experiments. Because the initial state of the system is completely uniform at every height, nothing would happen if the surface fluxes were turned on. The heat and water that are added at the surface would have to be transported upwards by diffusion, because there can only be convection (in a closed system) if
there is an initial perturbation of the system. In practice this would mean that the computer accuracy would be dominating in the emergence of turbulence. This would imply a strong dependency on the used computer. In order to prevent this undesired effect, small random perturbations are added in both $q_l$ and $\theta_l$. Since the discrete starting values are not an exact physical description of the initial state of the system, the system needs some time to stabilize itself after a startup. Usually the first three hours of simulation are neglected.

2.8 Remaining properties

The timestep In order to choose a timestep, the criterion is used that the Courant number ($Co$) should be smaller than 1. This dimensionless number is defined as follows:

$$Co = \frac{v_{max}dt}{\min(\Delta x, \Delta y, \Delta z)}.$$  \hspace{1cm} (2.32)

In both cases, the velocities are always smaller than $10 \, ms^{-1}$. For a smallest grid size of 20 $m$ (in vertical direction), the timestep should be smaller than 2 seconds, hence a timestep of 1 second was used in the detailed simulations.

The parallelization To speed up the simulation, the LES-code is parallelized so that there can be multiple processors working on a simulation. This is done by dividing the domain of the LES into $n$ parts, where $n$ stands for the number of processors (usually a power of 2). The division of the domain takes place in the $y$-direction. The consequence of the division is that variables at the edge of the sub-domains should be communicated after every timestep of the LES.

Staggered grid The LES has a staggered grid implemented in order to avoid oscillatory effects, that appear if every variable is calculated at the same position, at regular distances. A staggered grid means that a velocity is defined at the face of a gridbox. The other variables, like the temperature, pressure and water content, are defined in the center of the gridbox.
2.8 Remaining properties
Chapter 3

Lagrangian Particle Dispersion Model

The usage of Lagrangian Stochastic models is very common in atmospheric science. Many research groups from all over the world are (or were) using this kind of model. In such a model the trajectories of massless particles are calculated by means of a random-walk scheme. This means that the Navier-Stokes equations from equation 2.11 are not solved, but the particle motion is described by using a statistical description of the random velocity field. See for examples of these atmospheric stochastic models e.g. Wilson and Sawford [39], Kos et al. [18], Rao [24], Franzese et al. [8], Stohl and Thomson [32], Warland and Thurtell [36], Kljun et al. [16], Stohl et al. [31], K. Luhar and Britter [13], Reynolds and Iacono [25], Borgas and Sawford [3], Sawford and Yeung [23], Das and Durbin [6] and Du et al. [7]. The principle has also been applied in oceanographic research by Brickman and Smith [4].

Another way of investigation of turbulent flows, is the application of particle tracking. Now the particles are moved by a velocity field that is calculated by solving the Navier-Stokes equations. Research on particle tracking has been performed by, amongst others: Kenwright and Lane [14], Darmofal and Haimes [5] and Lane [20]. A combination of Direct Numerical Simulation (DNS) and particle tracking has been investigated by Yeung and Pope [40] and Kontomaris et al. [17]. Unfortunately, DNS is not possible in the atmosphere, because of the high Reynolds number of $\sim 10^7$.

3.1 Particle tracking in an LES

The main goal in this thesis is to implement a Lagrangian Particle Dispersion Model (LPDM) into the LES in order to calculate the particle trajectories online. This idea is also applied by, amongst others: Mason [21], Weil et al. [37], Gopalakrishnan and Avissar [11], Kim et al. [15] and Uliasz and Sorbjan [35]. The particles are massless and infinitesimally small. The particle subroutine will run parallel to the LES, so that at every moment, it is possible to get an output from the particle scheme, together with the output of the LES. It is also necessary to parallelize the particle scheme to be able to track as many particles as possible, without slowing the LES down for too much. The equation that needs to be solved in order to track a particle is the following:

$$\frac{dx_{i,p}}{dt} = \tilde{u}_i(x_p, t)$$  \hfill (3.1)

Where $\tilde{u}_i$ are the resolved velocities in the $x$-, $y$- and $z$-direction and $x_p$ are the coordinates of the particle. With the resolved velocities at every gridpoint at hand, from the LES, there
3.2 The interpolation scheme

are four important points of attention. These are:

1. spatial interpolation scheme
2. integration scheme
3. subgrid scheme
4. boundary handling scheme

At every timestep, the LPDM obtains the discrete, resolved velocities in three directions from the LES. After this, the LPDM has to interpolate these velocities for each particle, because the particles can move freely between the gridpoints. Then the new positions of the particles are calculated using the integration scheme. Since the LES only gives the resolved velocities, there is need for an extra scheme to account for the influence of subgrid turbulence. The input velocities for the integration scheme are divided into a resolved and a subgrid part. At the end of the LPDM, the boundary handling scheme makes sure that the particles stay within the domain of the LES.

3.2 The interpolation scheme

A point of attention in interpolation is that the LES employs a staggered grid. This means that a velocity is defined at all faces. The other variables, like the temperature, pressure and water content, are defined in the center of the gridbox, see figure 3.1. Although this looks complicated, it turns out that for 1 velocity component, a staggered grid turns into a shifted regular grid.

Figure 3.1: An illustration of a staggered grid in 2D.

Although there are many sophisticated interpolation schemes available from literature, in
the LPDM, a simple tri-linear interpolation scheme is used:

\[ u_p = (1 - dx) (1 - dy) (1 - dz) \quad u_A \]
\[ + \quad dx (1 - dy) (1 - dz) \quad u_B \]
\[ + \quad dx dy (1 - dz) \quad u_C \]
\[ + \quad (1 - dx) dy (1 - dz) \quad u_D \]
\[ + \quad (1 - dx) (1 - dy) dz \quad u_E \]
\[ + \quad dx (1 - dy) dz \quad u_F \]
\[ + \quad dx dy dz \quad u_G \]
\[ + \quad (1 - dx) dy dz \quad u_H . \]

Here the \( u_X \) are defined as shown in figure 3.2. There can be up to 10 million particles in the domain and if the simulation lasts for several hours, with a timestep of 2 seconds, then a complicated interpolation scheme like cubic splines, might take too much computation time, compared to the time needed to compute a timestep in the LES. Some tests will be performed in order to see whether the used interpolation scheme is sufficient in accuracy. These tests will involve the calculation of horizontally averaged statistics, by putting particles at a rigid position at either the center, or at an edge of a gridbox. Since the particles can not move, any difference in statistics will then be caused by the interpolation scheme. The results can be found in the next chapter.

### 3.3 The integration scheme

With the right velocities at hand, it is possible to make an estimate for the particle position after one timestep. There are numerous ways to do so, the simplest being Euler’s integration scheme:

\[ x_{i,n+1} = x_{i,n} + v_i(\overline{x_n}, t) dt \]
3.3 The integration scheme

Now the 1st order Euler-scheme is not the best scheme available. There are many different, higher order schemes that will allow the particles to follow the local streamlines in a better way. A few commonly used schemes are:

\[ x_{i,n+1}^* = x_{i,n} + v_i(\vec{x}_n, t)dt \]  \hspace{1cm} (3.4)

\[ x_{i,n+1} = x_{i,n} + \frac{1}{2} \left( v_i(\vec{x}_n, t) + v_i(\vec{x}_n^*, t) \right) dt \]

This method is called Heun’s method, also known as a 2nd order Runge-Kutta method. Another popular, second order method is the Adams-Bashfort scheme:

\[ x_{i,n+1} = x_{i,n} + \left[ \frac{3}{2} v_i(\vec{x}_n) - \frac{1}{2} v_i(\vec{x}_{n-1}) \right] dt \]  \hspace{1cm} (3.5)

