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Particle and droplet dynamics at cloud-environment interfaces

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January 2021

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*Submitted in part fulfilment of the requirements for the degree of
Doctor of Philosophy in Civil and Environmental Engineering of Imperial College London
and the Diploma of Imperial College London*

I hereby declare that all the work presented in this thesis is my own. Any contribution or work from others has been appropriately acknowledged or referenced.

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2nd January 2021

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Acknowledgements

Thank you Maarten, for the trust you showed in me while selecting me for this PhD position, for being incredibly patient throughout the four years, for not missing a single weekly meeting, for being tough but always fair, for always pushing me to do a little bit more to make a good publication a little bit better, for your attention to detail, for making me do a million iterations, for the post-midnight drinking in Paris and Torino, and for being the best supervisor I could have asked for and for being a genuinely good human being.

Thank you Elena for being who you are and for making every day in the basement a little bit more bearable, for all the conversations and keeping me up-to-date with everything that goes on in the lab, and for being a very good friend to me and Reshma. I am not going to that graduation ceremony unless you do as well!

A big thank you to every one in the lab I have had the pleasure of spending time with over the last four years: Sonja, Emily, JP, Birgit, Ivo, Lili, Carolanne, Cleo, Joanna, Emma, Rakib, Joanna, Daniel, the Toms, Li, Mark, Constantin, Alex. You guys are some of the kindest and friendliest people I have ever known.

I have really enjoyed the ESR meetings and all credit is due to my fellow COMPLETE ESRs, especially Tai, Sara and Marco. I will not forget the 1am walk to see the Eiffel tower (I am looking at you Tai!), all the dancing in Warsaw, hiking up Zugspitze, the extravagant dinners in Torino, the pubquiz in London and the beer festival in Gottingen. Thank you for all the memories!

I will be remiss if I do not acknowledge the contributions from Dr Thijs Heus and Dr John Craske towards this thesis. Thank you Thijs for all the stimulating skype discussions and thank you John for always being ready to help with all my questions, SPARKLE or otherwise.

Reshma, I cannot even begin to imagine where I would be without you. Words cannot describe what you mean to me. Thank you for keeping me sane through the last four years, for climbing mountains with me (literally and figuratively), for letting me annoy you for the last 18 years, for trying to play wife, and for being so brave through your pregnancy in such tough times. Here is to another 50 years of togetherness with kochapayi! To my parents, who have never denied me anything in spite of not having much. Thank you for showing me that working

hard and being kind matters more than anything else. This thesis is dedicated to you two.

Abstract

In this thesis, the correlation between mixing and entrainment/detrainment at the cloud edge, and the dynamics of particles/droplets is investigated. At the edge of a cloud, entrainment of unsaturated environmental air plays a very crucial role. Evaporation of cloud droplets exposed to unsaturated air results in the formation of a negatively buoyant layer, commonly referred to as the subsiding shell in literature. A systematic study of the dynamics of the subsiding shell using direct numerical simulations demonstrates the self-similar characteristics of the flow in the shell. A canonical setup is developed whereby a developing temporal plume is used as a paradigm for a small portion of the edge of a cloud. Characteristic scales for the shell thickness, buoyancy and velocities are identified using integral relations from van Reeuwijk and Craske (2015). Results reveal a buoyancy driven shell with the in-shell mean velocity being passive and slaved to the buoyancy. Different interfaces are identified at the cloud edge as a result of the generation of the subsiding shell. This includes a Turbulent-Non Turbulent Interface (TNTI) which is detected by applying thresholds on the enstrophy. Lagrangian particles crossing the TNTI exhibit sharp jumps in enstrophy and buoyancy when compared to traditional cloud boundaries which are shown to be dynamically unimportant.

A study of the effect of gravity on clustering in a polydisperse distribution of droplets in isotropic homogeneous decaying turbulence is performed. The radial distribution function is used to quantify clustering and analysis reveals that gravity suppresses clustering in sedimenting droplets due to reduced droplet-turbulence interaction times. Comparisons are also made with analytical and empirical relations and very good agreement is observed.

Different aerosol concentrations (clean and polluted clouds) are simulated by varying the initial size distribution of droplets, and the resulting effect of entrainment on the droplet size distributions and shell strength is investigated. Simulations reveal a dynamical positive feedback where droplet evaporation increases the turbulent kinetic energy which further drives entrainment and evaporative cooling. The droplet size distribution is found to be broader for initial size distributions with a larger mean droplet radius but smaller particle concentrations (clean clouds).

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List of Symbols

The following is not an exhaustive list but includes the most frequently used symbols in the thesis. Additional symbols are defined within individual chapters.

N	Particle number concentration	m^{-3}
D	Particle diameter	m
w_T	Particle fall velocity	ms^{-1}
α	Shape parameter	$[-]$
λ	Slope parameter	$[m^{-1}]$
N_t	Total number concentration	$[m^{-3}]$
Z	Radar reflectivity factor	dBz
θ	Potential temperature	K
q_v	Specific humidity of water vapor	$kgkg^{-1}$
p_0	Reference pressure	Nm^{-2}
p	Pressure	Nm^{-2}
T	Absolute temperature	K
R_d	Specific gas constant for dry air	$Jkg^{-1}K^{-1}$
R_v	Specific gas constant for water vapor	$Jkg^{-1}K^{-1}$
m	Total mass of moist air	kg

m_d	Mass of dry air	kg
m_v	Mass of water vapor	kg
m_l	Mass of liquid water	kg
q_l	liquid water specific humidity	$kgkg^{-1}$
q_t	total water specific humidity	$kgkg^{-1}$
$q_{t,0}$	total water specific humidity of the environment	$kgkg^{-1}$
q_s	Saturation specific humidity	$kgkg^{-1}$
θ_0	Potential temperature in the environment	K
θ_l	Liquid water potential temperature	K
θ_v	Virtual potential temperature	K
L	Latent heat of vaporization	Jkg^{-1}
c_p	Specific heat capacity of air	Jkg^{-1}
e	Vapor pressure	Pa
e_s	Saturation vapor pressure	Pa
ρ_f	Density of air	kgm^{-3}
ρ_p	Density of water	kgm^{-3}
S	Supersaturation	—
m_p	Mass of particle	kg
m_f	Mass of fluid	kg
$\mathbf{u}$	Flow velocity vector	ms^{-1}
$\mathbf{v}$	Particle velocity vector	ms^{-1}

$\mathbf{X}$	Particle position vector	m
$\mathbf{g}$	Gravity vector	ms^{-2}
R	Particle radius	ms
μ	Dynamic viscosity of air	$kgm^{-1}s^{-1}$
ν	Kinematic viscosity of air	m^2s^{-1}
τ_p	Particle relaxation time	s
Γ^D	Dynamic collision kernel	m^3s^{-1}
Γ^K	Kinematic collision kernel	m^3s^{-1}
Γ^g	Gravitational collision kernel	m^3s^{-1}
C_d	Condensation rate per unit mass	—
k_a	Thermal diffusivity of air	m^2s^{-1}
D_v	Molecular diffusivity of water	m^2s^{-1}
r	Particle separation distance	m
R_c	Radius of collision sphere	m
w_r	Radial component of relative velocity	ms^{-1}
g	Radial distribution function	[—]
η	Kolmogorov length scale	m
b	Buoyancy	ms^{-2}
b_c	In-cloud buoyancy	ms^{-2}
w_c	In-cloud vertical velocity	ms^{-1}
τ_c	Nudging time scale	s

L_c	Length of initial cloud layer	m
b_s	Saturation buoyancy	ms^{-2}
x_b^-	Inner boundary of shell	m
x_b^+	Outer boundary of shell	m
η_b	Self-similarity variable	$[-]$
l_s	Shell thickness from DNS data	m
$\bar{k}$	Mean turbulent kinetic energy	m^2s^{-2}
$\bar{\varepsilon}$	Turbulent dissipation rate	m^2s^{-3}
τ	Turn over time for largest eddy in the shell	s
l_e	Length scale for largest eddy in the shell	m
c_0, c_1, c_2	Coefficients for power law	m
St	Stokes number	$-$
Sv	Settling velocity dimensionless parameter	$-$
Re_p	Particle Reynolds number	$-$
r_c	Cross-over length scale	m
u_η	Kolmogorov velocity scale	m
t_η	Kolmogorov time scale	m
Re_λ	Taylor Reynolds number	$-$
$\langle k \rangle_v$	Volume averaged turbulent kinetic energy	m^2s^{-2}
u_e	Integral velocity scale	ms^{-1}
t_e	Integral time scale	s

L_e	Integral length scale	m
$\langle \varepsilon \rangle_v$	Volume averaged turbulent dissipation rate	$m^2 s^{-3}$
u_{rms}	Root mean square of the turbulent velocity fluctuations	ms^{-1}

Chapter 1

Introduction

Uncertainties and biases in the representation of cloud processes and their radiative properties in Global Climate Models (GCMs) are believed to be one of the largest uncertainties in understanding changes in the climate system. These uncertainties are considered to be responsible for the spread in modelled climate sensitivities and other regional errors in cloud radiative effects (Boucher et al. [2013](#)).

Clouds involve physical and chemical processes extending over a large range of spatial and temporal scales. Turbulence, like clouds, is ubiquitous and the relationship between turbulence and cloud microphysics is a major research problem and rightly so. Turbulence plays a very important role in the formation, evolution and dissipation of a cloud. Cloud-turbulence interactions also take place across a wide range of scales ranging from large-scale engulfment at cloud edges, to droplet-turbulence interaction at the smallest scales as shown in figure 1.1. Different degrees of complexity arise in the representation of clouds and microphysics based on the spatial and temporal resolutions of the models. Clouds are being represented on a more individual basis in recent operational models and it is important that the understanding of mixing and microphysics in cloud structures are improved.

Of special interest are warm (no ice formation), shallow (non-precipitating) cumulus clouds as they contribute more significantly to cloud fraction than larger clouds, and are prevalent over both ocean and land (Norris [1998](#); Koren et al. [2008](#)). A significant area of current research in meteorology is dedicated to the interfaces of clouds with the dry troposphere air as this involves

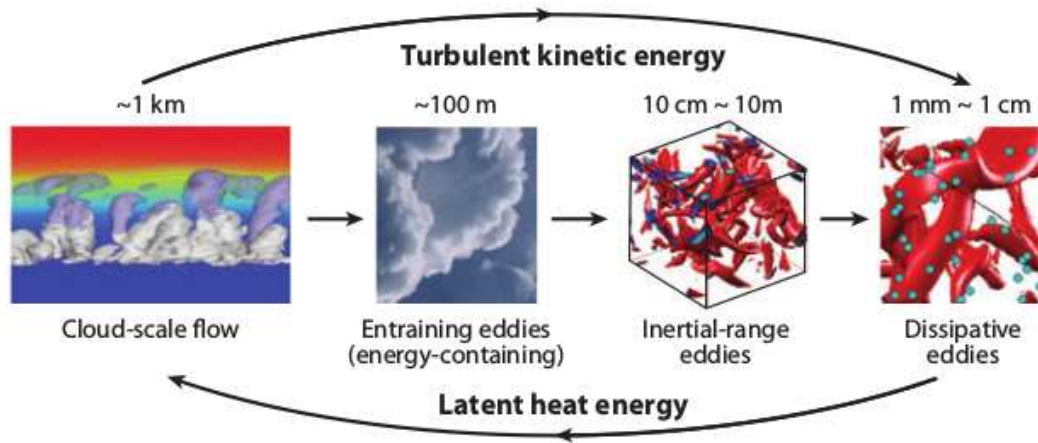


Figure 1.1: Interaction across different scales in clouds. Reproduced with permission from Grabowski and L.-P. Wang (2013).

rapid thermodynamic and micro-physical changes in cloud properties (de Rooy et al. 2013).

Even to an everyday observer, the three-dimensional and turbulent nature of a cumulus cloud, and the sharp interface between a cloud and the clear environment are obvious. At these highly convoluted and irregular edges, there is large-scale entrainment of dry environment air into the cloud. The transfer and transport of vertical momentum, moisture and heat by convection through the clouds is determined by the rate of entrainment and detrainment (de Rooy et al. 2013). In addition to such large scale interactions, entrainment also sets off a series of events that cascade down to the smaller scales. The entrained air is normally drier than the cloudy air, and this causes the cloud droplets close to the boundary to evaporate. The resulting evaporative cooling leads to the formation of a negatively buoyant layer hence establishing a horizontal buoyancy gradient across the cloud edge. This increases the complexity at the edge of a cloud. In order to understand the effects of clouds on the global climate, it is important to understand how entrainment affects cloud microphysics, as well as the role of interactions at extremely small-scale processes in determining the macroscopic properties of clouds like lifetime, extent, radiative properties and precipitation efficiency (Shaw 2003).

Regardless of resolution, there are certain processes which are a weak point in cloud models. These are the representation of cloud microphysics, precipitation and cloud-aerosol interaction (Boucher et al. 2013). Certain key processes have been identified as affecting the microphysics of warm clouds. These include droplet nucleation on Cloud Condensation Nuclei (CCN) at

the cloud-base, consequent adiabatic growth above the base, changes to the cloud droplet size distribution due to entrainment (including addition of new CCN) and subsequent dilution, and collision-coalescence. In this thesis, we focus on the role of entrainment on modifying the droplet size distributions as well as the effect of entrainment on cloud-aerosol interactions. Collision-coalescence is also studied, but at the edge of a cloud where the effects of entrainment are felt the most.

Entrainment of unsaturated air at the cloud-environment interface is capable of diluting the droplet population, can shrink the droplets through evaporation and can also introduce additional CCN. This has been shown to be one of the reasons for the broadening observed in cloud droplet size distributions (Jensen, Austin, et al. 1985; Jensen and Baker 1989; Pinsky and Khain 1997; Lasher-trapp, Cooper, and Blyth 2005). The entrainment of dry air also leads to fluctuations in the local supersaturation field which can lead to droplets arriving at the same point experiencing different supersaturation histories. This can cause differences in the droplet growth histories and hence a broader droplet size distribution than in an adiabatic parcel. (Cooper 1989; Srivastava 1989; Gerber 1991; Shaw 2003).

Another interesting process where turbulence and droplets interact is preferential concentration: particles or droplets that are heavier than the carrier fluid in which it is dispersed tend to accumulate or form 'clusters'. These clusters are formed in regions of high strain and low vorticity thus leading to inhomogeneities in the particle concentration (Maxey 1987; K. D. Squires and Eaton 1991; L.-P. Wang and Maxey 1993; Eaton and Fessler 1994; Fessler, Kulick, and Eaton 1994). This is important since the theory of droplet collision in clouds and even some elements in radiative transfer is based on the assumption that droplets are randomly distributed (Saffman and Turner 1956; Kostinski 2001). The role of gravity on preferential concentration has not been extensively studied. Gravity can play an important role at the edge of a cloud, especially on larger droplets formed due to collision-coalescence (Perrin and Jonker 2015). In this thesis, the role of gravity on preferential concentration is also explored.

One aspect of the interaction between particles/droplets and small-scale turbulence can be seen in the localized mixing at the cloud edge which results in the evaporation of water droplets leading to absorption of latent heat and the formation of a cold layer of mixed air. This

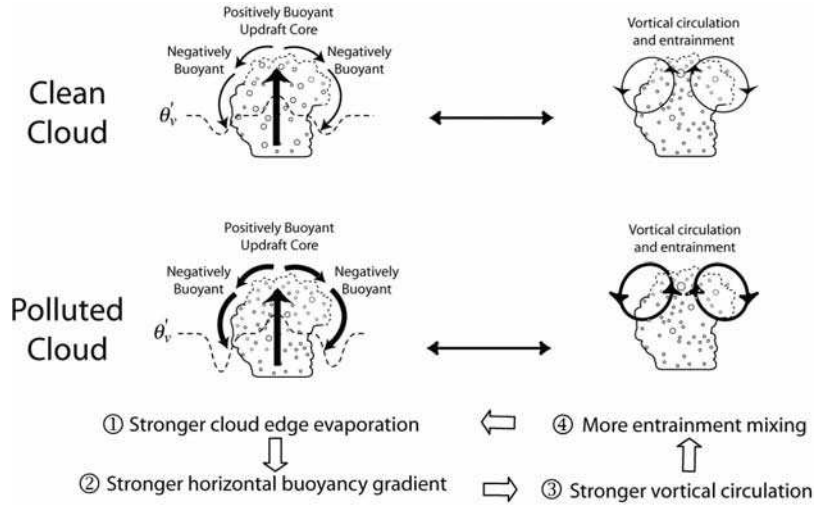


Figure 1.2: Evaporation-entrainment feedback mechanism. Reproduced from Small et al. (2009) with permission.

negatively buoyant 'shell' of subsiding mixed air has been observed in aircraft observations and numerical simulations (Jonas 1990; Heus and Jonker 2008; Katzwinkel et al. 2014). A positive feedback loop is created between droplet dynamics and small-scale turbulence with evaporation increasing the turbulence intensity in the mixing layer and the increased mixing driving further evaporation as shown in figure 1.2 (Small et al. 2009). The important aspects of droplet dynamics that has to be modelled in order to study these interactions are the tracking of individual particle/droplet Lagrangian trajectories and the changes in droplet size associated with condensation/evaporation and collision-coalescence. In the following section, the different methods of modelling a cloud edge is introduced.

1.1 DNS as a computational tool to study cloud edges

Cloud observational campaigns and experimental studies in cloud chambers and other setups are well complemented by numerical simulations of both individual and entire fields of clouds. Numerical simulations resolving individual clouds are dominantly Large Eddy Simulation (LES) studies. An LES simulation for shallow cumulus convection resolving the smallest cloud would have a relatively fine resolution of $\Delta x = \Delta y = \Delta z = 25m$ with a horizontal computational domain size of $25km \times 25km$ (Heus and Seifert 2013). Even though LES captures the large scale processes very well, these simulations are unable to resolve the finer details of cloud-edge mixing. Direct Numerical Simulation (DNS) studies are much more effective when it comes

to capturing small-scale dynamics as they resolve scales down to the Kolmogorov scale which are the smallest scales in the velocity field in a multi-scale turbulent flow. To study the effects of large scale turbulent mixing and entrainment at cloud edges on its microphysics, DNS offers a very good opportunity to develop idealized, canonical setups where the effect of different processes can be studied by carefully choosing domains and including only relevant physical processes/ microphysics.

Modelling a cloud edge is quite a challenging task given the complexity of the processes and the range of spatial and temporal scales involved. Entraining eddies in a cumulus cloud with a mean dissipation rate $\varepsilon = 10^{-2} m^2 s^{-3}$ have a length scale $l_e \approx 100m$ and a time scale $t_e \approx 100s$. The smallest scales of mixing in a cloud core or at the cloud edge are the Kolmogorov scales with length scale $\eta \approx 1mm$ and time scale $t_\eta \approx 0.04s$ (Grabowski and L.-P. Wang 2013). In this thesis, the micro-scale mixing at a cloud-clear air (environment) interface is simulated using DNS. In DNS, the turbulent flow is resolved down to the Kolmogorov scale, but the effects of large scale eddies which play an important role in actual clouds are not considered due to computational limitations. As is common to DNS studies of cloud turbulence, highly idealized initial and boundary conditions are used and the final stages of the entrainment-mixing process (after engulfment by large scale eddies) are simulated.

DNS studies of the cloud edge adopt a developing mixing layer as a paradigm for a small region at the edge of a cloud (Andrejczuk, Grabowski, et al. 2004, 2006, 2009; Kumar, Schumacher, and Shaw 2013, 2014; Götzfried et al. 2017). These setups are inspired by numerous experimental and computational studies on shearless mixing layers which are interfaces between two region with different turbulence intensities but the same mean velocity (Gilbert 1980; Veeravalli and Warhaft 1989; Tordella and Iovieno 2006, 2011). A similar sharp and well-defined interface exists between highly turbulent cumulus clouds and the less turbulent environment (Shaw 2003), which makes such setups relevant in studying lateral entrainment. Studies of the entrainment of inertial particles in shearless mixing layers also exists, which though ignoring the thermodynamic processes (phase changes), extensively studies particle behaviours across these interfaces (Good, Gerashchenko, and Warhaft 2012; Ireland and Collins 2012; Gerashchenko and Warhaft 2013).

A setup which is closely related to the shearless mixing layers is that of a temporal plume, where a buoyant plume that is evolving in time rather than space represents the cloud layer (Krug et al. 2017). One of the advantages of such a setup is that especially for studies focused on the dynamics at the interfaces, the vertical and span-wise directions can be considered to be homogeneous which means that statistics can be obtained by simply averaging over these directions without accounting for different mean-flow states (details in chapter 4). A similar two-layer temporal plume setup is considered in this setup and builds on the work done by Abma, Heus, and Mellado (2013) and Perrin and Jonker (2015).

In this thesis, multiple approaches are adopted for the numerical simulations. Canonical setups are created in such a way that the complex processes at the cloud edge and feedback between turbulence and droplet dynamics can be disentangled. In chapters 4 and 5, a fully Eulerian specification of air, water vapour and liquid water is adopted. In chapters 6 and 7 where droplet dynamics and its interaction with small-scale turbulence are extensively studied, a hybrid Eulerian-Lagrangian framework is adopted with an Eulerian approach for the air and water vapour fields and a Lagrangian approach for water droplets.

1.2 Project scope

This PhD project is part of the Marie Skłodowska-Curie Action European Training Network 'COMPLETE' (Cloud MicroPhysics and Telemetry), which aims to develop an interdisciplinary training network that will prepare early stage researchers with both scientific and industry-oriented skills that will advance our understanding in multi-scale complex natural phenomena in clouds. The principal research objectives of COMPLETE are to:

- 01.** characterize the direct interaction between cloud dynamics, thermodynamics and micro-physics at centimetre and meter scales;
- 02.** develop new telemetry methods for in-situ measurements of aerosols, turbulence, temperature, pressure and chemical content;
- 03.** improve cloud edge/interface models to improve predictions of mixing efficiency, temperature inversion, entrainment and detrainment;

- 04.** compare in a Lagrangian framework, radiative measurements and data obtained inside warm clouds;
- 05.** transfer the knowledge acquired by field and laboratory Lagrangian measurements and DNS modelling towards the climate/weather modelling community.

The research to be undertaken by COMPLETE is structured by formulating sets of five hypotheses which sets the departing points for the research program. The foundation of this thesis is based on one of these hypotheses which is presented below,

"Understanding the dynamics of turbulent-non turbulent cloud interfaces is fundamental to correlate the mixing and entrainment/detrainment processes and the sizing and spatial distribution of particles. To gain insight into droplet behaviour at the edge of clouds, laboratory experiments and high resolution direct numerical simulations must be carried out to study the conditioned statistics of inertial sub-Kolmogorov particles in shearless turbulent-non turbulent and turbulent-turbulent mixing layers."

In line with this hypothesis, we aim to understand the dynamics of cloud-edge mixing and the dynamics of particles/droplets at the different cloud-environment interfaces using numerical techniques in this thesis. The numerical code SPARKLE will be used to perform direct numerical simulations on a cloud-environment model. Initial work will focus on the behaviour of cloud boundaries using a bulk condensation scheme that describe the flow and processes in the domain under study. The work progresses into a more actual representation of cloud edges and SPARKLE is complemented with a microphysics routine to develop a model which is more representative of actual cloud conditions. A detailed study of the behaviour of particles at the cloud boundaries and the effect of entrainment on the cloud droplet size distributions is performed. The specific aims and objectives are now detailed.

This thesis aims to study cloud-turbulence interaction and hence improve the understanding of the role of entrainment at cloud edges on the different cloud microphysical processes. The main objectives are:

1. Understand the dynamics of flow in a subsiding shell at the edge of shallow cumulus clouds using a bulk condensation scheme.

2. Identify the different interfaces at the edge of a cloud and study the dynamics of massless particles crossing these interfaces.
3. Analyse the effect of gravity on the preferential concentration and geometric collision rates of a polydisperse distribution of sub-Kolmogorov sized inertial droplets in isotropic homogeneous decaying turbulence.
4. Study the effect of aerosol perturbations on cloud properties (strength of the subsiding shell, droplet size distribution etc) by varying the initial sizes of a monodisperse distribution of cloud droplets that can grow through condensation and collision-coalescence.

1.3 Thesis structure

The thesis is structured in such a way that the effects of cloud microphysics are introduced in a step-by-step process, with an incremental increase in modeling complexity. In chapter 2, a detailed description of the physics of cloud droplet growth is presented along with the modeling approach taken in this thesis. Chapter 3 provides details on the implementation of the cloud microphysics routine in SPARKLE and its validation. In chapter 4, we study the dynamics of subsiding shells in shallow cumulus clouds using a bulk condensation scheme to mimic cloud thermodynamics in an Eulerian framework. We then proceed to a Lagrangian framework in chapter 5, and study particle behaviour during entrainment and detrainment across the different interfaces at a cloud edge. In chapter 6, the effect of gravity on droplet clustering and collision in isotropic homogeneous turbulence is studied. In chapter 7, the effect of aerosol perturbations on the cloud shell strength and droplet size distribution is studied. Finally, in chapter 8, the results from the entire thesis are summarized and conclusions are drawn.

Chapter 2

Modeling of cloud microphysics

In this chapter, different methods of modeling cloud microphysics are introduced. A detailed theoretical description of the basic thermodynamic variables and the physics of cloud droplet growth is presented. A conceptual introduction and a statistical formulation of the droplet collision-coalescence process is also given.

The set of physical processes governing the formation of cloud droplets and ice crystals, their growth, and their fallout as precipitation is referred to as cloud microphysics. These processes act on the scales of cloud droplets and hydrometeors (with diameters of the order of micrometers to millimeters), which means that their effects are parameterized in numerical weather prediction models. Some of the significant processes are nucleation, condensation growth by vapor diffusion, collision and coalescence, freezing and melting (figure 2.1). Capturing these processes accurately in cloud models is extremely difficult due to the large number of particles, wide variety of microphysical species and the complex nonlinear interactions among different processes. The main microphysical species are: water vapor, cloud droplets, rain droplets, cloud ice crystals, snow, rimed ice, graupel and hail. Since we deal only with warm shallow clouds in this thesis, we discuss only the formation, growth and decay of water vapor and cloud droplets. The importance of cloud microphysical processes are numerous. An important microphysical process is the latent heating associated with the condensation of water vapor (and also sublimation and freezing) and the cooling due to the evaporation of droplets. This is a key element of climate dynamics and can drive phenomena such as convectively generated cold pools and mid-tropospheric mesoscale convective vortices. Also, the sedimentation of

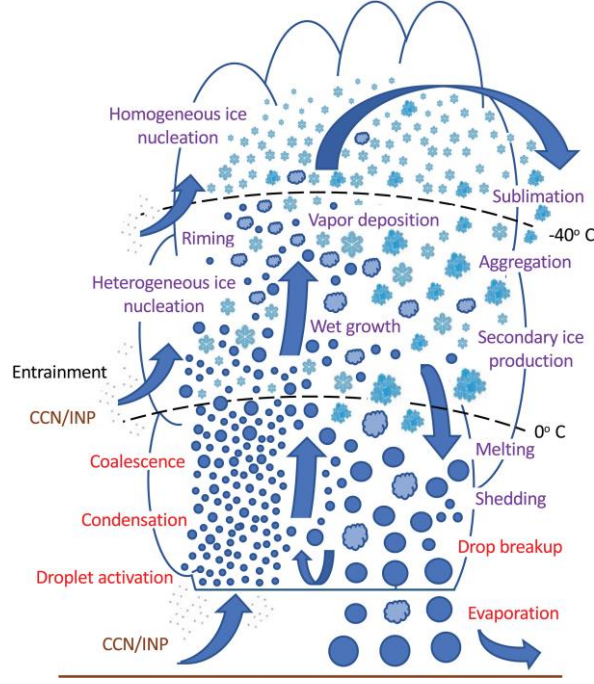


Figure 2.1: Microphysical processes in a typical cumulonimbus cloud. The processes shown in red involve only liquid drops and in purple involves ice particles or both liquid and ice. Figure reproduced from (Morrison et al. 2020).

larger particles results in precipitation. Microphysical processes also affect the radiative budget through cloud shading, absorption and emission of radiation etc.

Most current numerical weather prediction models and global climate models employ an Eulerian approach for modelling the sparse population distribution of cloud droplets and ice particles. There are two main classes of parameterizations using the Eulerian approach: *Bulk* and *Bin* schemes. These are differentiated by how they represent the evolution of the *size distribution*, which relates the total particle number concentration per unit volume (N) to particle diameter (D) for each of the different microphysical species.

The general form of the kinetic microphysics equation that governs the evolution of a hydrometeor population is given by (Morrison et al. 2020)

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla f - \frac{1}{\rho} \frac{\partial(\rho w_T f)}{\partial z} = \left(\frac{\partial f}{\partial t} \right)_{\text{diff}} + F_1 + F_2 + \dots F_N. \quad (2.1)$$

where $f(\mathbf{x}, t, \mathbf{q})$ is a distribution function representing the hydrometeor population in a location given by the vector $\mathbf{x}$ at time t and the vector $\mathbf{q}$ represents the particle attributes. A common attribute is the particle diameter D in which case equation 2.1 represents the evolution of

the particle size distribution. Other possible attributes are ice particle aspect ratio, dissolved solute mass etc, but for the sake of clarity, the attribute considered in this section is D . Also, $\mathbf{u}$ is the velocity vector, $\left(\frac{\partial f}{\partial t}\right)_{\text{diff}}$ is diffusion in physical space, w_T is the particle fall (sedimentation) velocity, and $F_1, F_2, \dots, F_N$ are the individual microphysical processes that affect f like condensation, freezing etc. In standard Eulerian schemes, equation 2.1 is solved by predicting a set of microphysical state variables related to f .

In *Bulk* schemes, bulk hydrometeor properties that depend only on $\mathbf{x}$ and t are taken as the state variables. These are usually expressed as weighted integrals, or *moments*, of f over $\mathbf{q}$ (D for the size distribution), i.e. $M_k = \int_{D_{\min}}^{D_{\max}} D^k f(D) dD$ for the k th order moment of f . Prognostic equations are formulated for one or more moments of the distribution function f . A closure problem then arises since the rate of change of a predicted moment of a given order depends on the moments of other orders. The closure is usually provided by assuming an analytical functional form for f , usually a gamma function or a logarithmic function. An example of a commonly used three parameter gamma distribution is given by

$$f = N_0 D^\alpha e^{(-\lambda D)}, \quad (2.2)$$

where N_0 is an intercept parameter, α is a shape parameter that gives a measure of the spectral width, and λ is the slope or scale parameter.

Each moment is associated with one predicted parameter: the intercept parameter N_0 can be related to the total number concentration N (the zeroth order moment M_0), the shape parameter α can be related to the radar reflectivity factor Z (the sixth order moment M_6), and the slope parameter λ can be related to N_0 and the mass fraction q (the third order moment M_3). Hence three prognostic equations for the moments are required to determine the three parameters uniquely. However it is common to follow an approach where only one or two moments are predicted and the remaining parameters are prescribed as constant or diagnosed.

There are three main classes of bulk parameterizations: single, double and triple moment schemes based on the number of predicted parameters. For a detailed list of works using the three schemes, see the reviews by Grabowski, Morrison, et al. (2019) and Morrison et al. (2020). Single moment parameterizations predict the mass fraction q_c of species with the

prognostic parameter being λ , and N_0 and α kept constant. Double-moment schemes have prognostic equations for both q_c and N with λ and N_0 determined prognostically, and α kept a constant. Finally, triple-moment schemes have an additional prognostic variable, Z , hence having three prognostic variables λ , N_0 and α . The single or double moment schemes are the most widely used schemes for operative parameterizations. The bulk schemes are effective and computationally cheaper than bin schemes and are considered the workhorses of the operational climate and weather prediction models (Grabowski, Morrison, et al. 2019).

In *Bin* schemes (also referred to as *spectral* schemes), the particle size distribution is calculated by solving the explicit microphysical equations for the different species. Therefore, no initial expression of the size distribution is assumed similar to the gamma distribution in the bulk schemes. The function f is discretized over $\mathbf{x}$, t and $\mathbf{q}$, where $\mathbf{q}$ is usually the particle radius or diameter. The size distribution is hence calculated over a finite difference size/radius grid consisting of tens to several hundred bins. These schemes predict state variables within a model volume over the size interval of the distribution (bins). The number of equations to be solved is proportional to the number of bins and the number of species. Typically the bin schemes have about 200-300 prognostic variables while bulk schemes have 6-18 variables. Due to the higher accuracy of bin schemes, they serve as 'benchmarks' against which bulk schemes are developed and tested (Grabowski, Morrison, et al. 2019).

Another approach which has become popular over the last 10 years is the Lagrangian particle based method where the particle population is represented by *super-particles* or *super-droplets* which are discrete ensembles of cloud and precipitation particles (Andrejczuk, Reisner, et al. 2008; Shima et al. 2009; Sölch and Kärcher 2010). In these schemes, a set of ordinary differential equations that evolve as a collection of super-particles replace the partial differential equation given by equation 2.1. Each super-particle represents a group of real particles/hydrometeors and maintain a trajectory following the fluid flow. They also grow or shrink as they move with the flow. Each super-particle has a parameter called the *multiplicity* which represents the total number of particles with similar properties as that of the super-particle. The Lagrangian schemes are considered to be a good alternative approach with advantages coming from replacing the partial differential equations with ordinary differential equations for the transport

and growth of the super-particles, which eliminates the numerical diffusion associated with Eulerian approaches. However insufficient number of super-particles in a given simulation may introduce errors (Grabowski, Morrison, et al. 2019).

In view of the need to resolve very small scales to capture the different processes in a turbulent cloud, DNS is the only approach capable of explicitly simulating the growth of individual cloud particles. In DNS, spatial and temporal flow scales down to the Kolmogorov scales are resolved along with explicit modelling of individual hydrometeors which comes at a high computational cost. Hence, the majority of the DNS studies focus on the effect of turbulence on the cloud droplet growth due to condensation and collision-coalescence (Shaw 2003; Devenish et al. 2012; Grabowski and L.-P. Wang 2013, and references therein).

In this thesis, both Eulerian and Lagrangian approaches are adopted for representing the microphysical processes of condensational droplet growth and collision-coalescence. In chapters 4 and 5, a fully Eulerian specification of air, water vapour and liquid water is adopted. These are governed by the continuity equations, the Navier-Stokes equations and convection-diffusion equations for two active scalars. In chapters 6 and 7, where droplet dynamics and its interaction with small-scale turbulence are extensively studied, a hybrid Eulerian-Lagrangian framework is used with an Eulerian approach for the air and water vapour fields and a Lagrangian approach for water droplets. In the following sections, detailed definitions of the thermodynamic variables and the theory behind the modelling of the droplet dynamics is discussed.

2.1 Thermodynamic variables

The thermodynamics of dry convection can be represented using two variables: the potential temperature θ , and the specific humidity q_v . These quantities remain conserved for adiabatic and isobaric mixing. The potential temperature θ is defined as the temperature an air parcel would have if adiabatically brought to a height where the pressure is p_0 , which (by convention) is usually taken as $p_0 = 1 \times 10^5 \text{ Pa}$. Combining the first law of thermodynamics and the ideal gas law $p v = R T$, where R is the gas constant, $v = V/M$ is the specific volume of the system with volume V , mass M , pressure p and temperature T , an expression for the potential temperature

is given by

$$\frac{T}{\theta} = \left(\frac{p}{p_0} \right)^{\frac{R}{c_p}}. \quad (2.3)$$

The quantity $\Pi = \left(\frac{p}{p_0} \right)^{\frac{R}{c_p}}$ is called the Exner function and is an important parameter in atmospheric modelling. Since we are dealing with dry convection, $R = R_d$ is the specific gas constant of dry air.

The specific humidity q_v is the ratio of the mass of water vapour in an air parcel to the total combined mass of dry air and water. The mass fractions of liquid water (q_l) and ice (q_i) can be defined in a similar way, i.e.

$$q_v = \frac{m_v}{m}, \quad q_l = \frac{m_l}{m}, \quad q_i = \frac{m_i}{m}. \quad (2.4)$$

where $m = m_d + m_v + m_l + m_i$ is the total mass of the air parcel including dry air and water, and the indices d , v , l and i indicate the mass of dry air, water vapor, liquid water and ice phase respectively. Since only warm clouds are considered in this thesis, m_i will be neglected.

Describing the thermodynamic state in moist convection is more complex than dry convection due to phase changes of water. Using q_l , two new variables can be defined to describe the temperature and humidity in moist convection processes. These are the liquid water potential temperature θ_l , and the total water mass fraction q_t (Betts 1973). These quantities are conserved for moist adiabatic processes, including phase changes between vapour and liquid water, and will be defined below.

The total water mass fraction q_t is the ratio of the mass of water (both vapour and liquid) in an air parcel to the mass of the total moist air in the same air parcel. Hence,

$$q_t = q_v + q_l. \quad (2.5)$$

The liquid water potential temperature θ_l specifies the temperature that a moist air parcel would have if it is reversibly transferred to a reference pressure and a reference state where all the

liquid water has evaporated. Betts (1973) derives θ_l as

$$\theta_l \approx \theta \exp\left(-\frac{L}{c_p} \frac{q_l}{T}\right), \quad (2.6)$$

where the approximation follows from using the dry values for the specific heat (c_p) and gas constant (R_d) for a moist air parcel, i.e. $c_{pm} = c_p$ and $R_m = R_d$ and L is the latent heat of vaporization of water. A Taylor series expansion around $q_l = 0$ gives

$$\theta_l \approx \theta - \frac{L}{c_p} \frac{\theta}{T} q_l. \quad (2.7)$$

The gas law for a moist air parcel can be expressed as

$$p = \rho R_d T_v. \quad (2.8)$$

The effect of water vapor and liquid water on the density can be expressed through the virtual temperature T_v . It is defined as the temperature that a given air parcel of a particular temperature and pressure would have if the parcel was completely free of water. It is given by the expression

$$T_v = T \left(1 + \left(\frac{R_v}{R_d} - 1\right) q_v - q_l\right), \quad (2.9)$$

where R_v is the specific gas constant for water vapor. The corresponding virtual *potential* temperature is defined as

$$\theta_v = \frac{T_v}{\Pi}. \quad (2.10)$$

2.2 Bulk condensation scheme

In the Eulerian framework, the prognostic variables used to describe the thermodynamic state of air are θ_l and q_t . The effect of cloud microphysics is captured through the variable q_l which is calculated using a bulk approach that was originally developed by Sommeria and Deardorff (1977) and is quite commonly used in LES. In addition to the dry air and water vapor, the disperse liquid phase is also modeled as a continuum. The scheme was originally developed

to address shortcomings in existing condensation schemes in cloud models which assumed a computational grid volume to be completely saturated or unsaturated. Even with very good grid resolutions this could be a seriously flawed assumption since a large portion of grid cells with saturated air lie near or contain the cloud boundary which is highly convoluted. There are also possibilities of pockets of unsaturated air within the saturated cloud core due to merging of lateral clouds or entrainment. Sommeria and Deardorff (1977) developed a condensation scheme to derive the dependencies of the mean liquid water content ($\bar{q}_l$) on humidity statistics assuming a joint normal probability distribution of q_t and θ_l within a computational grid cell. Also implicit in this scheme is the assumption that supersaturation effects are neglected, i.e. all moisture above the water vapor saturation value q_s is liquid water.