Finally, the 4th order Runge-Kutta scheme has to be mentioned, as it is the most common 4th order interpolation scheme:

\[ k_1 = v_i(\vec{x}_n, t)dt, \]  \hspace{1cm} (3.6)

\[ k_2 = v_i(\vec{x}_n + \frac{1}{2} k_1, t + \frac{1}{2} dt)dt, \]  \hspace{1cm} (3.7)

\[ k_3 = v_i(\vec{x}_n + \frac{1}{2} k_2, t + \frac{1}{2} dt)dt, \]

\[ k_4 = v_i(\vec{x}_n + k_3, t + dt)dt, \]

\[ x_{i,n+1} = x_{i,n} + \frac{1}{6} (k_1 + 2k_2 + 2k_3 + k_4). \]

Although this thesis does not go into the details of the different integration schemes, a few general comments on the integration schemes can be formulated:

- speed
- accuracy
- stability
- applicability

**speed** The integration scheme has to be used at every timestep of the particle subroutine and for every particle. Since the number of particles is usually very high (>100,000) in order to maintain statistical convergence, it becomes very important for any scheme involved in tracking the particles to be as fast as possible. As an example: a detailed simulation carried 1.3 million particles and the integration scheme was called 3 times at every timestep of the LPDM, while the simulation lasted for 15 hours. This example gives a total number of loops through the integration scheme of about 10^{11}. The demand for a fast algorithm points towards the simple Euler scheme. A higher order scheme will take more time. The goal is to have the LPDM using no more than 50% of the total computation time.

**accuracy** In general higher order integration schemes will be more accurate. This makes it very likely that the fast 1st order Euler scheme will give poor results. The demand for accuracy is conflicting with the demand for speed. Fortunately there is a limit on this. Since the velocities, that are the input of the integration scheme, are filtered in the LES, there are no rapid changes in the velocity possible. In this thesis, some tests are performed to see...
whether the 2nd order Adams-Bashfort scheme is indeed outperforming the 1st order Euler scheme and whether it is good enough to be used in production runs. If it turns out that the 2nd order Adams-Bashfort scheme is performing better than the 1st order Euler scheme, then it might become necessary to implement a 4th order scheme (e.g. Runge-Kutta), to see if that would further increase the performance of the LPDM. The tests will be described in the next chapter.

**stability**  In order to make the LPDM unstable, the velocity that is used to advect the particles must become infinite. In the LPDM this velocity is interpolated from the velocities that are resolved in the LES. This means that if the LES is stable, then the LPDM is stable. In this thesis the LES is assumed to be stable, so there were no problems regarding the stability of the integration schemes.

**applicability**  This requirement concerns the discretization of the velocity field in time. Some integration schemes require more than 1 velocity field (e.g. Heun, 4th order Runge-Kutta) per timestep. These intermediate velocity fields are not present in LES, unless the timestep of the particle scheme is chosen twice the timestep of the LES. But then it is highly questionable if the increased accuracy of the 2nd order integration method, will balance the decreased performance due to the larger timestep.

In the LPDM, there are 3 options for the integration scheme available. These are: the 1st order Euler scheme, the 2nd order Heun scheme and the 2nd order Adams-Bashfort scheme. It is now possible to choose per simulation, which scheme will be used. Because of the modular approach, it is very easy to add more integration schemes into the subroutine in the future.

### 3.4 The subgrid scheme

Although there is already a subgrid scheme present in the LES, a second subgrid scheme is needed for the LPDM. This is due to the fact that the input to the particle subroutine consists of resolved velocities, that are unable to fully describe the particle motions. Especially at the bottom of the domain and at the inversion, there is a lot of subgrid turbulence that is not resolved by the LES. A criterion for an subgrid scheme is that particles that are uniformly spread in the domain, should remain uniformly distributed. In order to meet this well-mixed condition, a Langevin model is adopted based on the research of Thomson [34]. An adaptation towards LES has been made by Weil et al. [37]. For more information on Langevin equations and solving them by means of solving the Fokker-Planck equation, see e.g. Pope [23].

The equation that needs to be solved is (3.1). In this equation \( \tilde{u}_i \) stands for the filtered velocity. The velocity that is used to advect a particle, is composed of a resolved part and a fluctuating, subgrid part. This will lead to an expansion of equation (3.1):

\[
\frac{dx_{i,p}}{dt} = \tilde{u}_i(x_{p}; t) + u'_i(x_{p}; t),
\]

(3.8)

where the \( \tilde{u}_i \) are resolved by the LES. The random subgrid velocity components \( u'_i \) are assumed to behave as a Markov process. This means that the velocity at the next timestep is
3.4 The subgrid scheme

a function of the velocity at the present timestep. From theory it follows that the evolution of $u'_i$ can then be described by the following stochastic differential equations (also called a Langevin equation):

$$\begin{align*}
du'_i &= a_i(\vec{x}, \overline{u}, t)dt + b_{ij}(\vec{x}, \overline{u}, t)d\xi_j,
\end{align*}$$

(3.9)

where $a$ and $b$ are functions of $\vec{x}$, $\overline{u}$ and $t$. The total velocity $\overline{u}$ is the sum of the resolved velocity and the subgrid velocity. The $d\xi_j$ is a component of a Gaussian white noise. The $b_{ij}$ term determines the distribution of the random velocity forcing and is chosen to be consistent with the Lagrangian structure function in the inertial subrange:

$$b_{ij} = (C_0 \epsilon)^{1/2}.$$  

(3.10)

The $C_0$ is the Langevin-model constant ($= 4 \pm 2$; Thomson [34], $4.3 \pm 0.3$; Rizza et al. [26]), $\epsilon$ is the dissipation rate. The density function of the phase-space (i.e. ($\vec{x}$, $\overline{u}$)-space) distribution of the particles will be denoted by $f(\vec{x}, \overline{u}, t)$. For a Gaussian random forcing, the $a_i$ term has to satisfy the Fokker-Planck equation. This equation governs the evolution of the Lagrangian PDF ($f_L(\vec{x}, \overline{u}, t)$) in phase space and gives the solution to a stochastic differential equation:

$$\frac{\partial f_L}{\partial t} = \frac{1}{T_L} \frac{\partial(\overline{u} f_L)}{\partial \overline{u}} + \frac{\sigma^2}{T_L} \frac{\partial^2 f_L}{\partial \overline{u}^2}. 
$$

(3.11)

Here $\overline{u}$ is the total velocity and $T_L$ is the Lagrangian time scale. For a well-mixed distribution, the Lagrangian PDF should be equal to the Eulerian PDF, since if the particles are well-mixed, then the particles completely fill the domain in both cases, thus giving identical results. Thomson argues, that the $a_i$ term in equation 3.9 can be calculated from the Fokker-Planck equation using the Eulerian PDF. More information about the derivation can be found in Thomson [34]. In Weil et al. [37], the following equation for the subgrid velocities is derived:

$$\begin{align*}
du'_i &= -f_s C_0 \epsilon u'_i \frac{\sigma^2_{sgs}}{2\sigma^2_{av}} dt + \frac{1}{2} \left( \frac{1}{\sigma^2_{sgs}} \frac{d\sigma^2_{sgs}}{dt} u'_i + \frac{\partial \sigma^2_{sgs}}{\partial x_i} \right) dt + (f_s C_0 \epsilon)^{1/2} d\xi_i.
\end{align*}$$

(3.12)

Here $f_s$ is a coefficient that takes into account that there is no need to model the entire velocity, since there is already a part resolved by the LES. The variance of the subgrid velocity, $\sigma^2_{sgs}$ is equal to $\frac{2}{3} \epsilon$, where $\epsilon$ is the subgrid turbulent kinetic energy. A parameterization of $f_s$ is given by:

$$f_s = \frac{\sigma^2_{sgs}}{\sigma^2_{av} + \sigma^2_{sgs}},$$

(3.13)

where the overline means an average over a horizontal plane. The $\overline{\sigma^2_{av}}$ is the horizontally averaged resolved variance:

$$\overline{\sigma^2_{av}} = \frac{1}{3} \sum_i (\overline{u_i} - \overline{\overline{u}})^2.$$ 