This approach should be not be confused with the bulk microphysics schemes. However, in this thesis, the condensation scheme from Sommeria and Deardorff (1977) is referred to as a bulk scheme to differentiate it from the scheme used in the Lagrangian framework where q_l can be calculated by counting the number of liquid droplets in each grid cell (see section 2.3.2).

The core of the scheme lies in the calculation of the saturation specific humidity q_s as a function of the absolute temperature T and pressure p , i.e. $q_s \equiv q_s(T, p)$. Since supersaturation effects are not considered, if $q_t < q_s$, then $q_t = q_v$. We can then calculate q_l using

$$q_l = \begin{cases} q_t - q_s & \text{if } q_t > q_s \\ 0 & \text{if } q_t \leq q_s \end{cases} \quad (2.11)$$

The saturation specific humidity $q_s(T, p)$ is calculated as follows. First, a liquid water temperature T_l corresponding to θ_l is defined as

$$T_l = \Pi \theta_l. \quad (2.12)$$

Now $q_s(T, p)$ can be calculated using a Taylor expansion around $T = T_l$

$$q_s(T, p) = q_{sl} + \left(\frac{\partial q_s}{\partial T} \right)_{T=T_l} (T - T_l) + O(\Delta T^2), \quad (2.13)$$

where $q_{sl} = q_s(T_l, p)$. For ideal gases, the specific humidity of saturated water vapor can be expressed using the saturation vapor pressure e_s as

$$q_{sl} = \frac{e_s(T_l)}{p - \left(1 - \frac{R_d}{R_v}\right) e_s(T_l)} \frac{R_d}{R_v}, \quad (2.14)$$

where $e_s(T_l)$ is the saturation vapour pressure calculated using the Tetens formula (Tetens 1930)

$$e_s(T_l) = e_{s,0} \exp \left[a \frac{T_l - T_{trip}}{T_l - b} \right], \quad (2.15)$$

with constants $e_{s,0} = 610.78$ Pa, $T_{trip} = 273.16$ K, $a = 17.27$ and $b = 35.86$.

The gradient $\frac{\partial q_s}{\partial T}$ is obtained from the Clasius-Clapeyron equation,

$$\left(\frac{\partial q_s}{\partial T} \right)_{T=T_l} = \frac{L q_{sl}}{R_v T_l^2}. \quad (2.16)$$

Substituting equations 2.14, 2.15 and 2.16 into equation 2.13 yields

$$q_s = \left(\frac{1 + \beta_1 q_t}{1 + \beta_1 q_{sl}} \right) q_{sl}, \quad (2.17)$$

where

$$\beta_1 = \left(\frac{L}{R_v T_l} \right) \left(\frac{L}{c_p T_l} \right). \quad (2.18)$$

2.3 Droplet Dynamics

The phenomena governing the behaviour of droplets at cloud-environment boundaries are not well understood in spite of years of research. The full thermodynamic coupling between the turbulent flow and the dispersed droplets that are able to grow or evaporate depending on local conditions, collide with each other and also settle out of the flow due to the effect of gravity, adds to the complexity at cloud boundaries. Studying droplet-turbulence interaction requires a hybrid Eulerian-Lagrangian framework to implement the multiphase flow involving the turbulent air and water droplets. The Eulerian description of the turbulent velocity, temperature and water

vapour fields are combined with the Lagrangian description of an ensemble of cloud water droplets. The cloud droplets are modelled as small rigid inertial point spheres which are subjected to Stokes drag and gravitational settling. Additional complexity can be added by allowing the droplet size to increase or decrease by diffusion and collision-coalescence.

2.3.1 Equation of motion

Building on the works of Basset (1888), Boussinesq (1903), Oseen (1927), Tchen (1947) and Corrsin and Lumley (1956), Maxey and Riley (1983) reformulated the equation of motion for a small rigid sphere in a non-uniform flow as,

$$\begin{aligned}
 m_p \frac{d\mathbf{v}}{dt} = & \underbrace{(m_p - m_f)\mathbf{g}}_1 \\
 & + \underbrace{m_f \frac{D\mathbf{u}}{Dt}\bigg|_{\mathbf{X}(t)}}_2 \\
 & - \underbrace{\frac{1}{2}m_f \left(\frac{d\mathbf{v}(t)}{dt} - \frac{d}{dt} \left(\mathbf{u}(\mathbf{X}, t) + \frac{1}{10} R^2 \nabla^2 \mathbf{u}|_{\mathbf{X}(t)} \right) \right)}_3 \\
 & - \underbrace{6\pi\mu R \mathbf{V}(t)}_4 \\
 & - \underbrace{6\pi\mu R^2 \int_0^t \frac{d\mathbf{V}(\tau)}{d\tau} \frac{d\tau}{[\pi\nu(t-\tau)]^{\frac{1}{2}}}}_5
 \end{aligned} \tag{2.19}$$

where

$$\mathbf{V}(t) = \mathbf{v}(t) - \mathbf{u}(\mathbf{X}(t), t) - \frac{1}{6} R^2 \nabla^2 \mathbf{u}|_{\mathbf{X}(t)}$$

Here $\mathbf{X}(t)$ and $\mathbf{v}(t)$ are the particle position and velocity vectors at time t , m_p is the mass of a sphere of radius R , m_f is the mass of fluid displaced by the sphere, $\mathbf{u} = (u, v, w)$ is the fluid velocity vector with u , v and w as the horizontal, transverse and vertical components respectively, μ is the dynamic viscosity of the fluid and $\mathbf{g} = -g \hat{z}$ where $g = |\mathbf{g}|$ is the acceleration due to gravity and $\hat{z}$ is a unit vector pointing in the positive vertical axis $\hat{z}$. Also, d/dt is a

time derivative in a reference frame moving with the particle and D/Dt is the time derivative following the fluid element.

The terms on the RHS of equation 2.19 correspond to the different forces acting on the spherical particle. The first term is the buoyancy force, the second term is the force on the particle exerted by the undisturbed flow field (fluid pressure gradient and viscous stresses), the third term is the added mass which represents the force required to accelerate the mass of the fluid surrounding and moving with the sphere (the increment being one-half the mass of the fluid displaced i.e. $1/2m_f$), the fourth term is the viscous drag force and the fifth term is the Basset history force. The terms containing $R^2\nabla^2\mathbf{u}$ are the Faxén correction terms which account for the non-uniformity of the flow at scales comparable to the particle diameter and is proportional to $\nabla^2\mathbf{u}$ (Faxén 1922).

This form of the equation of motion for a rigid particle is quite complicated and the evaluation of all the forces requires significant computational efforts. Simplifications can be made to the equation so that only the dominant forces for the problem being studied are determined. The Faxén correction terms become significant mainly in the case of finite-sized particle where the particle diameter D is of the order of η and are usually neglected when $D \ll \eta$ (Calzavarini et al. 2009). For problems in the aerosol regime which involves solid or liquid particles in air, and with a density ratio $\rho_p \gg \rho_f$, the added mass effect and the pressure forces are negligible compared to the Stokes drag. The Basset history force, though of a smaller order of magnitude to the Stokes drag, has been shown to influence particle motion and to be responsible for 10% of the particle acceleration (Mei, Adrian, and Hanratty 1991; Elghobashi and Truesdell 1992; Armenio and Fiorotto 2001; Bergougnoux et al. 2014; Olivieri et al. 2014). However calculating this force is numerically quite challenging as the entire history of the particle acceleration is required. Due to the the added computational cost in computing this, the force is usually neglected in DNS studies of cloud droplet growth (Kuerten 2016; Götzfried et al. 2017). Simplifying equation 2.19 gives

$$m_p \frac{d\mathbf{v}}{dt} = 6\pi R\mu (\mathbf{u}(\mathbf{X}, t) - \mathbf{v}(t)) + m_p \mathbf{g}. \quad (2.20)$$

Dividing by the particle mass m_p reveals an equation of motion that represents a balance between

the viscous drag force produced by the motion of the sphere relative to the surrounding fluid, and the force due to gravity:

$$\frac{d\mathbf{v}}{dt} = \frac{[\mathbf{u}(\mathbf{X}, t) - \mathbf{v}(t) + w_T]}{\tau_p}, \quad (2.21a)$$

$$\frac{d\mathbf{X}}{dt} = \mathbf{v}(\mathbf{X}, t). \quad (2.21b)$$

where $\tau_p = \frac{2\rho_p R^2}{9\mu}$ is the particle relaxation time, $w_T = \tau_p \mathbf{g}$ is the Stokes terminal velocity and ρ_p is the density of water. The particle relaxation time is defined as the characteristic time scale of the particle for relaxing and reacting to changes in the fluid flow.

2.3.2 Condensational growth

Condensational growth is a highly effective process in the early stages of cloud evolution when droplets are a few micrometers in size (Pruppacher and Klett 1978b). Droplet growth due to condensation in a cloud core has been studied extensively using Eulerian-Lagrangian models (Vaillancourt, Yau, and Grabowski 2001; Vaillancourt, Yau, Bartello, et al. 2002; Celani, Falkovich, et al. 2005; Celani, Mazzino, et al. 2007; Lanotte, Seminara, and Toschi 2009; Gotoh, Suehiro, and Saito 2016). The approach adopted by Vaillancourt, Yau, and Grabowski (2001) is followed in this thesis to model the condensational growth of droplets. Droplet growth by diffusion in a turbulent flow involves the transport of water vapor from the environment to the droplet surface, and the transfer of temperature (through latent heat release) from the droplet surface into the environment as well as into the liquid droplet (Sedunov 1974). This transport happens mainly through the process of molecular diffusion. The transport through convection, commonly referred to as the ventilation effect¹, can be neglected for droplets of radius less than $30\mu m$ (Sedunov 1974). Explicitly resolving these processes through a system of three convective-diffusive equations for water vapor and temperature (inside and outside) is highly prohibitive since this would require spatial resolutions of the order of micrometers (droplet diameter). The processes involved in condensational droplet growth can however

¹When a droplets is large, it settles through air with a significant speed hence distorting the spherical symmetry of the vapor field. The vapor field attempts to equilibriate around the droplet surface through steady state diffusion hence enhancing the effective diffusivity and conductivity.

be parameterized as a function of the local ambient conditions defined by the temperature and water vapor fields in each grid cell (Pruppacher and Klett 1978b; Vaillancourt, Yau, and Grabowski 2001). This assumption was justified by Vaillancourt, Yau, and Grabowski (2001) through a comparison of the characteristic time scales of the approach to steady state of the different diffusive processes. For an isolated droplet, the relaxation time of the droplet surface temperature² is identified as the slowest time scale involved in condensational growth. An analysis of the ratio of this droplet time scale to the fastest time scale of the ambient conditions (either the Kolmogorov time scale or the sedimentation time scale³) reveals that for droplets smaller than $20\mu m$ and $\varepsilon < 100cm^2s^{-3}$, the time scale ratios are much smaller than 1, hence rendering the steady state condensation assumption valid. This results in the following equation for the condensational growth of a droplet (Pruppacher and Klett 1978b),

$$\frac{dR^2}{dt} = 2KS. \quad (2.22)$$

Here R is the droplet radius, S is the supersaturation defined as $S = e/e_s(T) - 1$, where the vapor pressure e is calculated from the relation $q_v = \frac{(R_d/R_v) e}{p - e (1 - R_d/R_v)}$ and K is a constant given by $K^{-1} = \frac{\rho_p R_v T}{e_s(T) D_v} + \frac{L \rho_p}{\rho c_p k_a T} \left(\frac{L}{T R_v} - 1 \right)$ (R. R. Rogers and Yau 1989, Chapter 9). Droplets grow in regions of positive supersaturation and evaporate in regions of negative supersaturation. The effect of the condensational growth of the droplet is captured in the evolution equations of the temperature and water vapour through the condensation rate. Implementation details of this routine is given in section 3.4

2.4 Collisions between cloud droplets in DNS

Droplet collision is one of the most important processes in raindrop formation. In Eulerian microphysics schemes like the bulk and bin schemes, collision in clouds are treated by solving stochastic collection equations (Pruppacher and Klett 1978c). A common practise in DNS is to account for the effects of collision by considering droplets as finite volume particles that

²The surface temperature of the droplet changes due to latent heat release during condensation of water vapor from the environment onto the droplet surface.

³The sedimentation time scale is the time it takes for a droplet to sediment across the smallest eddy, i.e., η/w_T

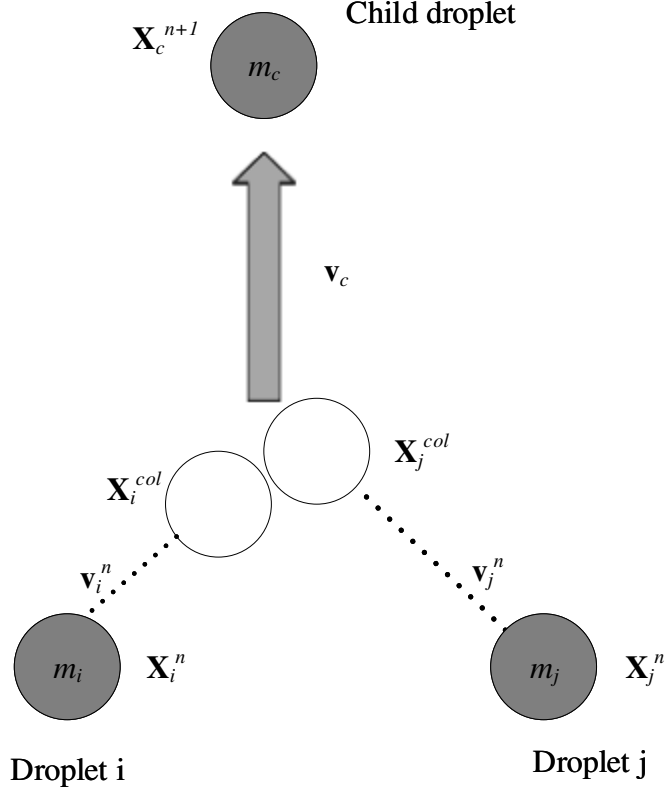


Figure 2.2: Schematic of the collision-coalescence process.

collide and coalesce. DNS studies make use of algorithms that describe particle collision in molecular dynamics simulations. A very popular example is the scheme in Allen and Tildesley (1987, Chapter 3) where hard sphere molecular dynamics is solved. This scheme is implemented in two main steps, the first being the calculation of collision times and the second being the implementation of collision dynamics. Figure 2.2 shows a schematic of the collision-coalescence process of two droplets i and j initially at time t^n . The particles collide at a time t_{col} resulting in the formation of a child droplet of mass m_c and velocity $\mathbf{v}_c$.

2.4.1 Calculation of collision time

In this section, the equations which are solved to determine the time at which two droplets collide is introduced. If two hard spheres i and j , of diameter D , positions $\mathbf{X}_i(t)$, $\mathbf{X}_j(t)$ and velocities $\mathbf{v}_i(t)$, $\mathbf{v}_j(t)$ collide at $t + t_{ij}$, the following equation holds:

$$|\mathbf{X}_{ij}(t + t_{ij})| = D. \quad (2.23)$$

where $\mathbf{X}_{ij} = \mathbf{X}_i - \mathbf{X}_j$. Introducing the relative velocity $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$, and assuming this velocity to be constant over the time interval t_{ij} , we have

$$|\mathbf{X}_{ij}(t + t_{ij})| = |\mathbf{X}_{ij}(t) + \mathbf{v}_{ij}t_{ij}|, \quad (2.24)$$

which can then be rewritten into a quadratic equation in t_{ij}

$$|\mathbf{v}_{ij}|^2 t_{ij}^2 + 2b_{ij}t_{ij} + |\mathbf{X}_{ij}|^2 - D^2 = 0, \quad (2.25)$$

where $b_{ij} = \mathbf{X}_{ij} \cdot \mathbf{v}_{ij}$. The following situations can now be identified,

1. if $b_{ij} > 0$, there is no collision since the spheres are moving away from each other,
2. if $b_{ij} < 0$ and $b_{ij}^2 - |\mathbf{v}_{ij}|^2(|\mathbf{X}_{ij}|^2 - D^2) < 0$, no collision occurs since the roots are complex.

The smaller of the two positive roots corresponds to collision and is taken as the collision time,

$$t_{ij} = \frac{-b_{ij} - (b_{ij}^2 - |\mathbf{v}_{ij}|^2(|\mathbf{X}_{ij}|^2 - D^2))^{1/2}}{|\mathbf{v}_{ij}|^2}. \quad (2.26)$$

2.5 Collision dynamics

The next phase of the collision involves the collision dynamics. Two common cases are elastic collision and coagulation (or coalescence). In the case of elastic collision, the change in velocity of the colliding pair follows from the conservation of energy and linear momentum and the requirement that the impulse acts along the line of centres (Allen and Tildesley 1987, Chapter 3). Assuming conservation of total linear momentum and kinetic energy, the change in velocity $\delta\mathbf{v}_i (= -\delta\mathbf{v}_j)$ for two colliding spheres of equal masses is given by,

$$\mathbf{v}_i(t + t_{ij}) = \mathbf{v}_i(t) + \delta\mathbf{v}_i, \quad (2.27)$$

$$\mathbf{v}_j(t + t_{ij}) = \mathbf{v}_j(t) - \delta\mathbf{v}_i \quad (2.28)$$

where $\delta\mathbf{v}_i = -(b_{ij}/D^2)\mathbf{x}_{ij}$ and $b_{ij} = \mathbf{x}_{ij} \cdot \mathbf{v}_{ij}$ is now calculated at the point of impact.

For implementing coagulation, it is assumed that all colliding pairs coagulate with 100% efficiency. Two colliding spheres produce a child sphere whose size is determined from the conservation of mass (M. Chen, Kontomaris, and McLaughlin 1999; Reade and Collins 2000a),

$$m_c = m_i + m_j, \quad (2.29)$$

$$D_c = \sqrt[3]{D_i^3 + D_j^3}, \quad (2.30)$$

where m_c and D_c are the mass and diameter of the child droplet, and the density of the child droplet is assumed to be the same as that of the parents. The velocity of the child sphere ($\mathbf{v}_c$) is determined from the conservation of translational momentum

$$m_c \mathbf{v}_c = m_i \mathbf{v}_i + m_j \mathbf{v}_j, \quad (2.31)$$

$$\mathbf{v}_c = \frac{D_i^3 \mathbf{v}_i + D_j^3 \mathbf{v}_j}{D_c^3}. \quad (2.32)$$

Finally, the coordinates of the center of the child droplet at the instant of collision is expressed as

$$\mathbf{X}_c = \frac{\mathbf{X}_i + \mathbf{X}_j}{2}. \quad (2.33)$$

2.6 Collision statistics

In this section, the statistical formulation of the collision-coalescence process is introduced. The growth of cloud droplets through the process of collision-coalescence is mainly governed by three consecutive and interrelated processes: 1) geometric collision (rate of geometric overlaps) due to particle-turbulence interaction, (2) collision efficiency due to local aerodynamic interactions between particles, and (3) coagulation efficiency as determined by droplet surface sticking characteristics (L.-P. Wang, Wexler, and Y. Zhou 1998). In this thesis, the aerodynamic interactions between droplets are neglected. A 100% coagulation efficiency is assumed, i.e. all colliding droplets are assumed to coalesce into one bigger droplet. Also, collisions between more than two droplets at the same time are not considered.

Consider a bidisperse system of particles of radius R_1 and R_2 in turbulent flow. The average

geometric collision rate per unit volume $\dot{N}_c$ is

$$\langle \dot{N}_c \rangle = \Gamma_{12}^D \langle n_1 \rangle \langle n_2 \rangle, \quad (2.34)$$

where Γ_{12}^D is the *dynamic* collision kernel which is a measure of the probability of particles geometrically overlapping, $n_1 = N_1/V$ and $n_2 = N_2/V$ are the particle number densities, and N_1, N_2 are the total number of particles of the respective sizes in a domain with volume V . The symbol $\langle \cdot \rangle$ denotes averaging over time. For a monodisperse system of particles the expression becomes (L.-P. Wang, Wexler, and Y. Zhou 1998; Y. Zhou, Wexler, and L.-P. Wang 2001)

$$\langle \dot{N}_c \rangle = \Gamma_{11}^D \frac{\langle n \rangle^2}{2}, \quad (2.35)$$

where Γ_{11}^D is the *dynamic* collision kernel for collisions between droplets of the same size.

Employing a realistic model of turbulence in clouds in their seminal work on droplet collisions to test the role of turbulence in initiating rainfall, Saffman and Turner (1956) formulated a kinematic description of the average geometric collision kernel Γ_{12}^K between particles of two arbitrary size groups. As explained succinctly in Devenish et al. (2012), Γ_{12}^K can be defined as the volume influx of droplets of radius R_2 to a droplet of radius R_1 over the surface of a collision sphere (which has a radius $R_c = R_1 + R_2$ and is centred about the centre of droplets of radius R_1 (figure 2.3)). The Saffman-Turner collision kernel can be expressed as

$$\Gamma_{12} = - \overline{\int_{w_r < 0} w_r dS}, \quad (2.36)$$

where $w_r = \mathbf{w} \cdot \mathbf{r}/|\mathbf{r}|$ is the radial component of the relative velocity $\mathbf{w}$ between two particles with separation vector $\mathbf{r}$. In this case, w_r is calculated at the collision radius, $r = R_c$. In isotropic turbulence, the bar denotes a spatial mean. To evaluate the integral, Saffman and Turner (1956) assumed that the relative velocity $\mathbf{w}$ is incompressible, which means that the influx and outflux over the collision sphere surface are equal. Hence $-\overline{\int_{w_r < 0} w_r dS} = \frac{1}{2} \overline{\int_{sphere} |w_r| dS} = 2\pi r_c^2 \overline{|w_r|}$. The final expression for the average kinematic collision kernel Γ_{12}^K per unit time between two arbitrary particle size groups (body-force-free, inertia-less particles of size less than η) in a

turbulent flow is

$$\Gamma_{12}^K = 2\pi R_c^2 \langle |w_r|(r = R_c) \rangle. \quad (2.37)$$

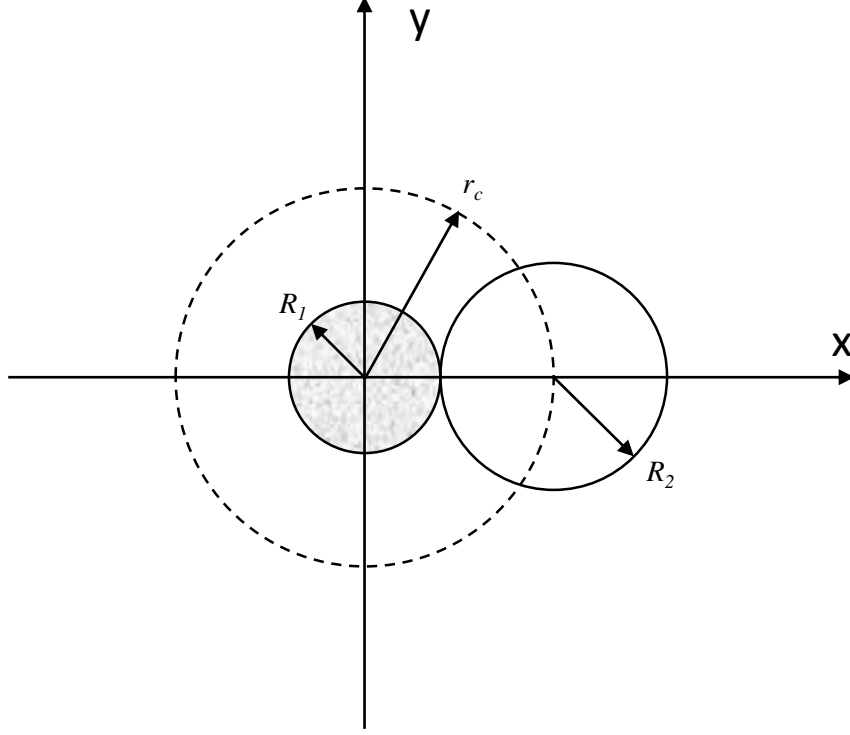


Figure 2.3: The collision sphere in the $\hat{x} - \hat{y}$ plane.

For the basic case of gravitational collision-coalescence of a bidisperse system of droplets falling through quiescent air under the influence of gravity and the hydrodynamic forces associated with their motion, the collision kernel for hydrodynamic capture can be expressed as (Pruppacher and Klett 1978a),

$$K_{12} = \pi R_c^2 |w_{T,1} - w_{T,2}| E_c. \quad (2.38)$$

Here, $w_{T,1}$ and $w_{T,2}$ are the sedimenting velocities of the droplets of radius R_1 and R_2 respectively, and E_c is the collection efficiency. The average of the magnitude of the radial relative velocity $\langle |w_r|(r = R) \rangle = 0.5|w_{T,1} - w_{T,2}|$. The collection efficiency E_c is the ratio of the actual collision cross section πy_c^2 to the geometric cross section πR_c^2 , where y_c is the critical horizontal distance between two droplets below which coalescence is certain to occur (Pruppacher and Klett 1978a; Devenish et al. 2012). If coalescence is assumed to occur anytime when

$y_c < R_c$, then collection efficiency is equal to the collision efficiency which is determined by the droplet-droplet interactions. The gravitational geometric collision kernel Γ_{12}^g is then given by

$$\Gamma_{12}^g = \pi R_c^2 |w_{T,1} - w_{T,2}|. \quad (2.39)$$

The formulation in equation 2.37 assumes that the particle concentration field is uniform in space and the averaging is an ensemble averaging in homogeneous turbulence. However particles have a tendency to accumulate in regions of low vorticity and high strain rate due to an inertial bias (Maxey 1987; K. D. Squires and Eaton 1991; L.-P. Wang and Maxey 1993; Eaton and Fessler 1994; Fessler, Kulick, and Eaton 1994). This preferential concentration can significantly enhance the average collision rates since the local collision rates are proportional to the square of the local concentrations. The effect of preferential concentration is quantified using a statistical quantity introduced by Sundaram and Collins (1997) called the Radial Distribution Function (RDF) which is the ratio of the actual pair concentration to that in a uniform suspension. Hence the most common kinematic formulation for the geometric collision rate of a bidisperse distribution is given by (Sundaram and Collins 1997; L.-P. Wang, Wexler, and Y. Zhou 1998, 2000a),

$$\Gamma_{12}^K = 2\pi R^2 \langle |w_r(r = R_c)| \rangle g_{12}(r = R_c). \quad (2.40)$$

Here, the angular brackets denote averaging over all possible directions of $\mathbf{r}$ in addition to the ensemble averaging over all pairs or averaging over space and time for a homogeneous and stationary system. The RDF is denoted by g_{12} and calculated at each instance of time as,

$$g_{12}(r; t) = \frac{\psi_{12}/V_{\delta_r}}{N_1 N_2 / V}, \quad (2.41)$$

where ψ_{12} is the number of pairs of particles of size R_1 and R_2 found at a separation distance r falling in a spherical shell of inner radius $r_i = r - \delta$, outer radius $r_o = r + \delta$, volume V_{δ_r} and centered on a particle of size R_1 .

Chapter 3

Implementation and validation

In this chapter, the DNS code SPARKLE is introduced. A Lagrangian particle tracking routine and collision-coalescence algorithm and their implementation in SPARKLE are discussed. The validation of these routines is presented. A novel test case, which was developed to validate the different aspects of the Lagrangian particle tracking routine, is also introduced. A detailed step-by-step description of the collision algorithm implemented in SPARKLE is given.

3.1 SPARKLE

The code used in this thesis is SPARKLE, which is a DNS code which solves the incompressible Navier-Stokes equations under the Boussinesq approximation. In addition to the buoyancy, an arbitrary number of scalars can be simulated with the code. The governing equations of SPARKLE are

$$\nabla \cdot \mathbf{u} = 0, \quad (3.1a)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} + b \vec{e}_z, \quad (3.1b)$$

$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = K \nabla^2 \chi, \quad (3.1c)$$

where $\mathbf{u} = (u, v, w)$ is the velocity vector with u , v and w as the horizontal, transverse and vertical components respectively. The buoyancy $b = \beta g \theta$ where θ is the potential temperature, β is the constant coefficient of thermal expansion which is assumed to be equal to $1/\theta_0$ and $\vec{e}_z$ is the unit vector along the positive vertical direction. The variable χ represents the scalar, P is

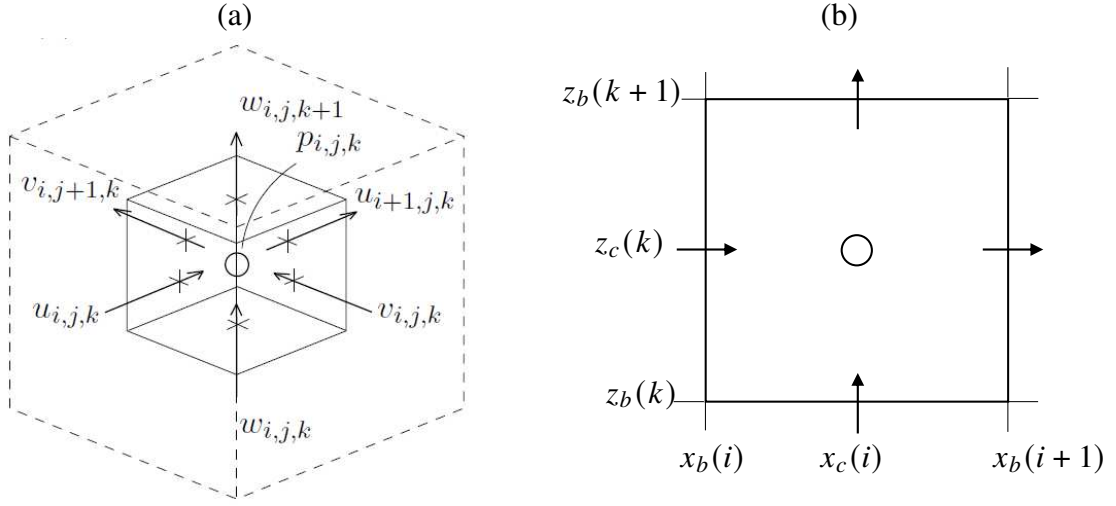


Figure 3.1: (a) A single computational cell showing the staggered arrangement of the variables. The arrows $\rightarrow$ represent the location of flux and $\circ$ represents the location of the transported quantity. (b) Two-dimensional section of a cell centred grid cell.

the kinematic pressure, ν is the kinematic viscosity and K is the scalar diffusivity.

SPARKLE is based on a symmetry-preserving finite volume discretisation (Verstappen and Veldman 2003), and is accurate to fourth order in space. A two-dimensional decomposition along the $\hat{y}$ and $\hat{z}$ directions is employed to parallelize the computations. Details of the numerical scheme, parallelization and boundary conditions are provided in the appendix of Craske (2015) and Craske and van Reeuwijk (2015). Variables are arranged in a staggered manner over the grid with the transported variables defined on the centre of a control volume while the fluxes are defined on face centres. A standard single computational cell in SPARKLE is shown in figure 3.1. The velocity component u is defined at (x_b, y_c, z_c) , v is defined at (x_c, y_b, z_c) , w is defined at (x_c, y_c, z_b) and the scalars are defined on the centre of the cell (x_c, y_c, z_c) . Here, the subscript c stands for the centre coordinate and b stands for the boundary coordinate.

3.2 Implementation of the bulk condensation scheme

For the Eulerian approach adopted in chapters 4 and 5, the prognostic variables for the active scalars $\chi = (\theta_l, q_t)$. As described in section 2.2, the liquid water mass fraction q_l is diagnosed from θ_l and q_t using the bulk condensation scheme at each time step. The buoyancy b (introduced in chapter 4) is then calculated using the value of q_l . Central to the scheme implementation is the calculation of the saturation specific humidity q_s in each grid cell as a function of the

ambient temperature T and pressure p (equation 2.17). The following steps make up the bulk condensation scheme which will be used in chapters 4 and 5.

1. Calculate the Exner function using equation (2.3). The ambient pressure p_0 is assigned a value of the pressure calculated at an altitude of 1000m. This is because the shallow cumuli considered in this thesis are low altitude clouds usually found between 200m - 2000m.
2. Calculate q_s in each grid cell using equations (2.12), (2.14) and (2.17).
3. Calculate q_l in each grid cell using equation (2.11).

3.3 Implementation of microphysics routine

In chapters 5 and 6, results are discussed for the interaction between cloud microphysical effects and small-scale turbulence. In this section, the cloud microphysics routine implemented in SPARKLE will be discussed. The main components of this routine are the Lagrangian particle tracking routine and a collision-coalescence routine. The implementation and validation of these routines are presented in the following subsections. We build on the microphysics routine used in Woittiez, Jonker, and Portela (2009) and Perrin and Jonker (2015). This routine was originally implemented in the second order version of SPARKLE. As part of this thesis, the routine has been implemented in the fourth order version of SPARKLE and the following changes/additions have been made:

1. Four new particle time-integration schemes have been implemented and validated.
2. The particle communication routine has been validated.
3. A tricubic interpolation scheme has been implemented and validated.
4. The collision algorithm has been improved and validated.

Detailed descriptions of the interpolation routines and time integration schemes used to solve the particle equation of motion is provided. The different steps involved in implementing the collision algorithm in SPARKLE is also clearly detailed.

3.3.1 Lagrangian particle tracking routine

In chapter 2, the equations of motion that govern the particle trajectory and velocity were introduced (equation 2.21). These equations are implemented in SPARKLE through the Lagrangian particle tracking module. The module consists of three main routines:

1. The particle interpolation routine to interpolate instantaneous flow velocities from the cell face centres ($\mathbf{u}_i$) to instantaneous particle location; ($\mathbf{u}(\mathbf{X}, t)$),
2. The time integration routine to advance particle positions and velocities in time;
3. The particle communication routine to identify and transfer particles at processor boundaries to respective neighbouring processors.

3.3.2 Interpolation schemes

Two schemes have been implemented to interpolate the velocities at cell boundaries to the particle locations:

1. Trilinear interpolation
2. Tricubic interpolation

These two schemes will be discussed below.

Trilinear interpolation

In the generic form of trilinear interpolation, points are linearly interpolated within a three-dimensional unit cube using the values at the vertices of the cell. The lower left vertex is considered as the origin as shown in figure 3.2. The interpolated value at a location (x', y', z') inside this cube is given by,

$$\begin{aligned} u_{x'y'z'} = & u_{000} (1 - x')(1 - y')(1 - z') + u_{100} x(1 - y')(1 - z') + u_{110} x' y' (1 - z') + \\ & u_{010} (1 - x') y' (1 - z') + u_{001} (1 - x') (1 - y') z' + u_{101} x' (1 - y') z' + \\ & + u_{111} x' y' z' + u_{011} (1 - x') y' z' \end{aligned} \quad (3.2)$$

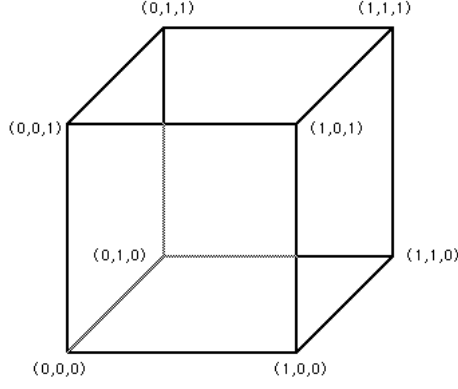


Figure 3.2: Eight vertices of a unit cube surrounding the interpolation point (x', y', z') .

where u_{ijk} is the value at vertex (i, j, k) .

Since the velocities in the SPARKLE grid cells are calculated at the cell face centers, a translation is required to align with the origin. Additionally, a scaling is required to transform the grid cell into a unit cube. To apply equation 3.2 to the SPARKLE grid, the following transformations are to be done (considering the interpolation of flow velocity component u to the particle location)

$$x' = \frac{(x_p - x_b(i))}{\Delta x} \quad (3.3)$$

$$y' = \frac{(y_p - y_c(j))}{\Delta y} \quad (3.4)$$

$$z' = \frac{(z_p - z_c(k))}{\Delta z} \quad (3.5)$$

where (x_p, y_p, z_p) are the particle coordinates at a time t , (x_b, y_c, z_c) are the coordinates of the particle cell face centre at which the flow velocity component u is calculated and $\Delta x, \Delta y$ and Δz are the grid cell sizes. To calculate the v and w components at the particle location, the grid face center values are changed to (x_c, y_b, z_c) and (x_c, y_c, z_b) respectively.

Tricubic interpolation

Tricubic interpolation is a method employed to obtain values of a grid defined function at arbitrary locations in 3D space. In most cases where tricubic interpolation is employed, it is desirable to preserve the function values as well as the continuity or smoothness of derivatives of the function during interpolation.