(3.14)

The form of equation 3.12 is equal to the form of a Langevin equation. The first term is a viscous term that tends to diminish the velocity fluctuations. The second term relates the particle velocity to the subgrid TKE. This relation is important, since the subgrid TKE is a measure for the amount of unresolved turbulence. Finally, the last term gives a random fluctuation similar to Brownian motion.
3. Lagrangian Particle Dispersion Model

3.5 The boundary handling scheme

The boundary conditions for the particles are related to the boundary conditions of the LES. Relevant for the particles are:

- at bottom: no-slip conditions, \( \tilde{u} = \tilde{v} = \tilde{w} = 0 \)
- at top: free surface, \( \frac{\partial \tilde{u}}{\partial z} = 0, \frac{\partial \tilde{v}}{\partial z} = 0, \tilde{w} = 0 \)
- at sides: periodic boundary conditions

Near the bottom and at the top, linear interpolation will take place between nearest grid-points and the boundary. Furthermore, at the bottom and at the top of the domain, particles that hit the boundary will be perfectly reflected. Note that the possibility of massless particles hitting the boundaries is only possible in combination with a very large timestep or with the use of the subgrid model. The no-slip conditions at the bottom, gives rise to relatively large gradients in the lowest grid boxes, since any velocity goes from any value to zero in the lowest grid box. The main goal of the top boundary condition is to prevent a particle from moving outside the domain.

Like in the LES, the parallelization makes the handling of the boundary conditions in the y-direction a little bit different from that in the x-direction. If a particle moves across the upper boundary in x-direction, then it comes in at the lower boundary again. In the y-direction, the particle that moves across the upper boundary, is moved to the next processor and comes in from the lower boundary again. In order to cope with the problem of individual processors having a changing number of particles, a dynamic list structure was used for particles at every processor. With this so called linked list the movement of particles between processors became easier. A particle crossing the y-boundary will be removed from the list of the old processor and then added to the list of the new processor. Every list contains as many records as there are particles inside the domain of the processor, while every record consists of as many entries as wished. The boundary handling scheme also has to be called for intermediate results (necessary for some interpolation schemes, e.g. Heun), because a new velocity can only be calculated, if a particle is inside the domain of the LES.
3.5 The boundary handling scheme
Chapter 4

Validation of the \textit{LPDM}

After the implementation of the particle routine, the question remains whether the particles do accurately follow the local streamlines. It is not obvious that a complicated scheme as described in the previous chapter, will give good results. Several criteria can be formulated in order to get a grip on the accuracy of the \textit{LPDM}. These criteria can be divided into three groups:

1. The particle routine should be stable.

2. Particles that begin uniformly distributed, must stay that way. (This is the well-mixed condition, as mentioned in section 3.4)

3. If the particles are uniformly distributed, they should give the same statistics in Lagrangian way, as they would in an Eulerian frame.

In the remainder of this chapter these criteria will be used as a guideline in order to validate the \textit{LPDM} within the framework of the \textit{LES}. At the end of this chapter, some information will be given about the time consumption of the \textit{LPDM}.

4.1 Stability of the particle scheme

Although this requirement sounds rather simple, it is of the greatest importance, because the particle routine would be useless if there were any regions where the solution of the particle advection scheme would be unstable. Fortunately, the scheme has proven itself to be stable. Simulations of high resolution, carrying over a million particles had no problems reaching the end of the simulation. No particles were found having velocities in excess of the expected maximum velocity of 8 \textit{m/s}. However, when the particle routine was executed with the CBL initial conditions, there were serious problems regarding the stability of the \textit{LPDM}. It was found that there was a problem in combining the $\kappa$-scheme that is used in CBL simulations, with the sgs-scheme of the \textit{LPDM}. A $\kappa$-scheme is designed to advect scalars (e.g. $q_t$, $c$), in such a way that the scalar can never become negative. This keeps the \textit{LES} free from negative amounts of water or negative amounts of sgs-TKE.

The problem can be explained by looking at figure 4.1. In this figure, the line after 1 hour shows that the variable $f_s$ (equation 3.13) has a peak above the inversion height. This peak is induced by the fact that the sgs-variances go to zero in a slower way than the resolved-variances, above the inversion. Now the $\kappa$-scheme, that is used as an advection scheme
inside the LES is a dissipative scheme, hence it destroys some of the sgs-variances, so that the sgs-variances go to zero faster than they should and thereby the $f_s$ parameter goes to zero instead of having a peak. This is shown by the line after 10 hours. The fact that the $f_s$ parameter becomes equal to zero, means that the 1st term and the last term in equation 3.12 also become equal to zero. Because the only remaining term makes the velocity grow each time it is calculated, the LPDM became unstable. In this thesis the problem was solved by manually setting $f_s = 1$ for all cases. This means that the LPDM as used in this thesis is positioned in the middle of the models as posed by Weil et al. [37] and Thomson [34]. Thomson mimics all particle motion by a stochastic process, whereas Weil lets only the part that is not resolved in the LES be determined by a stochastic process. Although this adjustment seems a bit harsh, the scheme was again found to be stable. However, it may have an influence on the well-mixed condition or on statistics, derived from the LPDM.

### 4.2 The well-mixed condition

To check whether the LPDM satisfied the well-mixed condition, as posed by Thomson [34], a BOMEX-simulation was performed, containing over 10,000,000 particles in a domain of $256 \times 256 \times 160$ grid points. The domain was divided into 160 layers. At every timestep, the number of particles in every layer was counted. The simulation without the subgrid scheme resulted in figure 4.2. As can be seen in the figure, there is a large amount of particles at the bottom of the domain. This surplus of particles is grows in time to an amount of approximately 50%, where it stabilizes. It is clear that up to a relative height of 0.4 there is an influence on the number of particles present at every height. After the implementation of the subgrid scheme, the test was repeated. Figure 4.3 shows that only at the bottom there is a small surplus of particles of about 5%. This behavior is stable in time, so the LPDM is performing quite well with regard to the well-mixed condition. This is not perfect, but it is sufficient for current use, as the main application of this LES is the bulk of the domain.
4. Validation of the LPDM

Figure 4.2: The relative number of particles as a function of height as a result of a simulation without the subgrid scheme. The height is normalized with the height of the inversion, \( z_i = 2000 \) m. The reference number of particles is 65536 (256 \( \times \) 256).

It is also believed, that with the addition of a more physical surface handling scheme (e.g. Monin-Obukhov), this deficiency of the LPDM could be further reduced. A Monin-Obukhov scheme would include a logarithmic decay of velocities towards the bottom of the domain if the ABL were neutral. Since the ABL is (in this study) far from neutral, the profiles would slightly deviate from the logarithmic curve.

Figure 4.3: The relative number of particles as a function of height as a result of a simulation with the subgrid scheme. The height is normalized with the height of the inversion, \( z_i = 2000 \) m. The reference number of particles is 65536 (256 \( \times \) 256).
4.3 Comparison of Eulerian-Lagrangian statistics

When the particles are uniformly distributed and if there are enough particles, then the Lagrangian statistics should be equal to the Eulerian statistics. In the LES, several statistics are calculated in an Eulerian way. These include horizontal slab averages of velocities, variances and subgrid turbulent kinetic energy. In the following figures, these variables are shown, calculated both in an Eulerian and in a Lagrangian way.