The implementation of tricubic interpolation in SPARKLE involves a sequential application of one dimensional *Cubic Interpolants (CI)* along $\hat{x}$, $\hat{y}$ and $\hat{z}$. The tricubic interpolation can be achieved by a series of calls to a one-dimensional *CI*. The interpolated velocity u at a location (x', y', z') inside a unit cube is obtained by

$$u_{z'}(i, j, z') = CI_{z'}(u(i, j, k-1), u(i, j, k), u(i, j, k+1), u(i, j, k+2)), \quad (3.6)$$

$$u_{y'}(i, y', z') = CI_{y'}(u_z(i, j-1, z'), u_z(i, j, z'), u_z(i, j+1, z'), u_z(i, j+2, z')), \quad (3.7)$$

$$u(x', y', z') = CI_{x'}(u_{y'}(i-1, y', z'), u_{y'}(i, y', z'), u_{y'}(i+1, y', z'), u_{y'}(i+2, y', z')), \quad (3.8)$$

where $i, j, k \in \{-1, 0, 1, 2\}$ where 0 is the index of the cell in which the function is calculated and in this context, the cell where the particle is located. This results in 21 calls to the one-dimensional cubic interpolant (16 to CI_z , 4 to CI_y and 1 to CI_x).

The one-dimensional cubic interpolant takes the form of a Catmull-Rom spline (Catmull and Rom 1974). The formulation of the Catmull-Rom spline is derived below as a form of a cubic Hermite spline. A cubic Hermite spline is a spline where each piece is a third degree polynomial specified in Hermite form, i.e. by its values and first derivatives at the end points of corresponding domain interval. In general, a one dimensional interpolation polynomial $P(t)$ on an interval $t \in [0, 1]$ and with P_0 and P_1 as the starting and ending points, can be written as

$$P(t) = h_{00}(t)P_0 + h_{10}(t)m_0 + h_{01}(t)P_1 + h_{11}(t)m_1, \quad (3.9)$$

where m_0 and m_1 are the tangents at the limit boundaries, and $h_{00}, h_{10}, h_{01}, h_{11}$ are Hermite basis functions. To derive the Hermite basis functions, the cubic polynomial is first expressed as

$$P(t) = c_0 + c_1u + c_2u^2 + c_3u^3, \quad (3.10)$$

The following four constraints are applied next:

$$P(0) = P_0, \quad P(1) = P_1,$$

$$P'(0) = m_0, \quad P'(1) = m_1.$$

These constraints are combined with equation 3.10 to get

$$\begin{aligned}c_0 &= P_0, \\c_0 + c_1 + c_2 + c_3 &= P_1, \\c_1 &= m_0, \\c_1 + 2c_2 + 3c_3 &= m_1,\end{aligned}$$

From these four equations, c_0 , c_1 , c_2 and c_3 can be expressed in terms of P_0 , P_1 , m_0 and m_1 . The basis functions can then be obtained by grouping all terms of P and m

$$P(t) = (1 - 3t^2 + 2t^3)P_0 + (t - 2t^2 + t^3)m_0 + (3t^2 - 2t^3)P_1 + (-t^2 + t^3)m_1. \quad (3.11)$$

Hence $h_{00} = (1 - 3t^2 + 2t^3)$, $h_{10} = (t - 2t^2 + t^3)$, $h_{01} = (3t^2 - 2t^3)$ and $h_{11} = (-t^2 + t^3)$. The basis functions for the Hermite interpolants are shown in figure 3.3. For an arbitrary interval (x_i, x_{i+1}) , interpolation is done by mapping to the unit interval $[0,1]$ using the following formulation

$$P(t) = h_{00}(t)P_i + h_{10}(t)(x_{i+1} - x_i)m_i + h_{01}P_{i+1} + h_{11}(x_{i+1} - x_i)m_{i+1}, \quad (3.12)$$

where $t = (x - x_i)/(x_{i+1} - x_i)$. To interpolate a data set (x_i, P_i) for $i = 1, \dots, n$, the above procedure is applied in each data interval and appropriate definitions for tangents are made. This results in an interpolated curve made of piecewise cubic Hermite splines. In the formulation for the Catmull-Rom spline, the tangent at a particular point is specified using the previous and next point on the spline. This ensures built-in C^1 continuity while each segment of a Catmull-Rom spline is a Hermite spline. The tangent is specified as (for an arbitrary interval),

$$m_i = \zeta \frac{P_{i+1} - P_{i-1}}{x_{i+1} - x_{i-1}}. \quad (3.13)$$

The parameter ζ is the tension parameter and it affects how sharply the curve bends at the interpolated points. It is set to 0.5. Substituting equation 3.13 in 3.12 and rearranging, the geometry matrix for the Catmull-Rom spline can be expressed as

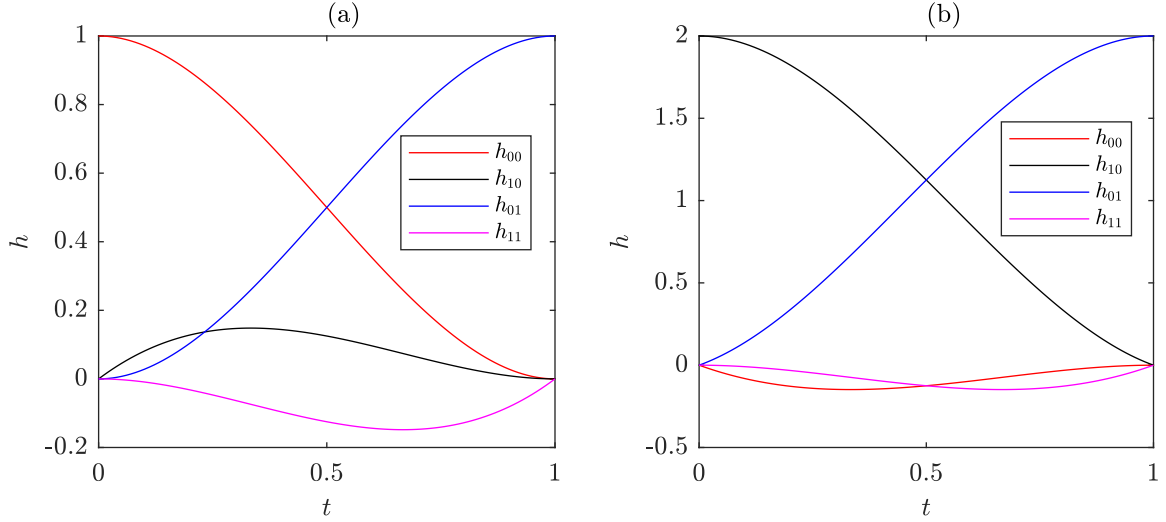


Figure 3.3: (left) Hermite basis functions (right) Basis functions for Catmull-Rom splines.

$$P(t) = 0.5 \begin{bmatrix} t^3 & t^2 & t & 1 \end{bmatrix} \begin{bmatrix} -1 & 3 & -3 & 1 \\ 2 & -5 & 4 & -1 \\ -1 & 0 & 1 & 0 \\ 0 & 2 & 0 & 0 \end{bmatrix} \begin{bmatrix} P_{i-1} \\ P_i \\ P_{i+1} \\ P_{i+2} \end{bmatrix}$$

The basis functions for the Catmull-Rom spline are shown in figure 3.3(b).

Care should be taken while choosing the particle time step Δt_p such that a particle never travels more than a grid cell. If this condition is not adhered to, an error occurs when the particle is communicated across the boundary while using the cubic interpolation method. There are only three ghost cells, and if the particle moves across more than one grid cell at the processor boundary, the cubic interpolant will have access to only one grid cell ahead of the particle grid cell, rather than the two cells it needs to successfully interpolate the velocities. Hence δt_p is chosen such that the particle movement is restricted to one grid cell, and this means that at the boundaries, the interpolant will have access to values from two ghost cells at all times.

3.3.3 Time-integration schemes

Explicit time integration schemes are implemented in SPARKLE to advance the position ($\mathbf{X}$) and velocities ($\mathbf{v}$) of the particles in the Lagrangian framework. These include *intermediate-step methods* like the Runge-Kutta schemes which make a number of estimations of the slope before determining the values at the next time step ($\mathbf{X}^{n+1}, \mathbf{v}^{n+1}$), and *multi-step methods* like the

Table 3.1: Time integration schemes.

Scheme	$\mathbf{f}$	ϵ
RK1	$\mathbf{f}_1 = \mathbf{f}(t^n, \mathbf{y}^n)$	$O(\Delta t)$
RK2	$\mathbf{f}_2 = \mathbf{f}(t^n + \frac{1}{2}\Delta t, \mathbf{y}^n + \frac{1}{2}\mathbf{f}_1\Delta t)$	$O(\Delta t^2)$
RK4	$\frac{1}{6}(\mathbf{f}_1 + 2\mathbf{f}_2 + 2\mathbf{f}_3 + \mathbf{f}_4)$	$O(\Delta t^4)$
AB2	$\frac{3}{2}\mathbf{f}(t^n, \mathbf{y}^n) - \frac{1}{2}\mathbf{f}(t^{n-1}, \mathbf{y}^{n-1})$	$O(\Delta t^2)$
AB3	$\frac{23}{12}\mathbf{f}(t^n, \mathbf{y}^n) - \frac{4}{3}\mathbf{f}(t^{n-1}, \mathbf{y}^{n-1}) + \frac{5}{12}\mathbf{f}(t^{n-2}, \mathbf{y}^{n-2})$	$O(\Delta t^3)$
$\mathbf{f}_3 = \mathbf{f}(t^n + \frac{1}{2}\Delta t, \mathbf{y}^n + \frac{1}{2}\mathbf{f}_2\Delta t)$ $\mathbf{f}_4 = \mathbf{f}(t^n + \Delta t, \mathbf{y}^n + \mathbf{f}_3\Delta t)$		

Adams-Bashworth schemes which make information of previous time steps and then determine $\mathbf{X}^{n+1}$ and $\mathbf{v}^{n+1}$ in one single step. The methodology of these schemes can be demonstrated by integrating in time a simple ODE of the form

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y}(t)). \quad (3.14)$$

Integrating both sides from t^n to t^{n+1} and setting $\mathbf{f} = \frac{1}{\Delta t} \int_{t^n}^{t^{n+1}} f dt$ gives,

$$\frac{\mathbf{y}^{n+1} - \mathbf{y}^n}{\Delta t} = \mathbf{f}, \quad (3.15)$$

where $\mathbf{f}$ is the average gradient on the interval $t^n < t < t^{n+1}$. The different time integration schemes implemented in the Lagrangian framework for SPARKLE are shown in table 3.1 along with the estimation of $\mathbf{f}$ using a Taylor series approximation in each of these schemes. The order of accuracy is shown by ϵ . A total of five particle time integration schemes have been implemented: first order Runge-Kutta (RK1 or forward Euler), second order Runge Kutta (RK2), fourth order Runge-Kutta (RK4), second order Adams-Bashworth (AB2) and third order Adams-Bashworth (AB3).

3.3.4 Particle communication across boundaries

SPARKLE is parallelized along the $\hat{y}$ and $\hat{z}$ directions. This means that as particles approach the boundary of a processor along these directions, they have to be transferred or 'communicated' across based on their velocities. This includes adding a new particle in the destination processor and deleting the same particle from the current processor. This is done through the following steps:

1. Once time integration is completed, a check is conducted to determine whether the new location of the particle lies within the current processor. If the new location lies on a neighbouring processor, the particle has to be sent (communicated) to the respective processor.
2. Identification of destination processor: A series of checks are conducted to determine whether the particle is to be transferred to the top, bottom, left, right or one of the four diagonal neighbouring processors.
3. Through a series of *MPI SENDRECV* commands, the particles are communicated across boundaries to the destination processor through an intermediary buffer.
4. Once communication is complete, an independent check is conducted in all the processors to identify the particles that have location vectors beyond their processor boundaries and are immediately deleted.

If the particle crosses the domain boundary along the periodic $\hat{x}$ or $\hat{y}$ boundaries, it is transferred to the first or last processor in the respective direction. If the particle crosses $\hat{z}$ domain boundaries, it is immediately deleted.

3.4 Condensational growth

The physics behind the condensational growth has been described in section 2.3.2 with the growth being governed by equation 2.22. In this section, the implementation details of the condensation rate C_d which introduces the feedback due to diffusive growth in the evolution

equations of the temperature and water vapour is given. It should be noted that these routines were directly transferred from the code used by Perrin and Jonker (2015).

The condensation rate per unit mass C_d is obtained by summing the rate of increase of mass of an individual droplet over all the droplets within a grid cell. In SPARKLE, C_d is calculated using the following relation,

$$\begin{aligned} C_d &= \frac{1}{m} \frac{dm_l}{dt} = \frac{1}{m} \frac{4}{3} \pi \rho_w \sum_{i=1}^{N_{p,c}} \frac{dR^3}{dt}; \\ &= \frac{1}{m} 4\pi \rho_w K S \sum_{i=1}^{N_{p,c}} R_i \end{aligned} \quad (3.16)$$

where $m = m_d + m_v + m_l$, ρ_w is the density of water, R_i is the radius of a droplet with index i and $N_{p,c}$ is the number of droplets in a single grid cell.

The resulting governing equations for the scalars are given by

$$\frac{\partial \theta}{\partial t} + \mathbf{u} \cdot \nabla \theta = \frac{L}{c_p} C_d + k_a \nabla^2 \theta \quad (3.17a)$$

$$\frac{\partial q_v}{\partial t} + \mathbf{u} \cdot \nabla q_v = -C_d + D_v \nabla^2 q_v \quad (3.17b)$$

where k_a is the thermal diffusivity of air and D_v is the molecular diffusivity of water.

We now discuss the numerical details of solving equation 2.21 and equation 2.22 in SPARKLE. Solving these equations are quite challenging in the presence of evaporating droplets. As droplets evaporate, the particle relaxation time $\tau_p \rightarrow 0$, which makes equation 2.21 stiff. Hence, equation 2.21 are solved by two time integration schemes: an Euler implicit scheme if the droplet $\tau_p < 0.5\Delta t$, and an explicit third-order Adams-Bashworth time-stepping scheme otherwise. Here, Δt is the Eulerian fluid time step. Additionally, if the radius of a droplet becomes smaller than $10^{-8}m$, it is carried along by the flow as a passive tracer.

The droplet radius (equation 2.22) is solved separately using an implicit method (Hall 1980). The supersaturation field can be derived from q_v and θ and therefore the numerical calculation is consistent with the treatment for the scalars q_v and θ . Hence in this method, the time integration is broken up into advection and microphysical contributions. The dynamic tendencies of the supersaturation field are determined by the advection of q_v and θ . The dynamic process and

the microphysical process are then combined to give the average supersaturation over the given time step. The steps involved are detailed below:

- The values of θ^* and q_v^* are calculated at an intermediate time-step t^* between t^n and t^{n+1} by considering just the advection terms in equations 3.17a and 3.17b and using forward time integration.
- The average supersaturation is implicitly solved for over the time step Δt , after which θ and q_v are updated with the microphysics contribution. This involves solving the following set of equations:

$$\begin{aligned}\theta^{n+1} &= \theta^* + \Delta t \frac{L}{c_p} \bar{C}_d \\ q_v^{n+1} &= q_v^* - \Delta t \bar{C}_d \\ S^{n+1} &= \frac{q_v^{n+1}}{q_s^{n+1}} - 1 \\ \bar{C}_d &= C_d \bar{S}\end{aligned}$$

The average supersaturation $\bar{S}$ is solved by iteration using the Newton-Rhapson method by assuming $\bar{S} = 0.5(S^{n+1} + S^n)$. This is then directly applied to equation 2.22.

3.5 Collision algorithm

The collision algorithm implemented in SPARKLE and used by Woittiez, Jonker, and Portela (2009) and Perrin and Jonker (2015) has been improved as part of this thesis. The new algorithm follows the general scheme in Allen and Tildesley (1987) where hard sphere molecular dynamics is solved. A broad description of such schemes was given in chapter 2 along with the equations to calculate the time of collision between a droplet pair. Here, the detailed step-by-step description of the algorithm implemented in SPARKLE is presented.

Calculation of the collision time is the most expensive part of the routine since all possible collisions between distinct pairs must be considered (Allen and Tildesley 1987). An efficient way is through the concepts of cell-indexing and neighbour lists and this is used extensively

in the algorithm implemented in SPARKLE. In this method, the cell in which a particle is residing at a particular time is identified, and the potential partners of a particle in a cell are found from all other particles in the cell plus the particles in the neighbouring cells. Since we only consider particles that can collide in a single time step and the particles do not travel more than a grid cell distance in a single time step, this means for each particle, partners are sought in a secondary grid of 3^3 cells. Considering N_p particles in a grid with $N_x \times N_y \times N_z$ cells and avoiding double counting, this requires $O\left(\frac{27}{2} \frac{N_p^2}{N_x N_y N_z}\right)$ operations. The list and number of particles in each cell is set up using the concept of linked lists after each time integration. This was already implemented by Woittiez, Jonker, and Portela (2009) and Perrin and Jonker (2015) for the second order version of SPARKLE and is validated as part of this thesis.

Figure 3.4 shows a detailed flowchart with the sequence of different steps followed in the new algorithm. Between successive instants $[t^n, t^{n+1}]$, particle pairs that are on a collision course can be identified using their trajectories determined by their locations $\mathbf{X}^n = \mathbf{X}(t^n)$ and velocities $\mathbf{v}^n = \mathbf{v}(t^n)$. Of all the multiple possible colliding pairs, the earliest colliding pair is identified and all the particles are integrated to the earliest colliding time t_{col} , i.e. $t_{col} = \min(t_{ij})$. Collision dynamics are implemented for the colliding pair, after which the next pair colliding at $t_{col} < \Delta t$ is identified ($\Delta t = t^{n+1} - t^n$). The particles are again integrated to this t_{col} and collision dynamics are implemented for this pair. A counter time variable t_{cur} keeps track of the time progress within the time step and colliding pairs are sought until the particles have reached t^{n+1} . In this thesis, particles are assumed to undergo only one collision within a particular step. However an option has been included in the algorithm which allows particles to undergo multiple collisions in a single time step. This requires an additional step where all possible collisions involving the newly collided pair are checked for and collisions are added or deleted. The four main steps in this algorithm are given below:

1. locate collisions and identify time of first collision
2. integrate all particle locations till first collision time;
3. execute collision dynamics for the colliding pair (equations 2.31, 2.32 and 2.33 for coalescence);

4. calculate collision statistics, ready for averaging and return to step 1.

The algorithm is shown diagrammatically in figure 3.4

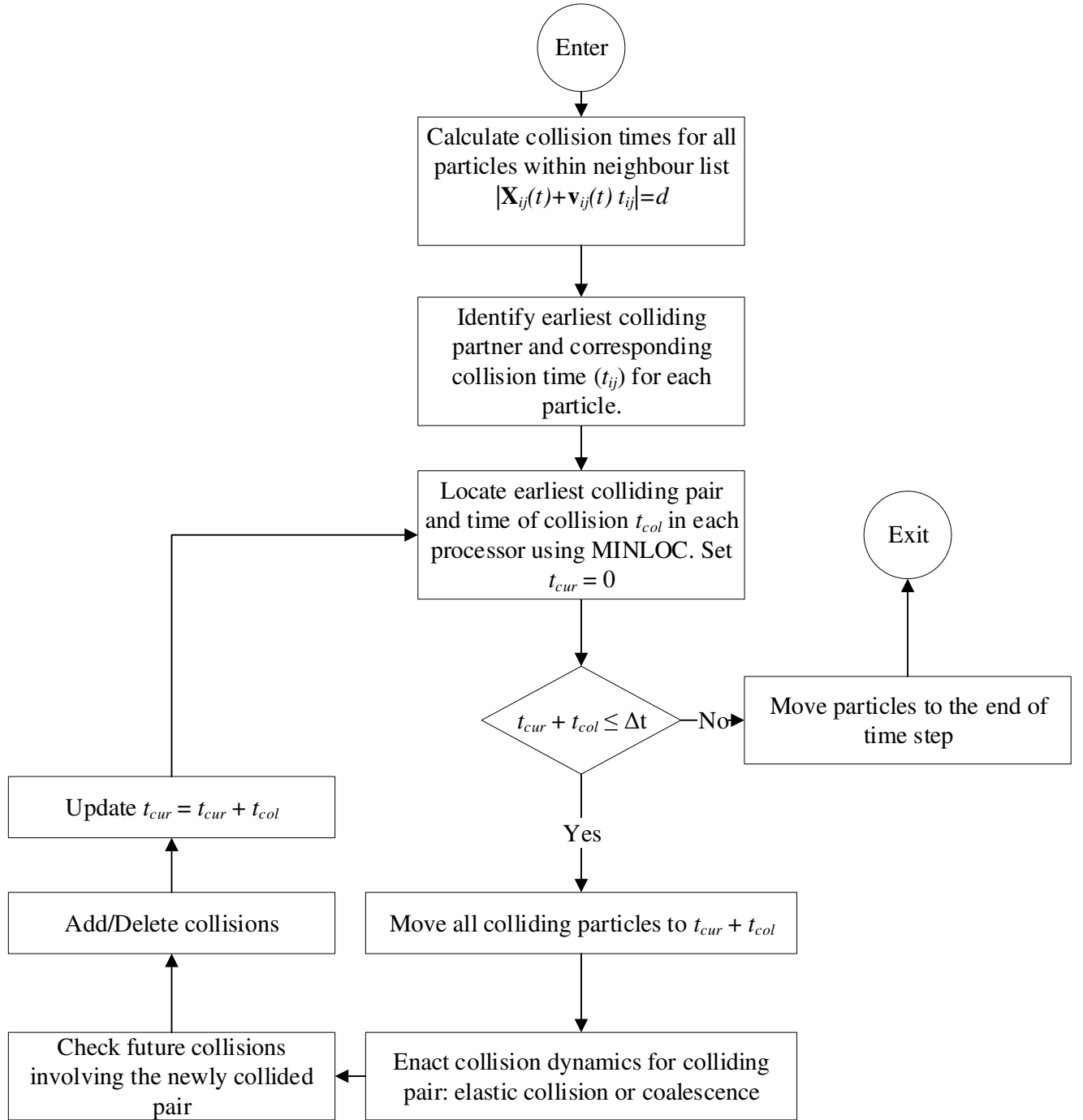


Figure 3.4: The collision algorithm implemented in SPARKLE

3.6 Validation

3.6.1 The translating Rankine vortex test case

A wide variety of test cases are available for validation of time integration and spatial interpolation schemes. A good example for such a test case is the transport of particles in a Rankine vortex. For this case, an exact solution exists to calculate the trajectories of particles inside the vortex. However, implementing the Lagrangian particle tracking routine in SPARKLE demands a very specific test case that allows the validation of the integration schemes, interpolation schemes, particle communication across processor boundaries and the periodic domain boundaries (along the $\hat{x}$ and $\hat{y}$ directions). A test case which involves particle transport inside a Rankine vortex would allow us to validate the integration and interpolation schemes. However to validate communication across processor and domain boundaries, the vortex has to translate across the domain. Hence we create a test case by imposing a uniform horizontal mean flow in the simple Rankine vortex test case. This is a novel test case which was developed as part of this thesis. The exact solution for the trajectories of particles following a *spiral* trajectory inside the translating Rankine vortex is derived, and the accuracy of the different schemes is compared against this analytic solution.

A Rankine vortex model is given by a combination of a rigid-body rotation within a core surrounded by a decay of angular velocity. This can be described in cylindrical coordinates by considering an azimuthal flow, i.e. $u_r = u_z = 0$ and $u_\theta = f(\theta)$ such that

$$u_\theta = \begin{cases} \omega \tilde{r}, & \tilde{r} < R_0, \\ \frac{\omega R_0^2}{\tilde{r}} & \tilde{r} > R_0 \end{cases}$$

where ω is the angular velocity, R_0 is the radius of the vortex core, and $(\tilde{r}, \tilde{\theta}, \tilde{z})$ are the cylindrical coordinates. Hence the tangential velocity increases linearly with radius inside the vortex and decreases with radius outside the vortex core with an infinite vorticity (singularity) concentrated at $\tilde{r} = 0$. The velocity components in cartesian coordinates for a Rankine vortex with axis along

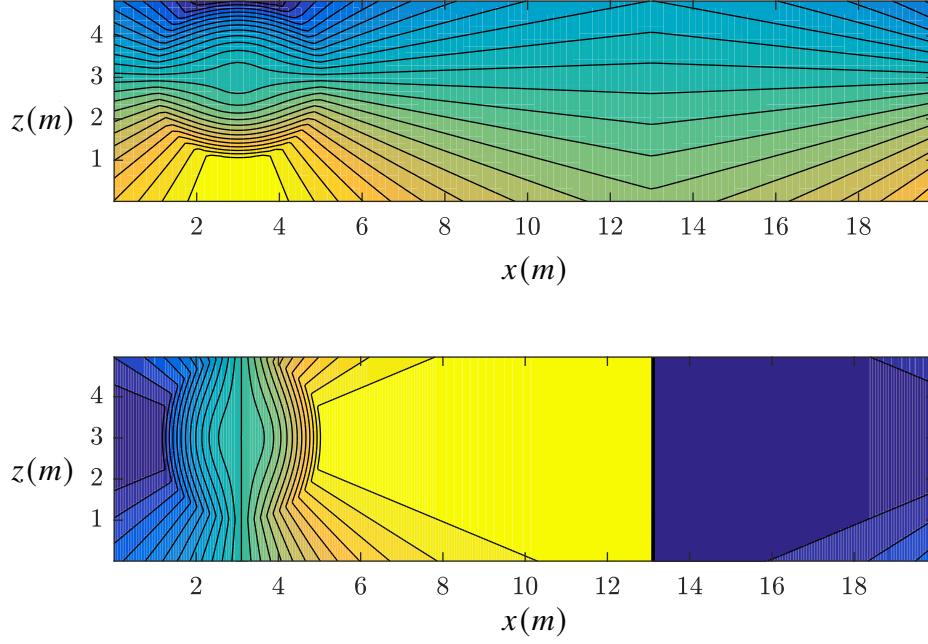


Figure 3.5: Velocity contour plots for the Rankine vortex (top) u and (bottom) w .

the $\hat{y}$ axis are then given by,

$$u = -\tilde{r} u_\theta \sin \tilde{\theta} \quad (3.18)$$

$$v = 0 \quad (3.19)$$

$$w = \tilde{r} u_\theta \cos \tilde{\theta} \quad (3.20)$$

A uniform mean flow U_0 is superimposed on u resulting in a translating Rankine vortex. The velocity fields for this translating vortex are shown in figure 3.5 (using periodic boundary conditions). The vortex has a radius $R_0 = 3m$ and is centered at $(x_{v0}, z_{v0}) = (3, 3)$. Fluid tracer particles are initially released inside the vortex core and their trajectories are followed. Variations on the test case follow from changing the axis of the vortex.

The exact solution for the fluid particle trajectories in a translating Rankine vortex (with axis along $\hat{y}$) is derived,

$$x(t) = x_v(t) + r_0 \cos \theta(t), \quad (3.21)$$

$$z(t) = z_v(t) + r_0 \sin \theta(t), \quad (3.22)$$

where

$$r_0 = \sqrt{(x_0 - x_{v0})^2 + (z_0 - z_{v0})^2}, \quad (3.23)$$

$$x_v(t) = x_{v0} + U_0 t, \quad (3.24)$$

$$\theta(t) = \theta_0 + u_\theta t, \quad (3.25)$$

$$\theta_0 = \tan^{-1} \left(\frac{z_0 - z_{v0}}{x_0 - x_{v0}} \right). \quad (3.26)$$

Here (x_0, z_0) and (x_{v0}, z_{v0}) are the positions of the tracer particle and the centre of the Rankine vortex core at $t = 0$.

3.6.2 Particle communication across processors

Figure 3.6 clearly shows the successful communication of particles across the processor boundaries (shown by the dotted line) along the $\hat{z}$ direction. A second order Adams-Bashworth scheme is used along with cubic interpolation. Particles cross multiple processor boundaries along $\hat{z}$ and also crosses the periodic $\hat{x}$ boundary. A simulation (not shown) was also performed with the axis of the Rankine vortex along $\hat{z}$ to check the particle communication across processor boundaries along $\hat{y}$.

3.6.3 Spatial interpolation

The translating Rankine vortex test case is used to analyse the performance of the two interpolation schemes explained in section 3.3.2 in determining the fluid velocities at the particle locations. The trajectories of a particle in a translating Rankine vortex are calculated using both the trilinear and the tricubic interpolation schemes and a fourth order Runge-Kutta scheme. An order-of-accuracy test is performed for the interpolation schemes. This is done by calculating a global truncation error given by

$$\epsilon = ||\mathbf{x}^n - \mathbf{x}(t_n)||, \quad (3.27)$$

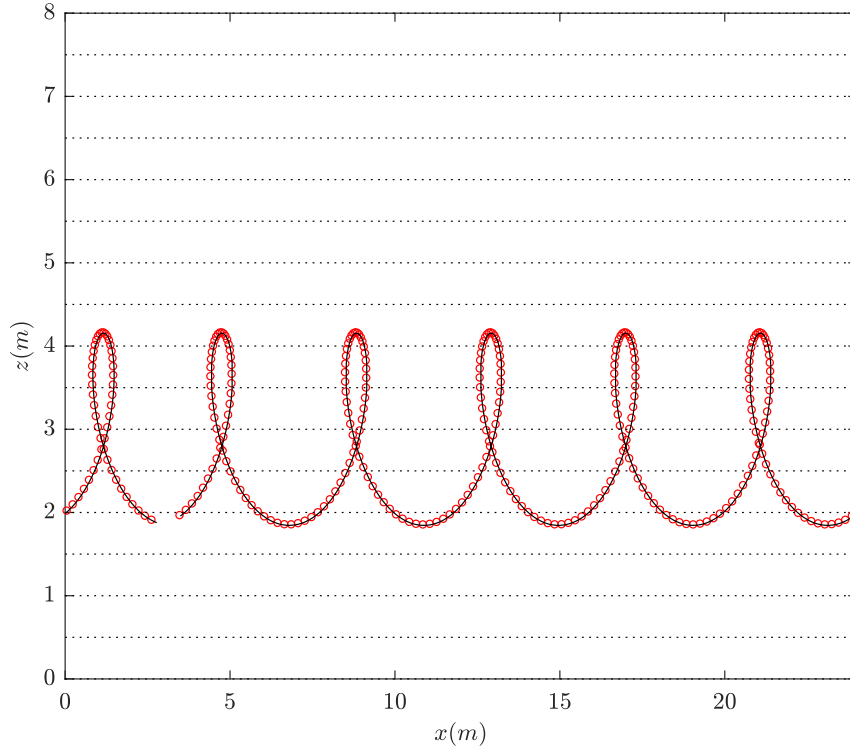


Figure 3.6: Trajectories of a particle travelling across different processor boundaries (dotted lines). The black solid line is the exact solution (equation 3.21) and the red circles are from the simulation. $U_0 = 0.25$; $R_0 = 3$; $x_{v0} = 3$; $z_{v0} = 3$.

which is the difference between the particle locations given by the numerical approximation $\mathbf{x}^n$, and the exact solution $\mathbf{x}(t_n)$ at the end of the simulation ($t = 16s$).

The trilinear interpolate is not actually linear, but instead a product of three linear interpolants as is clear in equation (3.2). However the interpolant is linear along lines parallel to the $\hat{x}$, $\hat{y}$ and $\hat{z}$ direction or if $\hat{x}$, $\hat{y}$ and $\hat{z}$ is kept constant. Along any other straight line, the interpolant is cubic. Since the translating Rankine test case is two-dimensional ($\hat{y}$ is kept constant), the interpolant would be quadratic and we expect a slope of 2 and this is indeed what is observed in figure 3.7.

For tricubic interpolation, a polynomial of degree 3 and order of accuracy 4 is used. The interpolation implementation involves a series of one dimensional interpolations (keeping the other two directions constant). Hence we expect a fourth order of convergence for error ϵ calculated from equation 3.27 and this is indeed what is observed in figure 3.7.

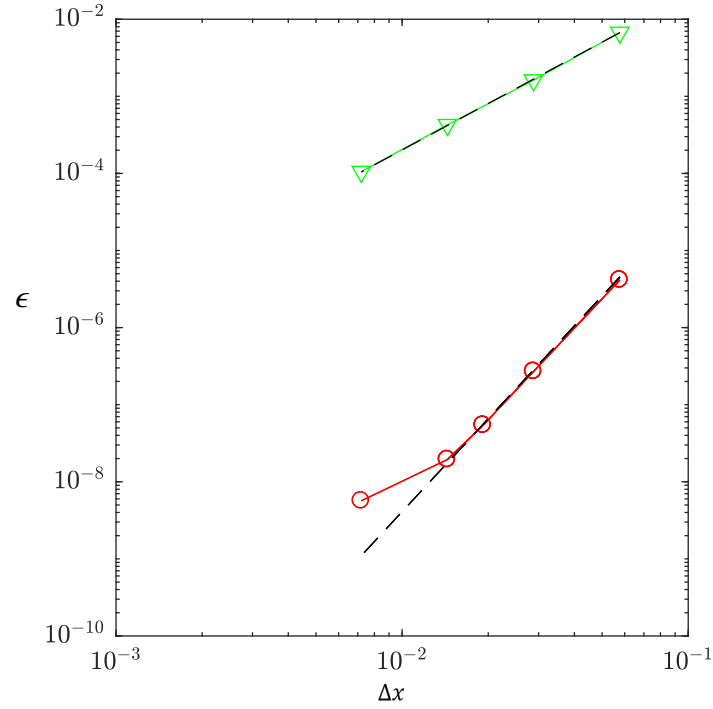


Figure 3.7: Global truncation error for the translating Rankine test case using different interpolation schemes. Green triangles: Trilinear interpolation, red circles: Tricubic interpolation. The dashed lines have slopes 2 and 4.

3.6.4 Time-integration schemes

An order of accuracy test is performed for the different time integration schemes by varying the time step Δt , and the convergence is studied. A domain of $20m \times 5m \times 5m$ was used. The convergence of the errors calculated using equation 3.27 is plotted in figure 3.8 and the expected order of accuracy was observed for the RK1 (Forward Euler), AB2, AB3 and RK4 time schemes.

3.6.5 Collision kernel

The collision statistics involves the calculation of the dynamic collision kernel, the radial distribution function and the radial relative velocities as detailed in section 2.6. The kinematic collision kernel has been validated against the dynamic collision kernel using DNS for both non-sedimenting inertial particles (L.-P. Wang, Wexler, and Y. Zhou 2000b; Y. Zhou, Wexler, and L.-P. Wang 2001) and sedimenting droplets (Ayala, Rosa, L.-P. Wang, and Grabowski 2008; Woittiez, Jonker, and Portela 2009). The test case used for validation is the case of settling particles in stagnant air for which an analytical expression for the collision kernel exists. In still

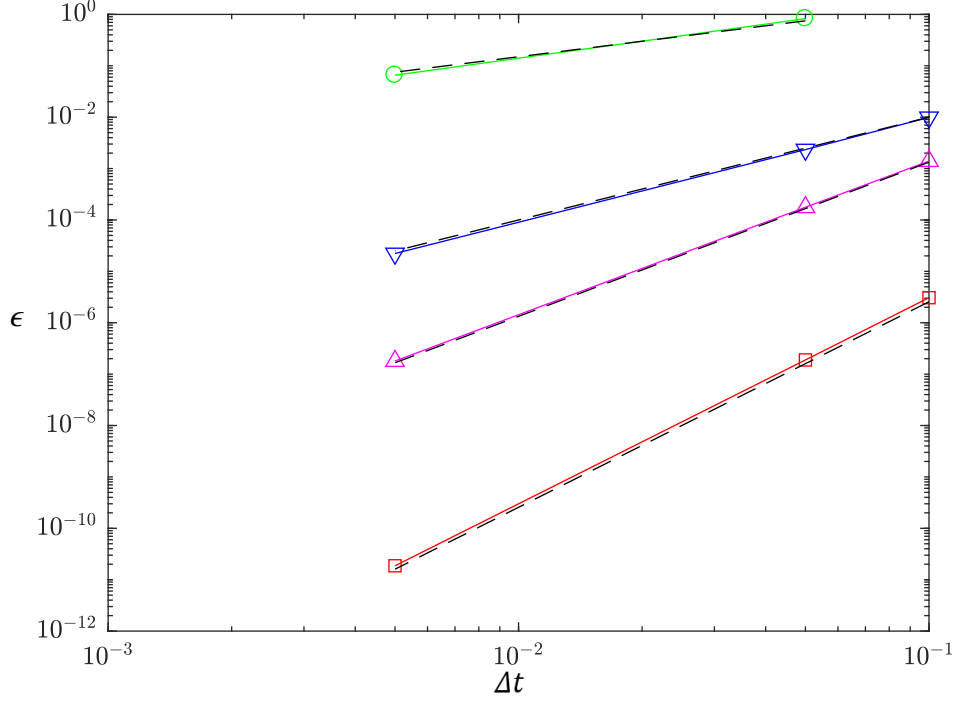


Figure 3.8: Global truncation error for the translating Rankine test case using different time integration schemes. Green circles: first order Euler, blue triangles: second order Adams-Bashworth, magenta triangles: third order Adams-Bashworth, red squares: fourth order Runge-Kutta

air, droplets sediment with a terminal velocity w_T . The average relative velocity for this case is

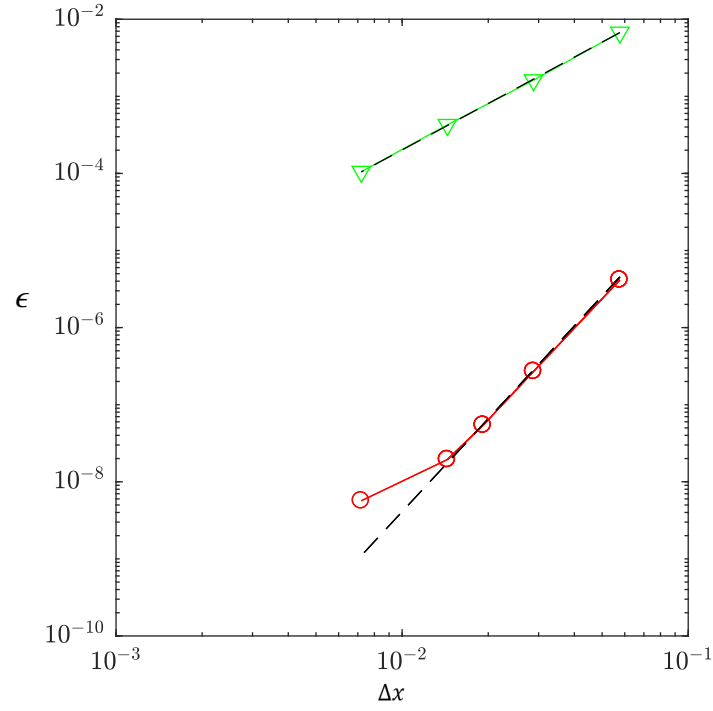
$$\langle |w_r^g| \rangle = 0.5 |w_{T,1} - w_{T,2}|, \quad (3.28)$$

where $w_{T,1}$ and $w_{T,2}$ are the terminal velocities of droplets of size R_1 and R_2 . By definition, the RDF is equal to one. Hence the gravitational collision kernel is

$$\Gamma_{12}^g = 2\pi R_c^2 \langle |w_r^g| \rangle, \quad (3.29)$$

where $R_c = R_1 + R_2$ is the radius of the collision sphere.