4.3.1 The BOMEX case

velocities The simplest comparison that can be made, is the comparison between the horizontally averaged velocities. In figure 4.4 and 4.5 the results of this comparison are shown for the BOMEX case. It can be seen that the results from the LPDM are in good agreement with the LES values.

variances Another quantity that can be used to compare the results of the LES with those from the LPDM, are the horizontally averaged, resolved variances. These results are shown in figure 4.6, 4.7 and 4.9. It is clear that the values from the LPDM are a little smaller than the values from the LES. This is most likely due to the fact that velocities have to be interpolated in the LPDM. This effect can be explained by looking at the definition of the variance:

\[ \sigma^2_u = \overline{(u - \overline{u})^2} = \overline{u^2} - \overline{u}^2 \]  

(4.1)

The overline means a horizontal average. Now it has just been shown that \( \overline{u} \), as measured by the LPDM is equal to the averaged velocity derived from the LES. Thus the difference has to be caused by the \( \overline{u^2} \) term. Now it is known that it matters whether the interpolation takes place before or after the squaring. In the LPDM the velocity is first interpolated and then squared. This gives rise to a slight underestimation of the resolved variances. Apart from this, the results from LES and LPDM show a great resemblance.

subgrid scale turbulent kinetic energy A third quantity that can be looked at is the sgs-TKE. The sgs-TKE should be equal to the sum of the three variances of the sub-grid velocities, divided by 2 (see equation 2.25). The results of that comparison are shown in figure 4.9. Also in this case the figure shows a good agreement of LES results and LPDM results.

4.3.2 The CBL case

velocities Also for the CBL case, the comparison is made between the horizontally averaged velocities. In figures 4.10 and 4.11 the results are shown. The results from the LPDM show reasonable agreement with the LES values. The values for the CBL case are more scattered. This is due to the fact that the average is closer to zero and the number of particles was about 6 times smaller than in the BOMEX case.

variances The second quantity that is used to compare the results of the LES with those from the LPDM, are the variances. The results for the CBL-case can be found in figures 4.12, 4.13 and 4.15. Here also, the values from the LPDM are a little smaller than the values from the LES. Here it is shown that this is a result of the interpolation of the velocities in the LPDM. The values of the LPDM lie between the values of a simulation with the LPDM.
4. Validation of the LPDM

Figure 4.4: Comparison between the instantaneous horizontally averaged $u$-velocities as obtained by standard LES output and the horizontally averaged $u$-velocities as calculated by the LPDM. The difference between the lowest points is caused by the fact that the simulation without the sgs-scheme gives more particles at the bottom and hence the average velocity is underestimated. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. This is a BOMEX case. The height is normalized with the height of the inversion, $z_i = 2000$ m.

Figure 4.5: Comparison between the instantaneous horizontally averaged $v$-velocities as obtained by standard LES output and the horizontally averaged $v$-velocities as calculated by the LPDM. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. This is a BOMEX case. The height is normalized with the height of the inversion, $z_i = 2000$ m.
4.3 Comparison of Eulerian-Lagrangian statistics

Figure 4.6: Comparison between the instantaneous horizontally averaged $u$-variances as obtained by standard LES output and the horizontally averaged $u$-variances as calculated by the LPDM, with or without sgs-scheme. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. This is a BOMEX case. The height is normalized with the height of the inversion, $z_i = 2000$ m.

Figure 4.7: Comparison between the instantaneous horizontally averaged $v$-variances as obtained by standard LES output and the horizontally averaged $v$-variances as calculated by the LPDM, with or without sgs-scheme. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. This is a BOMEX case. The height is normalized with the height of the inversion, $z_i = 2000$ m.
4. Validation of the LPDM

Figure 4.8: Comparison between the instantaneous horizontally averaged $w$-variances as obtained by standard LES output and the horizontally averaged $w$-variances as calculated by the LPDM, with or without sgs-scheme. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. This is a BOMEX case. The height is normalized with the height of the inversion, $z_i = 2000\ m$.

Figure 4.9: Comparison between the instantaneous horizontally averaged sgs-TKE as obtained by standard LES output and the horizontally averaged variances as calculated by the LPDM. This is a BOMEX case simulation. The sample time is at 2 hour after the restart of the simulation. The restart took place after 4 hours of simulation. The height is normalized with the height of the inversion, $z_i = 2000\ m$. 


4.3 Comparison of Eulerian-Lagrangian statistics

Figure 4.10: Comparison between the instantaneous horizontally averaged \( u \)-velocities as obtained by standard LES output and the horizontally averaged \( u \)-velocities as calculated by the LPDM. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case. The height is normalized with the height of the inversion, \( z_i = 775 \) m.

with non-moving particles at the center of the gridboxes and a simulation with non-moving particles at the edge of the gridboxes. Apart from this, the results from LES and LPDM show a great resemblance.

subgrid scale turbulent kinetic energy A third quantity that can be looked at is the sgs-TKE. The sgs-TKE should be equal to the sum of the three variances of the sub-grid velocities, divided by 2 (see equation 2.25). The results of that comparison are shown in figure 4.15. Also in this case the figure shows a good agreement of LES results and LPDM results.

4.3.3 The vorticity

An interesting quantity in turbulence research is the vorticity of the flow. The vorticity is defined as:

\[
\vec{\omega} = \nabla \times \vec{u}
\]

(4.2)

The vorticity was calculated inside the LPDM and averaged over the entire domain. It was anticipated that particles, advected without an sgs-scheme would have a lower vorticity, because they would be thrown out easier of the fastest spinning eddies. This numerical effect is due to the fact that a particle is advected with an integration scheme that has a certain timestep. During this timestep, a particle will travel in a straight line and hence the particle will be thrown out of the vortex. The results of this experiment are shown in figure 4.16. It can be seen that the particles that are advected without an sgs-scheme have a higher vorticity than the particles that were advected with the sgs-scheme. This unexpected result can be explained by combining figures 4.2 and 4.17. In figure 4.2 it can be seen that, without a sgs-scheme, there are more particles at the bottom of the LES. Figure 4.17 shows that at the bottom of the domain, the vorticity is highest. So this explains the higher overall vorticity for the LPDM without sgs-scheme. Furthermore, figure 4.16 shows that the implementation
4. Validation of the LPDM

Figure 4.11: Comparison between the instantaneous horizontally averaged $v$-velocities as obtained by standard LES output and the horizontally averaged $v$-velocities as calculated by the LPDM. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case. The height is normalized with the height of the inversion, $z_i = 775$ m.

Figure 4.12: Comparison between the instantaneous horizontally averaged $u$-variances as obtained by standard LES output and the horizontally averaged $u$-variances as calculated by the LPDM. In this figure 4 lines are plotted. The first are the averaged variances as obtained from the LES. The second is obtained by the LPDM with moving particles. The last two are obtained by putting non-moving particles at either the center or the upper edge of the gridboxes. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case. The height is normalized with the height of the inversion, $z_i = 775$ m.
Figure 4.13: Comparison between the instantaneous horizontally averaged $v$-variances as obtained by standard LES output and the horizontally averaged $v$-variances as calculated by the LPDM. In this figure 4 lines are plotted. The first are the averaged variances as obtained from the LES. The second is obtained by the LPDM with moving particles. The last two are obtained by putting non-moving particles at either the center or the upper edge of the gridboxes. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case. The height is normalized with the height of the inversion, $z_i = 775$ m.