Multiple simulations are performed with a bidisperse distribution of particles with radius $R_1 = 20\mu m$ and $R_2 = [25, 30, 35, 40]\mu m$. The simulations were performed on a cubic box of side $0.509m$ for $0.1s$ using $N_{p,1} = 4.5 \times 10^6$ and $N_{p,2} = 4.5 \times 10^6$ particles of radius R_1 and R_2 respectively. Particles were allowed to geometrically overlap with no special collision dynamics employed. The consistency of the kinematic formulation of the collision kernel (Γ_{12}^K) with the dynamic collision kernel (Γ_{12}^D) is displayed in figure 3.9(a) for bidisperse collisions



between sedimenting droplets in still air. The normalized value $\Gamma_{12}^K/\Gamma_{12}^D$ is one for all the simulations. Figures 3.9(b), (c) and (d) show comparisons between DNS values and theoretical predictions for the Kinematic collision kernel Γ_{12}^K (equation 3.29), the RDF g_{12} , and the average radial relative velocity $\langle |w_r| \rangle$ (equation (3.28)). There are statistical uncertainties in the RDF measurements, but still a very good agreement is observed for all three quantities between the two methods, providing further confidence in the implementation of the Lagrangian particle routines and collision statistics.

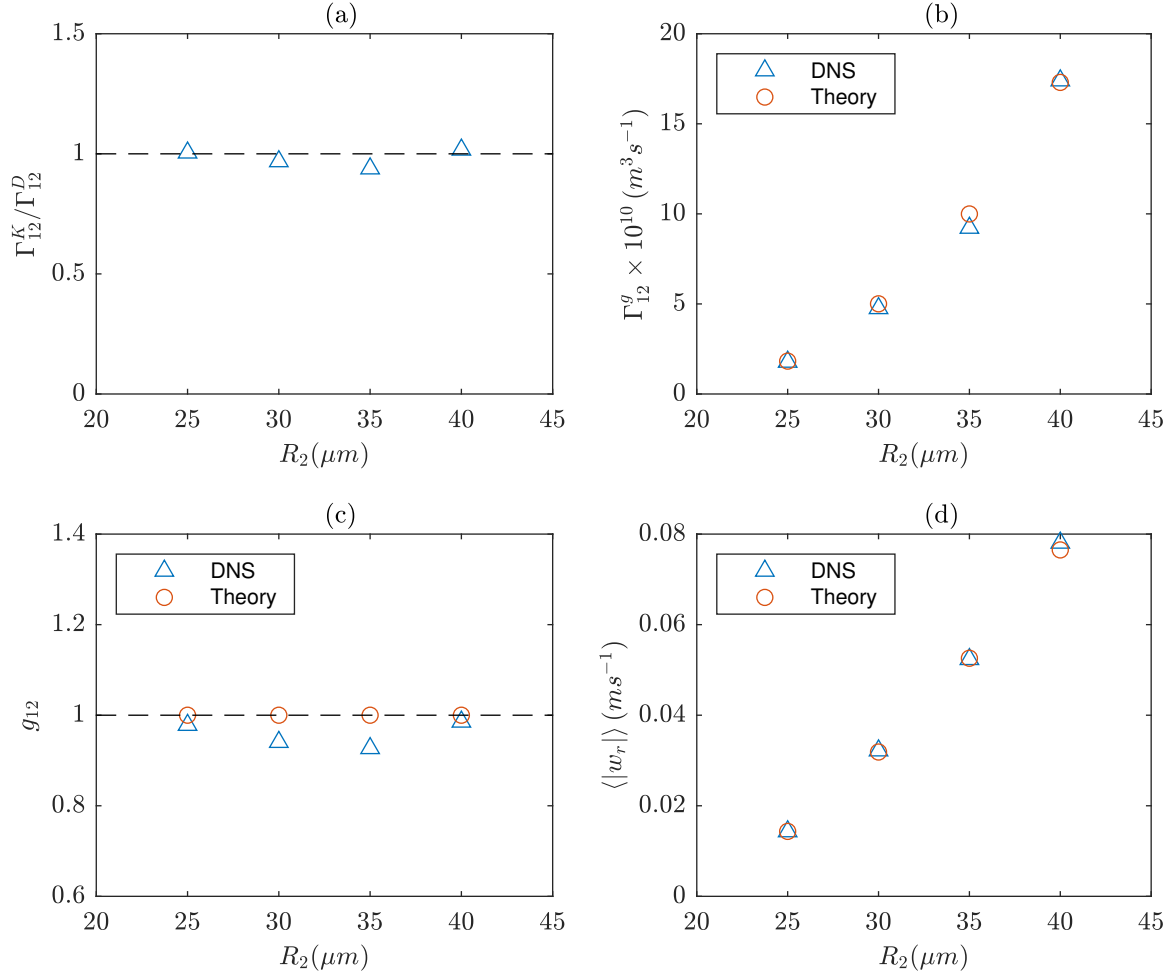


Figure 3.9: Validation of the gravitational collision terms for bidisperse collisions with $R_1 = 20 \mu\text{m}$ in stagnant air. (a) Ratio of kinematic collision kernel with dynamic collision kernel. (b) Kinematic collision kernel Γ_{12}^K (Theory refers to equation 3.29), (c) RDF g_{12} and (d) $\langle |w_r| \rangle$ (equation 3.28).

Chapter 4

Subsiding shells in shallow cumulus clouds

In this chapter, the dynamics of a subsiding shell generated at the lateral edges of shallow cumulus clouds is analyzed using direct numerical simulations. A canonical setup is developed in which the dynamic properties of the shell is analysed in the presence of an actively growing cloud. Self-similarity of the flow in the shell is explored and the characteristic scales are identified. A simple entrainment model is also developed. This chapter includes material from a publication by the author (Nair, Heus, and van Reeuwijk 2020).

4.1 Introduction

4.1.1 Background

Poor parameterizations of shallow cumulus convection in GCMs has been identified as one of the possible contributors towards the inter-model spread in climate sensitivity (Bony et al. 2015). An important factor in the parameterizations for the vertical convective transport of momentum, heat and moisture are the entrainment and detrainment rates of the environmental air into the cloud core, and the cloud core air into the environment, respectively (de Rooy et al. 2013). In a seminal paper, Stommel (1947) highlighted the importance of lateral mixing in a cumulus cloud. Mixing between a rising cloud and the environmental air drawn in by the cloud leads to a change in the mechanical and thermodynamic properties inside the cloud. An opposing school of thought developed with P. Squires (1958) proposing that vertical mixing causes the cloud to dilute from top-down, i.e. environmental air entraining from the cloud-top,

was responsible for mixing through 'penetrative downdrafts'. Leading the charge for cloud-top entrainment was Paluch (1979), who presented conserved variable diagrams of observations showing the source of entrained air inside the cloud at a level above or at the cloud top. Since then, numerous observational and model studies, especially using LES have shown that both lateral and vertical mixing occurs in clouds, with lateral mixing being the dominant contributor towards cloud dilution (Blyth, Cooper, and Jensen 1988; Taylor and Baker 1991; Heus, van Dijk, et al. 2008; de Rooy et al. 2013). Even though most operational climate models use parameterizations based on lateral mixing in a bulk approximation of entire fields of clouds, a precise picture of the mixing characteristics is still not available. Studies on fundamental understanding and parameterization of entrainment in cumulus clouds remain an active field of current research (de Rooy et al. 2013).

The turbulent mixing at cloud edges results in the formation of a 'shell' of negatively buoyant layer of air around the cloud which adds to the complexity in studying and parameterizing entrainment in shallow cumulus clouds. One of the early observations of the shell was done by Jonas (1990), who observed a thin descending layer of negatively buoyant air at the edges of developing and maturing shallow cumulus clouds. The observations were further corroborated using aircraft data from a large number of flight legs through cumuli (Rodts, Duynkerke, and Jonker 2003; Y. Wang, Geerts, and French 2009). A conspicuous dip in the profiles of the virtual potential temperature suggested that these shells were formed as a result of evaporative cooling due to entrainment and mixing with warm unsaturated environmental air. One of the first LES studies of the subsiding shells was performed by Heus and Jonker (2008). By analyzing the individual terms in the vertical momentum budget, it was concluded that the evaporative cooling was the driving force behind the subsiding shell. However, recent studies (Park, Gentine, et al. 2016; Park, Heus, and Gentine 2017) suggest that buoyancy reversal at the cloud edge occurs even in a modified LES where evaporative cooling is absent. Park, Gentine, et al. (2016) speculates that the downdrafts in the boundary layer are generated by overturning vortex-like circulations similar to Hill's vortex (Hill 1894) as proposed by Sherwood, Hernandez-Deckers, and Colin (2013), which are then strengthened by evaporative cooling in the cloud layer; while Park, Heus, and Gentine (2017) propose that they are generated instead by convective mixing

across vertical levels and condensation in the cloud.

The majority of mass-flux based parameterization schemes (Tiedtke 1989; Siebesma, Bretherton, et al. 2003; Neggers, Köhler, and Beljaars 2009), use a bulk parameterization to calculate the entrainment and detrainment rates into and from the cloud cores. In such approximations, the properties of the entrained and detrained air are considered to be that of the averaged properties of the environmental air and the cloud cores respectively. With the increase of resolution in weather models, cumulus convection has entered the grey zone (resolutions between 200 m to 10 km where turbulent and convective structures are partially resolved and partially parameterized), and has become partially resolved. At those resolutions, bulk parameterizations are no longer valid, and a more detailed understanding of mixing on a cloud-by-cloud is necessary (Neggers 2015). However, direct measurements of the entrainment and detrainment rates by Roms (2010) show values twice as high as the ones used in current parameterization schemes. This difference was attributed to the presence of these shells which makes it important to include the dynamics of the shell in parameterizations of cumulus clouds in GCMs (Dawe and Austin 2011; Park, Gentine, et al. 2016; Hannah 2017). Jonker, Heus, and Sullivan (2008a) suggested that the majority of the upward mass flux in the cloud core is compensated by the downward mass flux in the shell, thus rendering cumulus clouds much less effective mixers than previously thought.

Given that the typical width of the shell is usually close to the resolution of the LES, DNS studies are much more effective when it comes to capturing small-scale dynamics as they resolve scales down to the Kolmogorov scale. But DNS studies have been few, and always with simple idealized models. A DNS of the cloud edge was performed by Abma, Heus, and Mellado (2013) to explore the characteristics of the shell and to obtain scaling laws for its evolution under buoyancy reversing conditions. Since DNS resolves the entire turbulent spectrum, it is expensive and beyond current computational capabilities to resolve an entire cloud. Hence only the flow immediately around the cloud edge is considered. A highly idealized setup was used which ignores important properties such as in-cloud buoyancy, vertical velocity, turbulence and cloud microphysics. This idealization, as fairly mentioned in the work is "likely to create an overestimation of the strength of the subsiding shell". However the simulations in Abma, Heus,

and Mellado (2013) were highly transient to study the dynamic properties of the shell. The results from Abma, Heus, and Mellado (2013) were compared with observations by Katzwinkel et al. (2014) who performed measurements of the structure of cloud edges for trade wind cumuli. They studied turbulent, thermodynamic and microphysical structures. Since the measurements were taken over the trade wind region where there is a continuous development of the shallow cumulus clouds during the day, the shell properties were studied as the cloud evolves through different stages. They observed that the shell thickness varied according to the evolution stage of the cloud. This provides additional motivation to develop a setup which could simulate an actively growing cloud.

4.1.2 Recent progress in entrainment research

The importance of entrainment laws in Numerical Weather Prediction (NWP) models cannot be overstated since three dimensional turbulence is not fully resolved in such predictions (van Reeuwijk and Jonker 2018). There has been significant progress in the understanding of turbulent entrainment in clouds, mainly from the atmospheric sciences community (de Rooy et al. 2013, and references therein). However, entrainment is an important process of relevance for a plethora of other canonical flows including jets, plumes, wakes, mixing layers, boundary layers etc. These flows have been studied by the turbulence community which has made significant inroads in understanding the small-scale and integral aspects of entrainment especially in jets and plumes (da Silva et al. 2014; van Reeuwijk and Holzner 2014). However, despite the significant progress in the understanding of turbulent entrainment, it remains 'fragmented and case-specific' (van Reeuwijk and Jonker 2018). In the atmospheric community, fractional entrainment and detrainment rates are studied as a function of vertical height (from cloud base to top), as key parameters in mass flux parameterizations to determine the cloud core fields and mass flux profiles (Siebesma and Cuijpers 1995a; Siebesma, Bretherton, et al. 2003; de Rooy et al. 2013). In the turbulence community, entrainment models (Priestly and Ball 1955; Morton, Taylor, and Turner 1956) or entrainment relations are defined in terms of an entrainment coefficient α and an entrainment velocity scale $\hat{u}$. In this chapter, an attempt has been made to bridge the two communities by employing entrainment relations originally

developed for axisymmetric free shear flows like jets and plumes (van Reeuwijk and Craske 2015), to understand entrainment in clouds.

The turbulent entrainment is decomposed into contributions from turbulence production, buoyancy production and profile shape modifications by using the integral conservation equations for velocity, momentum and turbulence kinetic energy equations in van Reeuwijk and Craske (2015). This was later applied to an idealized sheared nocturnal boundary layer and adapted for wall-bounded flows by a further decomposition into inner and outer layer contributions (van Reeuwijk and Jonker 2018). The analysis in van Reeuwijk and Jonker (2018) concluded that the entrainment coefficient is determined mainly by the turbulence kinetic energy production in the outer layer with the inner layer contributions being negligible after a sufficient period of time. We aim to extend these relations to study turbulent entrainment in shallow cumulus clouds.

The goal of this work is to study the cloud-clear interface while taking the presence of the in-cloud buoyancy and updraft into account. The setup is to be designed as close to actual actively growing cloud conditions; with a distinct positively buoyant cloud core with updrafts, surrounded by a thin subsiding shell layer with downdrafts. The dynamic evolution of the shell under the effects of evaporative cooling and turbulent mixing is studied. We investigate if the flow reaches a self-similar regime thus establishing Reynolds number independence, and obtain scaling laws for the growth of the shell. A simplified model is also developed to quantify the turbulent entrainment in the cloud using the integral framework in van Reeuwijk and Craske (2015).

This chapter is structured as follows. In section 4.2, the case setup, governing equations and the details of the simulations are explained. In section 4.3, initial results that identifies the subsiding shell are presented. In section 4.4, the self-similarity aspects and characteristic scales of the flow are studied. Section 4.5 includes a theoretical analysis to identify the processes which govern the flow in the shell. In section 4.6, the results from all the simulations are compared to study how the shell properties are influenced by the initial thermodynamics of the cloud and environment. Finally, section 4.7 includes a discussion of the results from the simulations and concluding remarks.

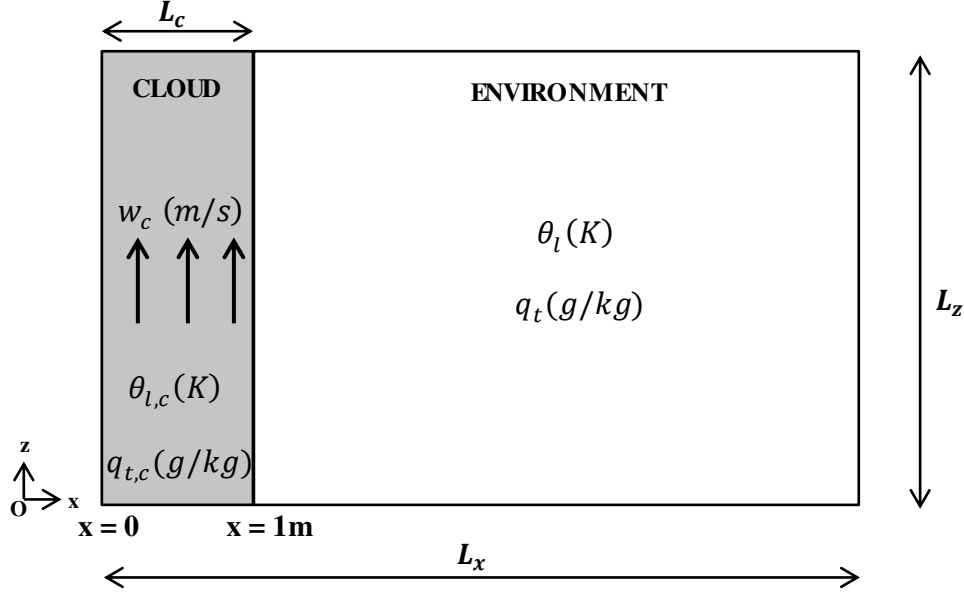


Figure 4.1: Two-layer cloud-environment simulation setup. A volumetric forcing is applied over the grey cloud region from $x = 0$ to $x = 1m$.

4.2 Simulations

4.2.1 Case setup

The simulations are temporal flow experiments in which the development of a small region at the edge of a shallow cumulus, including both the cloud and the surrounding environment, is studied. Specifically, we consider a two layer cloud-environment set-up, in which the domain is divided into a moist, positively buoyant cloud layer and a dry, neutrally buoyant environment layer, with the gravity vector aligned in the vertical direction $\hat{z}$ as shown in figure 4.1. The cloud has a positive buoyancy b_c and an in-cloud velocity w_c and hence resembles an actively growing cloud as defined in Katzwinkel et al. (2014). The liquid water potential temperature θ_l , and the total water mass fraction q_t , define the thermodynamic properties of the cloud and the environment. As in Abma, Heus, and Mellado (2013), the dominant mixing is assumed to occur locally and hence the influence of the cloud top and base can be neglected which makes the system statistically homogeneous in the vertical direction $\hat{z}$. This allows us to impose periodic boundary conditions on the top and bottom boundaries and in the span-wise direction if the

domain is large enough. Hence statistics can be obtained by averaging over the YZ -plane.