Figure 4.14: Comparison between the instantaneous horizontally averaged $w$-variances as obtained by standard LES output and the horizontally averaged $w$-variances as calculated by the LPDM. In this figure 4 lines are plotted. The first are the averaged variances as obtained from the LES. The second is obtained by the LPDM with moving particles. The last two are obtained by putting non-moving particles at either the center or the upper edge of the gridboxes. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case. The height is normalized with the height of the inversion, $z_i = 775$ m.
4. Validation of the LPDM

Figure 4.15: Comparison between the instantaneous horizontally averaged sgs-TKE as obtained by standard LES output and the horizontally averaged variances as calculated by the LPDM. The sample time is at 10 hour after the restart of the simulation. The restart took place after 3 hours of simulation. This is a CBL case simulation. The height is normalized with the height of the inversion, \( z_i = 775 \) m.

of the sgs-scheme makes the particles distribute more quickly towards a steady state. If we now take a closer look at figure 4.17 then it can be seen that the horizontally averaged, absolute vorticity does not depend on the used integration scheme nor on the usage of the subgrid scheme. However, the difference in sampling position is evident. The reason for this difference, is that, in order to calculate a derivative like \( \frac{\partial u}{\partial y} \), there is also a difference in the amount of interpolation that is needed to perform the calculation. At the center of a gridbox, there are more interpolation steps necessary than at the edge. This increased amount of interpolations gives rise to a lower averaged vorticity. All this leads to the conclusion that the interpolation scheme is a greater source of error, than the integration scheme is.

4.4 Computation time of the LPDM

After the LPDM was implemented and validated, it was possible to measure the time the LPDM spends in a certain subroutine. The results of such a measurement are shown in appendix C. Unfortunately, the measured simulation was so large, that it was impossible to combine the data of all 32 processors, so only the data from 1 processor is given. Because the particles were, more or less, homogeneously spread, this data should be representative for the total domain. It can be seen that in the simulation that contained over 10 million particles, the LPDM took about 30\% of the total computation time. From this 30\% the Adams-Bashfort 2nd order integration scheme took about 10\% of the time, while the interpolation schemes required 20\% of the time. Unfortunately, there are many parameters that can influence the performance of the LPDM. Especially the write statements can take a lot of time and memory. In the simulation described above, there were no write-statements included, only at the end something needed to be written. In the case of preparing a dataset for postprocessing, it is likely that the particles will be written every few seconds (LES time). With simulations of the LPDM, files have been created with a size of several Gigabytes, although this is in its turn very dependent on the format that is used to store the data and of course, of the amount of data that is written. A line of data contains at least the time, the
4.4 Computation time of the LPDM

Figure 4.16: The absolute vorticity, averaged over the entire domain for simulations with the LPDM. There are 5 different lines plotted. In the first 3 simulations, particles are released at the center of the gridboxes. In the following simulation, the particles start at the upper edge of the gridboxes (i.e. point G in figure 3.2). In the last simulation, the particles start at the upper edge of the cells, but there are also particles at the lower edge of the lowest gridboxes. In the first 2 simulations, the particles were allowed to move, whereas in the rest of the simulations they were kept at the starting position. The simulations lasted 10 hours, where the particles were inserted after 3 hours. This is a BOMEX case.

Figure 4.17: A snapshot of the horizontally averaged, absolute vorticity. The 4 different (although not distinguishable) lines denote two integration schemes, both with and without the sgs-scheme turned on. In the rest of the simulations the particles were kept at the starting position. In the first 5 simulations, particles are released at the center of the gridboxes. In the last simulation, the particles start at the upper edge of the gridboxes (i.e. point G in figure 3.2). This is a BOMEX case simulation. The snapshot was taken after 2 hours of simulation with the LPDM, where the particles were inserted after 3 hours. The height is normalized with the height of the inversion, $z_i = 2000 \, m$. 

position and the velocities of a particle, but it is possible to write a lot more data, like the higher order moments of the velocity, the sgs-TKE at the particle position, etcetera.
4.4 Computation time of the *LPDM*
Chapter 5

Conserved variable diagrams

In the world of atmospheric scientists, there exists a controversy that has lasted for over 5 decades now. The question is whether mixing of a cloud and the surrounding air can be described best by lateral mixing or by vertical mixing, figure 5.1. There is no discussion about the large part of air entering the cloud from below, since a rising thermal is generally accepted as the initiator of the formation of a cloud. With lateral mixing, environmental air is mixed into a cloud, mainly from the sides. While on the opposite, with cloud-top mixing, there is only mixing (between cloud and environment) at the bottom and at the top of a cloud. A cloud will always have properties that are based on the environmental air originating from below the cloud. The question is now, whether a cloud also has properties of environmental air originating from the top of the cloud, or also from the sides of the cloud. The answer to this question is vital in the modeling of clouds. More information, along with previous studies on this topic can be found in: e.g. Rogers and Yau [27], Blyth et al. [2], Blyth [1], Jonas [12], Paluch [22] and Squires [30]. In this chapter, first the arguments for lateral mixing will be discussed. After this, the arguments for cloud-top mixing will be examined. With the LPDM, it might be possible to create clear evidence for either one of these theories, at least within the LES framework.

Figure 5.1: The different views on mixing between cloud and environment. The left picture shows the concept of lateral mixing, whereas on the right the concept of cloud-top mixing is visualized.
5.1 Lateral mixing

In order to investigate the mixing properties of a cloud, a simulation was performed, containing 1.3 million particles. The particles were released uniformly throughout the domain and were allowed to move freely with the flow. Afterwards it was then possible to backtrack the trace of the particles, in order to determine whether they had entered the cloud at the side, at the bottom or at the top. The results of this simulation are shown in figure 5.2. This figure shows the number of particles that enters or leaves a cloud, as related to the relative height. This relative height is defined as the ratio of the particle height within the cloud, divided by the total cloud height. The pulse of particles entering the cloud from below can be clearly distinguished. Furthermore, it can be seen in the figure that there are particles passing the boundaries of a cloud at every height. There is no pulse of particles crossing the border of a cloud at the top. This could be an indication that lateral mixing is important.

5.2 Cloud-top mixing

An argument in favor of the cloud-top mixing version, is a conserved variable diagram, also called a Paluch diagram (Paluch [22]). In such a diagram, the total water content \( q_t \) is plotted against the liquid water potential temperature, \( \theta_l \). It is shown, that the assumption of linear mixing holds for these conserved variables. Now suppose that there is mixing between two parcels of air, with different values for \( q_t \) and \( \theta_l \). Then, because they are conserved variables, the mixture will have values for \( q_t \) and \( \theta_l \) that are directly proportional to the mixing ratio. This is shown for \( q_t \) in equation 5.1, where 2 parcels of air are mixed (1 and 2) to deliver the
5. Conserved variable diagrams

Figure 5.3: The original conserved variables diagram, as presented by Paluch [22]. The $Q$ is the total liquid water content $q_l$. SFC is the surface at 1.4 km. Cloud bottom CB is at 3.8 km. Cloud top was at 9-12 km and the observation level was at 5.2 km.

new parcel of air (3). The $\alpha$ is the mixing ratio.

$$q_{l,3} = \alpha q_{l,1} + (1 - \alpha)q_{l,2}$$

In 1979, Paluch was the first to do this analysis, by analysing data obtained from aircraft measurements. The results of her analysis are shown in figure 5.3. In this case, the wet equivalent potential temperature, $\theta_q$, is used as a conserved variable instead of $\theta_l$. $\theta_q$ is given as follows:

$$\theta_q \approx \theta_l + \frac{L}{c_p} \left( \frac{p}{p_0} \right)^{rac{R_d}{c_p}} q_l \approx \theta_l + 2.5 \times 10^3 q_l.$$  

The reason for this change is that the original conserved variable, $\theta_l$ is strongly correlated with $q_l$ (see equation 5.3). According to equation 5.4, $q_l$ is in turn strongly correlated with $q_t$, so a plot of $q_l$ against $\theta_l$ would be biased by this correlation. A derivation of this formula can be found in appendix B.

$$\theta_l \approx \theta - \frac{L}{c_p} \left( \frac{p}{p_0} \right)^{rac{R_d}{c_p}} q_t,$$

$$q_l = q_t + q_v.$$  

In figure 5.3 the horizontally averaged environmental curve is plotted as a line. The measured cloud points are also plotted. It turns out that the cloud points are on a line, from the
5.3 The choice of conserved variables

In the previous section, it was mentioned that the use of $\theta_l$ would lead to a strongly correlated result. Unfortunately, it turned out that in this case, the use of the wet equivalent potential temperature $\theta_q$ leads to another correlation. This can be explained by looking at figure 5.4. If, from this picture, the environmental curve is taken for a height from 0 to 3.2 km (as is the height of the BOMEX-case), then the environmental curve turns out to be a straight line. The mentioned correlations can be seen in figures 5.4 to 5.9. Here six conserved variable diagrams are shown, with the same data, but with different values for $\theta_x$. This variable is defined as follows:

$$\theta_x = \theta_l + c_x 10^3 q_t.$$  \tag{5.5}

The prefactor is dependent on the unit of $q_t$; it is $10^3$ because $q_t$ is given in [g/kg]. The $c_x$ is a constant that has to be chosen so that the figures become less correlated. Note that $c_x = 0$ gives $\theta_x = \theta_l$ and $c_x = 2.5$ gives $\theta_x = \theta_q$. The $c_x$ constant was varied from 0 to 2.5. In figure 5.6 the curvature is maximal, so the value $c_x = 0.7$ is used in the remainder of the research. Despite the fact that there is no physical background for the use of this variable, $\theta_x$ can be used, because it is a linear combination of two conserved variables and is therefore also a conserved variable.

Figure 5.4: A conserved variable diagram for one sampled cloud. Here $\theta_x = \theta_l$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloud base at 550 m and cloud top at 1750 m. The sample is taken after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.

environmental curve at about 1.5 km to the environmental curve at 8 km. This led Paluch to the conclusion that the measured cloud points contained a mixture of the properties of air from below cloud base and air that originates from a height of 8 km. This result from Paluch (and others) has been used as the main argument for the cloud-top mixing theory. In the remainder of this chapter, in similar figures the $y$-axis will be reversed, so that if $y$ increases, also the height increases.
5. Conserved variable diagrams

Figure 5.5: A different form of the same conserved variable diagram. Here $\theta_x = \theta_l + 0.6 \times 10^3 q_t$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloudbase at 550 m and cloud top at 1750 m. Output is given after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.

Figure 5.6: A different form of the same conserved variable diagram. Here $\theta_x = \theta_l + 0.7 \times 10^3 q_t$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloudbase at 550 m and cloud top at 1750 m. Output is given after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.
5.3 The choice of conserved variables

Figure 5.7: A different form of the same conserved variable diagram. Here $\theta_x = \theta_l + 0.8 \times 10^3 q_t$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloudbase at 550 m and cloud top at 1750 m. Output is given after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.

Figure 5.8: A different form of the same conserved variable diagram. Here $\theta_x = \theta_l + 10^3 q_t$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloudbase at 550 m and cloud top at 1750 m. Output is given after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.
5. Conserved variable diagrams

Figure 5.9: A different form of the same conserved variable diagram. Here $\theta_x = \theta_l + 2.5 \times 10^3 q_t \approx \theta_q$. The line represents the environmental values, whereas the points are cloudy points. The crosses represent heights of respectively 1000 and 1400 m. Also drawn are the positions of cloudbase at 550 m and cloud top at 1750 m. Output is given after 1 hour of simulation with the LPDM, which has started after 4 hours of simulation by the LES.

5.4 The setup of the case

In order to answer the question, whether mixing of a cloud and the surrounding air can be described best by lateral mixing or by vertical mixing, a simulation was performed, containing over 1 million particles ($128 \times 128 \times 80$). The particles were released after 4 hours of simulation by the LES. After 1 hour, the biggest cloud was selected and all particles that were at that time inside the cloud, were selected. A projection of the selected cloud is given in figure 5.10. There were 1731 particles selected. After the selection procedure, the simulation went on for another hour. Since the particle data was written every 30 seconds, it was possible to track the positions of the particles offline. Because all calculated variables were stored with the position of the particles, it was also possible to visualize the particles in a conserved variable diagram. The sample heights of 800, 1000 and 1400 m are shown in figure 5.10. For this cloud, cloudbase is at 550 m and cloud top at 1750 m. In order to ensure a sufficient number of particles, the particles were selected within a range of 40 m in height, centered around the observation heights of 800 m and 1000 m. A range of 20 m in height was used for the observation level of 1400 m. The cloud sample at 800 m contains 45 particles, the cloud sample at 1000 m contains 34 particles and the cloud sample at 1400 m contains 66 particles. The lowest two cloud samples contain a sample of a rising cloud, whereas at 1400 m the cloud is close to the top and the sample contains both rising air and descending air. The selected particles can be visualized in a Paluch diagram, at different timesteps.

5.5 Results of the case

The analysis of the conserved variable diagram, as introduced by Paluch, often leads to conclusions that are pointing towards cloud-top mixing as the dominant mixing process. In this section it will be shown, that it is possible to give an argument towards lateral mixing as the dominant mixing process in cumulus clouds, by using a Paluch diagram. In figures 5.11.
5.5 Results of the case

Figure 5.10: The projection of the selected cloud. The lines represent the sample heights. Selection time was after 1 hour of simulation with the \textit{LPDM}, which has started after 4 hours of simulation by the \textit{LES}.

$5.12$, $5.13$ and $5.14$ the history of the particles is shown in a Paluch diagram. This is done for a group of particles that is selected to be in the same cloud, at the same height, at the same time. If the conclusion of Paluch were true, then the particles should originate either from the bottom of the cloud, or from the top of the cloud. This would mean that the particles should spread in the Paluch diagram on a line towards cloud top or towards cloud bottom. For the sample heights of 800 m and 1000 m it can be seen that the particles do not do so. Instead they seem to originate from various positions approximately on the environmental curve, with a somewhat stronger correlation towards cloud bottom. This means that the particles were mixing laterally with environmental air, while there also were some particles originating from cloud bottom. The latter was not under discussion, since a rising thermal from the bottom is generally believed to be the cause of the existence of a cloud. However, the first conclusion is exactly the proof that is needed to make the statement, that lateral mixing is a better way to describe the mixing of environmental air into a cloud, than cloud-top mixing is.

However, for the sample height of 1400 m the results are pointing towards a different conclusion. There is an amount of particles originating from above observation height. This means that higher in the cloud, there is some influence from the top. This can be explained by the fact that a cloud contains more turbulence near the top and therefore some influence from cloud top can be expected higher in the cloud. In figure $5.15$ there are two lines plotted that show the two influences. For cloudy particles that are beneath 1000 m, the line that can be drawn through these points is clearly a straight line towards a height of approximately 800 m. The other line states that cloudy points higher than 1000 m are mixed with environmental air originating from a height of about 1650 m. These lines become even more visible if the values for the cloudy points are averaged over the height. This is done in figure $5.16$.

The conclusions as described above is even more supported by the figures $5.17$, $5.18$ and $5.19$. In these figures the previous heights of the same particles can be seen. In the case of cloud-top mixing, the particles should originate from heights that are well above observation height, or well below observation height. It can be seen from the figures, that for the sample heights of 800 m and 1000 m, the particles originate from all heights, with the majority originating from heights just below the observation height. For the sample height of 1400 m, there are also particles coming from above observation height. This also gives good
evidence for the lateral mixing concept to be the most appropriate in the bulk of the selected cumulus cloud. Only near the top there is some influence of a vertical mixing process.

### 5.6 Applicability of the results

Some remarks can be made of the results mentioned above. It is already mentioned that a difference in cloud height can affect the results in a conserved variable diagram. It is also possible that different types of clouds will have different mixing characteristics. Another topic of importance is the lifecycle of a cloud. A young growing cloud consists of a strongly buoyant updraft, with a lot of liquid water. This in contrast to a mature cloud, which has little liquid water left and has almost zero buoyancy. It can be expected that the mixing properties of such a young cloud, are different from the mixing properties of a large, mature cloud. A complication is also that, in growing clouds, it is hard to distinguish between lateral mixing and mixing at the increasing top. More research is needed in order to investigate the mixing properties of the different types and ages of clouds.
5.6 Applicability of the results

Figure 5.11: The history of the cloudy points at the sample height of 800 meter. Here $\theta_x = \theta_l + 0.7 \times q_t$. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. The line represents the environmental values, where a cross is drawn at the sample height. The cloudy points are visualized by points if they are a cloud and by a plus sign if they are not. Also visible are: cloud-base at 550 m and cloud-top at 1750 m.
Figure 5.12: The history of the cloudy points at the sample height of 1000 meter. Here $\theta_x = \theta_l + 0.7 \times q_t$. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. The line represents the environmental values, where a cross is drawn at the sample height. The cloudy points are visualized by points if they are a cloud and by a plus sign if they are not. Also visible are: cloud-base at 550 m and cloud-top at 1750 m.
5.6 Applicability of the results

Figure 5.13: The history of the cloudy points at the sample height of 1400 meter. Here $\theta_x = \theta_t + 0.7 \times q_t$. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. The line represents the environmental values, where a cross is drawn at the sample height. The cloudy points are visualized by points if they are a cloud and by a plus sign if they are not. Also visible are: cloud-base at 550 m and cloud-top at 1750 m.
Figure 5.14: The history of the cloudy points at the different sample heights. Here \( \theta_x = \theta_t + 0.7 \times q_t \). The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. The line represents the environmental values, where a cross is drawn at the sample height. The cloudy points are visualized by points if they are a cloud and by a plus sign if they are not. Also visible are: cloud-base at 550 m and cloud-top at 1750 m.
5.6 Applicability of the results

**Figure 5.15:** Two linear fits through the total of 1731 selected cloudy points, at 1 hour after the restart of the simulation. The two lines cross at a height of 980 m. Here $\theta_x = \theta_l + 0.7 \times q_t$. The restart took place after 4 hours of simulation. The line represents the environmental values, where the crosses are drawn every 100 m, starting with 700 m. The cloudy points are visualized by points, also visible are: cloud-base at 550 m and cloud-top at 1750 m.

**Figure 5.16:** Two linear fits through the horizontally averaged values of the cloudy points, at 1 hour after the restart of the simulation. The two lines cross at a height of 980 m. Here $\theta_x = \theta_l + 0.7 \times q_t$. The restart took place after 4 hours of simulation. The curved line represents the environmental values, where the crosses are drawn every 100 m, starting with 700 m. The cloudy points are visualized by points, also visible are: cloud-base at 550 m and cloud-top at 1750 m.
Figure 5.17: The time dependent heights of particles that are present in a cloud at an observation height (OB) of 800 m, at sample time. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. Cloud base (CB) is indicated at 550 m, cloud top (CT) is shown at 1750 m.

Figure 5.18: The time dependent heights of particles that are present in a cloud at an observation height (OB) of 1000 m. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. Cloud base (CB) is indicated at 550 m, cloud top (CT) is shown at 1750 m.
5.6 Applicability of the results

Figure 5.19: The time dependent heights of particles that are present in a cloud at an observation height (OB) of 1400 m. The sample time is at 1 hour after the restart of the simulation. The restart took place after 4 hours of simulation. Cloud base (CB) is indicated at 550 m, cloud top (CT) is shown at 1750 m.
Chapter 6
Conclusions and recommendations

This chapter will present some conclusions from this thesis, along with some remarks and recommendations. First the LPDM will be discussed, as it is implemented and running. After this, some attention will be given to the subgrid scheme and finally some results that are obtained with the LPDM will be discussed.

6.1 The LPDM

This section contains the conclusions that are directly related to the implementation and testing of the LPDM.

6.1.1 Implementation of the LPDM

The first conclusion is that the LPDM is implemented and working without problems. It is now possible to follow an amount of particles through time, as they travel within the domain. The LPDM has been proven to work with a total of over 10 million particles. The LPDM runs parallel to the LES and uses the resolved velocities from the LES. The particle scheme has to interpolate these velocities for each particle and then the new positions of the particles are calculated using the integration scheme and the subgrid scheme. At every timestep the boundary conditions are checked. These topics will be discussed in more detail in the following paragraphs.

The integration scheme In the production runs of the LPDM, usually the Adams-Bashfort 2nd order scheme was used. Although it was expected in advance that the 2nd order scheme would give better results than the 1st order scheme, the difference turned out to be rather small. The interpolation errors were shown to be dominating the results. Furthermore, since the velocities that are the input of the integration scheme, are filtered in the LES, there are no rapid changes in the velocity possible. Therefore the 2nd order Adams-Bashfort scheme will be good enough for current use, although it is always possible to implement a 4th order scheme, if after improvement of the interpolation scheme, it turns out to be necessary.

The spatial interpolation scheme In the LPDM the 1st order tri-linear interpolation scheme is used. Also because the velocities are filtered in the LES, it was not expected that there are large spatial variations in the domain. However, it turned out that in calculating derivatives, it mattered a lot whether they were calculated in the center of a gridbox, or at an edge of the
6.2 The LPDM in practice

gridbox. The conclusion is that the simple interpolation scheme is good enough for velocity calculations, but that it leads to large errors in calculations of derivatives.

The subgrid scheme  It was found that an extra subgrid scheme was needed for the particles, because the input to the particle subroutine consists of resolved velocities, that are unable to fully describe the particle motions. It was especially needed to avoid a build up of particles at the bottom of the domain. A stochastic subgrid scheme that has been adapted to work inside an LES was implemented.

The boundary handling scheme  The LPDM has the same boundary conditions as the LES, except that the particle scheme has perfect reflection implemented at the top and bottom of the domain. The latter requires some explanation, since massless particles normally do not hit the walls. The subgrid scheme is totally responsible for any particles running into the walls. It can be concluded that the boundary conditions do not give any problems in the LPDM

6.2 The LPDM in practice

6.2.1 Validation of the LPDM scheme

In order to validate the particle scheme and to make sure that it was implemented correctly, some tests were performed. After the comparison of several quantities that were calculated both by the LES and by the LPDM, it can be concluded that the LPDM is working as it should. Particles that are uniformly spread in the domain, should remain uniformly distributed. Without the subgrid scheme there was a number particles remaining at the bottom of the domain. This surplus of particles was continuously increasing to over 40% after just 2 hours of simulation. The use of the subgrid scheme has been shown to keep the surplus of particles at the bottom of the domain at approximately 5%. This is good enough for current use.

6.2.2 Computation time of the LPDM

With a simulation that contained over 10 million particles, the LPDM took about 30% of the total computation time. This is acceptable for current usage. Unfortunately, there are many parameters that can influence the performance of the LPDM. Especially the write statements take a lot of time and memory. These statements are very dependent on the format that is used to store the data and of course of the amount of data that is written. A line of data contains at least the time, the position and the velocities of a particle, but it is possible to write a lot more data, like the higher order moments of the velocity, the TKE at the particle position, etcetera.

6.2.3 The timestep of the LPDM

In the LPDM the timestep was set to be equal to the timestep of the LES. This means that in the test cases, a timestep of 2 seconds was used and in the production runs, a timestep of 1 second was used. Since the requirement for the timestep of the LES is more or less equal to the requirement of the LPDM, it seems reasonable to put the timestep of the LPDM at the
same value as the timestep of the LES. However the LPDM can handle almost every value of the timestep, as long as it is either a multiple of the timestep of the LES, or vice versa.

6.2.4 The $\kappa$-scheme and the subgrid scheme

Unfortunately, the implemented sgs-scheme becomes unstable if a $\kappa$-advection scheme is used. This is due to the dissipative properties of the $\kappa$-scheme, which makes that the $f_s$ parameter goes to zero, where it should not. This $f_s$ parameter is calculated by dividing the subgrid variances by the total variances. This problem is solved by manually setting the $f_s$ parameter to 1. The LPDM is thus positioned in the middle of the models as posed by Weil et al. [37] and Thomson [34]. However, the change of this parameter could have some influence on statistics.

6.3 Lateral or vertical mixing

In a conserved variable diagram, two conserved variables ($\theta_q$ and $q_t$) are plotted against each other. Such a diagram seems to be a major argument for top-bottom mixing as the best way to describe mixing of cloudy air with its environment. Recent research has come up with evidence towards lateral mixing. This conclusion is examined by looking at the time dependent conserved variable diagram, by means of an experiment with the LPDM.

6.3.1 Conserved variable diagram

It was possible to construct a conserved variable diagram, in the same way as Paluch [22]. The only problem was that the cumulus clouds that are investigated here, are much smaller than the clouds investigated by Paluch. This results in a diagram that contains a strong correlation between the two variables $\theta_q$ and $q_t$. This problem is solved by using a different conserved variable, $\theta_x \equiv \theta_l + 0.7 \times 10^3 q_t$, which has no physical background, but, since it is composed of a linear combination of two conserved variables, can be used legitimately.

6.3.2 Setup and results from the BOMEX-case

Simulations were performed on a $256 \times 256 \times 160$ grid, containing over 1,3 million particles. With the generated data, the particles could be followed back in time to see where they came from. If the conclusion of top-bottom mixing being the dominant mixing process were true, then the particles should originate either from the bottom of the cloud, or from the top of the cloud. It follows from the results, that the particles do not do so. Instead, for the sample heights of 800 m and 1000 m, they are found to originate from various positions approximately at the observation height, on the environmental curve, with a somewhat stronger correlation towards cloudbottom. This means that for these sample heights, the particles were mixing laterally with environmental air, while also some particles were originating from cloud bottom. For the sample height of 1400 m, there seem to be two processes acting on the cloud, since there are also particles originating from above observation level. These results clearly show that also in the form of a conserved variable diagram, lateral mixing can be seen as the dominant mixing process for the bulk of the cloud. Only near the top of the cloud, there seems to be an influence from vertical mixing from the top of the cloud.
6.3.3 Comments on the results

A difference in cloud height can affect the results in a conserved variable diagram. It is also possible that different types of clouds will have different mixing characteristics. Another topic of importance is the lifecycle of a cloud. In a young growing cloud, it can be expected that the mixing properties are different from the mixing properties of a large, mature cloud. A complication is also that in a growing cloud, it is hard to distinguish between lateral mixing and mixing at the increasing top. More research is needed in order to investigate the mixing properties of the different types and ages of clouds.

6.4 Future research

In the future, it might be necessary to make improvements based on the different parts of the LPDM. A more sophisticated interpolation scheme would be cubic splines. For the integration method, the 4th order Runge-Kutta scheme might be implemented. In the subgrid scheme there is the $f_s$ parameter that is manually set to 1. Some time has to be spent in order to see if there is a better solution to make the subgrid scheme stable in combination with the $\kappa$-scheme. It is believed, that with the addition of a Monin-Obukhov scheme for the bottom grid cells, the surplus of particles at the bottom of the domain can be further reduced. A Monin-Obukhov scheme would include an approximately logarithmic decay of velocities towards the bottom of the domain, instead of the present linear decay. Also the $LPDM$ currently works only with an equidistant grid. In the future adaptations might be made to make the $LPDM$ compatible with non-equidistant grids. Future research is also needed in order to determine whether it is worthwhile to use a larger timestep for the $LPDM$. It is not sure how much the combined $LPDM$-$LES$ would run faster and what would be the penalty in accuracy for choosing a larger timestep for the $LPDM$. With regard to the Paluch diagrams, the next step would be to look at more clouds while using even more particles, in order to obtain better statistics. Furthermore, the output from the $LPDM$ might be visualized in a virtual environment. Research towards this is already being performed and promises to be of great utility.
Appendix A

Derivation of potential temperature.

The following equations are used in the derivation of the potential temperature:

\[ p v = R_d T, \]  
\[ dh = v dp, \]  
\[ dh = c_p dT. \]  

(A.1)  
(A.2)  
(A.3)

These equations are the ideal gas law and two equations for a change in enthalpy, \( h \). In these equations \( p \) is the pressure, \( R_d \) is the gas constant for dry air, \( T \) is the temperature, \( v \) is the specific volume of air and \( c_p \) is the heat capacity of air. Combining all three equations gives:

\[ c_p dT = \frac{RT}{p} dp \]  

(A.4)

Rearranging delivers:

\[ \frac{dT}{T} = \frac{R}{c_p} \frac{dp}{p} \]  

(A.5)

Integration of this equation gives:

\[ \frac{T}{T_0} = \left( \frac{p}{p_0} \right)^{\frac{R}{c_p}} \]  

(A.6)

Now the potential temperature is defined as the temperature a parcel of air would have if it was brought adiabatically to the reference pressure \( p_0 \):

\[ \theta \equiv T_0 = T \left( \frac{p}{p_0} \right)^{\frac{R}{c_p}} \]  

(A.7)
Appendix B

Derivation of the wet equivalent potential temperature

The wet equivalent potential temperature \( \theta_q \), as used in equation 5.2, can be derived from the definition of \( \theta_q \) given by Paluch [22]:

\[
\theta_q = T \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})\gamma}{C_{p,a}T}} \exp\left[ \frac{q_v L \gamma}{C_{p,a} T} \right],
\]  
(B.1)

\[
\gamma = \frac{1}{1 + \frac{C_{p,w}}{C_{p,a}} q_l}.
\]

The variables are as defined in chapter 2. With \( C_{p,w} \approx 4C_{p,a} \) and \( q_l \approx 10^{-2} \), then \( \gamma \approx 1 \). If the approximation of \( \gamma \) is used and with the application of the expansion for \( e^x = 1 + x + O(x^2) \), then the equation can be approximated by:

\[
\theta_q = T \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} \left[ 1 + \frac{q_v L}{C_{p,a} T} \right].
\]  
(B.2)

This equals:

\[
\theta_q = T \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} \left[ 1 + \frac{q_v L}{C_{p,a} T} \right].
\]  
(B.3)

With \( q_v = q_t - q_l \), this becomes:

\[
\theta_q = T \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} + \frac{L}{C_{p,a}} \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} q_t - \frac{L}{C_{p,a}} \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} q_l.
\]  
(B.4)

Now the first and the last term together form \( \theta_l \) (equation 4.6):

\[
\theta_q = \theta_l + \frac{L}{C_{p,a}} \left( \frac{p}{p_0} \right)^{-\frac{(R_d/C_{p,a})}{C_{p,a}T}} q_t.
\]  
(B.5)

The following values are used:

- \( L = 2.5 \times 10^6 \text{Jkg}^{-1} \)
- \( C_{p,a} = 1004 \text{Jkg}^{-1} K^{-1} \)
• $p \approx 9 \times 10^4 Pa$
• $p_0 = 10^5 Pa$
• $R_d = 287 J/kg^{-1}$

With these values the final equation can be given:

$$\theta_q \approx \theta_l + 2.5 \times 10^3 q_t.$$  \hspace{1cm} (B.6)
Appendix C

Details of the time consumption of several parts of the LPDM

This appendix contains information about the performance of the LPDM. Because of the enormous amount of information, only the results from 1 processor are given. The usertime routine gives lots of details of internal processes, so for clarity, only the data that took more than 1% of the computation time is presented.

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Bibliography