In test simulations, it was observed that the negatively buoyant layer formed at the cloud edge grows at the expense of the cloud. The cloud-environmental air mixture soon exhausts the entire cloud layer and descends as a single fluid mass. This is a very transient process and does not provide an ideal setup to study the dynamic properties of the shell. In order to overcome this problem and study the properties of the subsiding shell in an actively growing cloud, a volumetric forcing is applied to the cloud layer which nudges the vertical velocity and thermodynamic properties of the cloud towards pre-defined values. We aim to study the dynamics of the shell in the presence of an actively growing cloud (positive buoyancy and vertical velocity) which is in the early stages of its lifetime. The nudging can be considered to be similar to replenishment from the cloud core and a means to maintain/delay the transition of a cloud into a more mature stage.

The governing equations in SPARKLE have been introduced in chapter 3. The volumetric forcing is added to the vertical momentum equation and the scalar transport equations giving

$$\nabla \cdot \mathbf{u} = 0, \quad (4.1a)$$

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla P + \nu \nabla^2 \mathbf{u} + b \vec{e}_z + \frac{w_c - w}{\tau} \vec{e}_z H(L_c - x), \quad (4.1b)$$

$$\frac{\partial \chi}{\partial t} + \mathbf{u} \cdot \nabla \chi = K \nabla^2 \chi + \frac{\chi_c - \chi}{\tau_c} H(L_c - x). \quad (4.1c)$$

where χ represents the scalars (θ_l, q_t) , K represents the diffusivity constants (κ, D) where κ is the thermal diffusivity of air and D is the molecular diffusivity of water. Parameters w_c and χ_c are the nudging values maintained in the cloud layer, H is the Heaviside function, L_c is the width of the initial cloud layer, $\vec{e}_z$ is the unit vector along the vertical direction and τ_c is a nudging time scale for the forcing.

The buoyancy of a moist air parcel is now introduced. The buoyancy b of any parcel at a particular level can be defined using the difference between the virtual potential temperatures of the parcel $(\theta_v, \text{equation 2.10})$ and the environment $(\theta_{v,0})$ at that level which results in the following equation

$$b = g (\theta_v - \theta_{v,0}) / \theta_0, \quad (4.2)$$

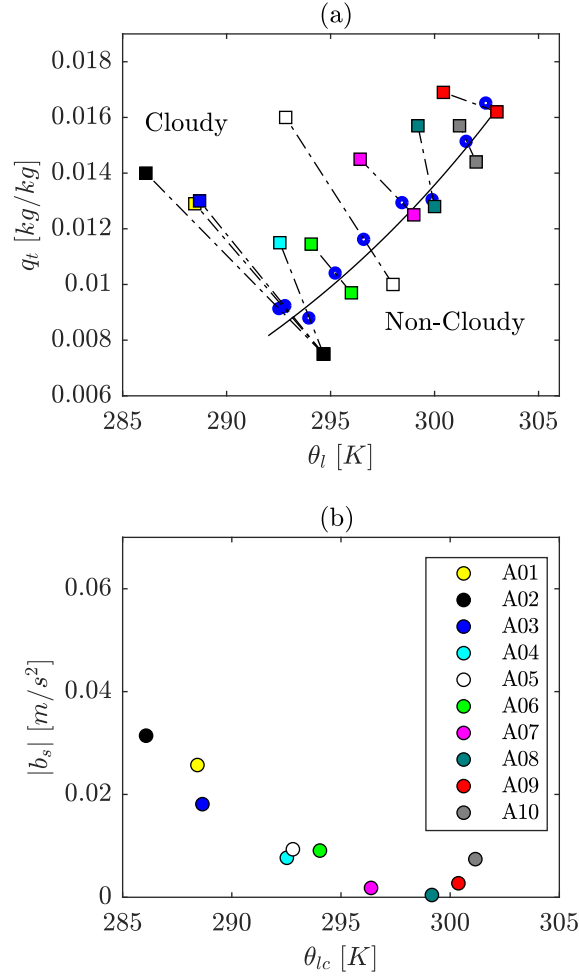


Figure 4.2: (a) Temperature-humidity diagram representing different initial states for cloud and environment. Black line represents the saturation curve, squares represent the properties of the initial states of the cloud and environment layer, and the dot-dash line represents the mixing line. The property of the mixed parcels with minimum mean buoyancy is represented by circles. (b) Magnitude of buoyancy minima in the shell b_s against θ_{lc} , the initial value of θ_l in the cloud for different simulations.

where θ_0 is a reference temperature which in this thesis, is set to be equal to the potential temperature of the environment. Substituting (2.10) in (4.2) gives

$$b = g \left(\frac{\theta - \theta_0}{\theta_0} - \left(1 - \frac{R_v}{R_d} \right) (q_t - q_{t,0}) - \frac{R_v}{R_d} q_l \right), \quad (4.3)$$

where θ_0 and $q_{t,0}$ are the environmental values, $R_d = 287.0 \text{ J kg}^{-1} \text{ K}^{-1}$ and $R_v = 461.5 \text{ J kg}^{-1} \text{ K}^{-1}$ are the gas constants for dry air and water vapour respectively. The bulk condensation scheme described in section 2.2 is used to diagnostically calculate q_l .

4.2.2 Simulation details

A temperature-humidity diagram relating q_t and θ_l is shown in figure 4.2. The continuous line represents the saturation curve. The initial values of the thermodynamic properties θ_l and q_t are represented by squares, where all the squares above the saturation curve represent the cloud and those below represent the environment. The range of initial cloud and environment properties vary from $\theta_l \approx 286K \rightarrow 303K$ and $q_t \approx 7.5g/kg \rightarrow 17g/kg$. Assuming linear mixing, the thermodynamic states of the cloud-environmental air mixture can be approximated to lie along a mixing line (dot-dash) between these two squares. The mean properties of the saturated mixtures for each of the simulations can then be considered to be lying on the saturation curve. The point where this mixing line crosses the saturation curve gives the properties of the critically saturated mixture, $\theta_{l,s}$ and $q_{t,s}$. These values can be used to determine the magnitude of the buoyancy minima in the shell b_s (shown in bottom panel of figure 4.2). The circles denote the point $(\theta_{l,s}, q_{t,s})$ obtained from the DNS for each of the simulations and they lie very close to the saturation curve hence showing that this approximation works well.

The cloud layer extends up to L_c in the cross-stream direction and the forcing is applied in this region. The initial buoyancy and vertical velocity distributions are homogeneous in the $\hat{z}$ and $\hat{y}$ directions. Periodic boundary conditions are imposed along these directions as well. Free-slip boundary conditions are imposed along the $\hat{x}$ direction. This setup results in the mean values having non-zero gradients only along the $\hat{x}$ direction. The forcing is applied across the cloud layer till $L_c = 1m$ over a time scale given by $\tau_c = L_c/w_c$. To ensure that results were not influenced by these arbitrary parameters, a sensitivity analysis was performed in which two test simulations were performed: the first by relaxing the nudging time scale to $2 L_c/w_c$, and a second simulation by doubling L_c to $2m$. The results obtained indicate that the flow dynamics are insensitive to the choice of L_c and τ_c (shown in appendix A).

The domain size is $30m \times 15m \times 15m$. The simulations are performed until the shell reaches about 70 percent of the domain width (in $\hat{x}$ direction) so as to avoid any effects from interference with the domain wall boundary.

The simulations named A01 - A10 vary in the initial θ_l and q_t of the cloud (θ_{lc}, q_{tc}) and environment (θ_{le}, q_{te}), and the strength of the cloud updraft w_c as shown in table 4.1. The

Table 4.1: Simulation parameters

Sim No	Grid size	$\Delta\theta_l$ (K)	Δq_t (gkg ⁻¹)	θ_{lc} (K)	q_{lc} (gkg ⁻¹)	w_c (ms ⁻¹)	t_{sim} (s)	b_s (ms ⁻²)	Re_λ	$\Delta x/\eta$
A01	3072 x 1536 x 1536	-6.2	5.4	288.5	3.0	0.81	148	-0.022	95.1	0.62
A02	1536 x 768 x 768	-8.1	6.3	286.1	4.3	0.96	120	-0.025	70.3	0.89
A03	1536 x 768 x 768	-5.9	5.5	288.7	3.0	0.81	120	-0.018	61.1	0.78
A04	3072 x 1536 x 1536	-2.1	4.0	292.6	1.3	0.67	148	-0.0073	90.3	0.33
A05	1536 x 768 x 768	-5.2	6.0	294.1	3.0	0.52	148	-0.0088	102.7	1.39
A06	1536 x 768 x 768	-1.9	1.8	292.8	0.8	0.31	180	-0.0088	36.5	0.76
A07	1536 x 768 x 768	-2.6	2.0	296.4	1.3	0.31	240	-0.0014	60.9	0.62
A08	1536 x 768 x 768	-0.8	2.9	299.2	0.9	2.03	100	-0.0002	47.8	0.52
A09	3072 x 1536 x 1536	-2.6	2.0	300.4	1.2	0.43	220	-0.002	53.8	0.30
A10	1536 x 768 x 768	-0.8	1.3	301.2	0.3	2.00	120	-0.007	64.7	0.82

difference in the initial values of the scalars $\Delta\theta_l = \theta_{lc} - \theta_{le}$ and $\Delta q_t = q_{tc} - q_{te}$ across the cloud-environment interface are shown in the third and fourth columns. The simulations are run for a duration given by t_{sim} . The remaining parameters shown in the table (to the right of the double-vertical line) are obtained from the simulation: the magnitude of the minimum mean buoyancy in the shell b_s , the Taylor Reynolds number $Re_\lambda = \sqrt{\frac{2}{3}} k \frac{\lambda}{\nu}$, where $\lambda = \sqrt{\frac{10\nu k}{\epsilon}}$ is the Taylor micro-scale, ν is the fluid kinematic viscosity, k and ϵ are the integral turbulent kinetic energy and dissipation respectively within the shell, and the resolution $r_x = \Delta x/\eta$ where η is the Kolmogorov length scale. The domain is discretized into a uniform grid of 3072 x 1536 x 1536 points for simulations A01, A04 and A09, and a grid of 1536 x 768 x 768 for all other simulations. The simulations were performed on the UK supercomputer ARCHER with A01 running on 683 nodes (using 16,384 cores) for 20 hours (CPU time).

4.3 Identification of shell

The turbulent mixing between the cool and moist cloudy air and the warm, dry environmental air, leads to evaporation (initially present only in cloudy area) until the mixture becomes critically saturated. The evaporative cooling at the mixing zone in the cloud edge results in the layer becoming negatively buoyant as the temperature scalar is no longer passive, and is coupled to the flow buoyancy. We refer to the negatively buoyant layer as the 'shell', and to the negatively

buoyant layer with negative vertical velocity as the 'subsiding shell'.

Figure 4.3 shows the development of the subsiding shell at the cloud boundary for simulation A01. The snapshots show the instantaneous buoyancy b and vertical velocity w at different time intervals for simulation A01. The white filaments correspond to zero magnitude, and red and blue layers represent positive and negative regions respectively. As found in Abma, Heus, and Mellado (2013), buoyancy drives the flow and the sharp interface between the cloud and the environment evolves to convoluted filaments. The layer at the edge of the cloud becomes negatively buoyant early on in the simulation, and the thickness of the shell increases with time. However even when b is negative, at earlier times, the velocity still remains positive or close to zero. As the shell thickens, we start seeing the formation of the subsiding shell.

Figure 4.4 shows profiles of the mean buoyancy $\bar{b}$ and the mean vertical velocity $\bar{w}$ of the developing flow at the cloud boundary. As mentioned in the introduction, the flow can be considered homogeneous over the vertical direction $\hat{z}$ and the span-wise direction $\hat{y}$. Hence all the quantities are averaged over the yz plane. Additionally the quantities are averaged over a time interval of $4s$. Hence the over-bar denotes statistics averaged over the homogeneous yz -plane and a time interval $t_{stat} = 4s$. For example, the mean buoyancy $\bar{b}(x, t)$ is calculated as,

$$\bar{b}(x, t) = \frac{1}{t_{stat}} \int_0^{t_{stat}} \left[\frac{1}{L_y L_z} \iint_{y\hat{O}z} b(x, y, z, t) dy dz \right] dt \quad (4.4)$$

Results are shown every $8s$ from $t = 48s$ to $t = 112s$ for simulation A01. We observe the formation of the negatively buoyant shell and its thickening with time. The magnitude of the minima for $\bar{b}$ and $\bar{w}$, $\bar{b}_{min}(t)$ and $\bar{w}_{min}(t)$ respectively, are also shown along with their respective locations along $\hat{x}$, x_b^0 and x_w^0 . The bounds of the negatively buoyant layer ($x_b^\pm$), and negative vertical velocity ($x_w^\pm$) are also shown. These are respectively, the locations along $\hat{x}$ where the quantities first turn negative (x_b^-, x_w^-) and then positive again (x_b^+, x_w^+).

Figure 4.4 clearly shows the shell growing and thickening with time. From figure 4.4(a), it is clear that after an initial transient period, the minimum buoyancy $\bar{b}_{min}(t)$ is time-invariant. This occurs when the cloud-air mixture is critically saturated as will be explained rigorously in section 5. Figure 4.4 also shows how x_b^- and x_b^+ shifts as the shell broadens with time. The

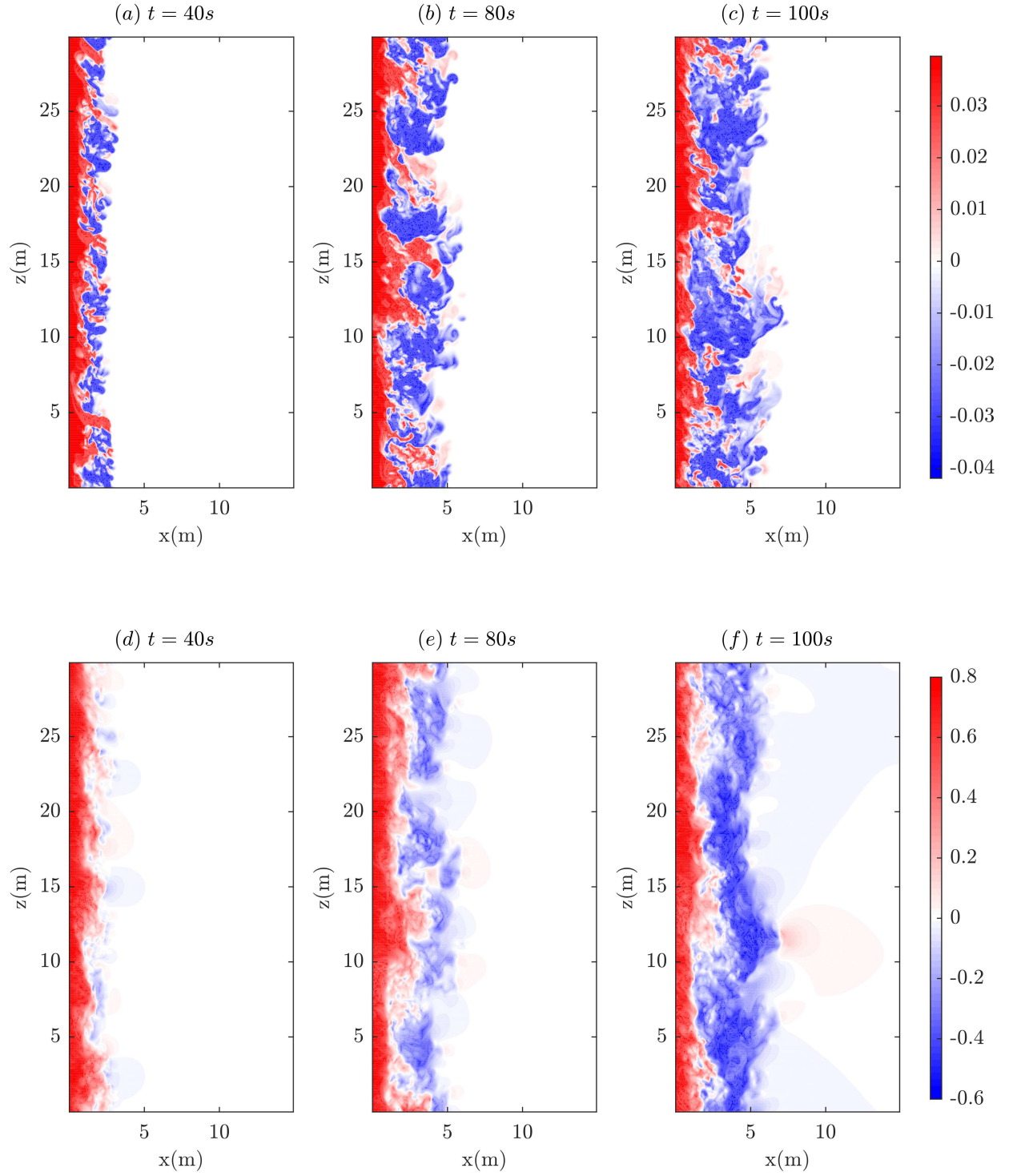


Figure 4.3: Instantaneous plots of the vertical cross-section of the flow in simulation A01. Top panel shows the evolution of buoyancy and bottom panel shows the evolution of vertical velocity. Red represents positive values and blue negative values with white representing zero.

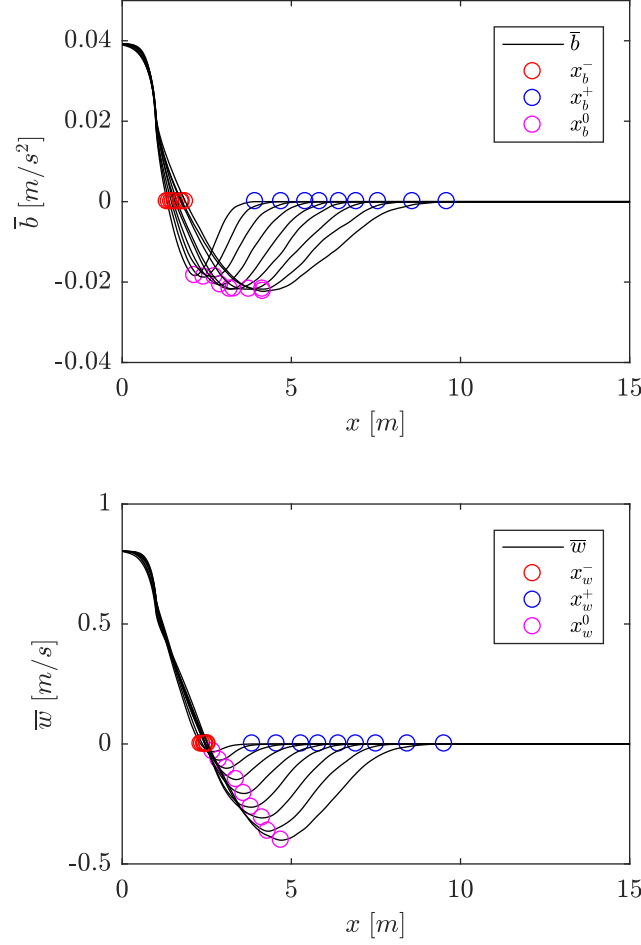


Figure 4.4: Time series of (a) mean buoyancy $\bar{b}$, and (b) mean vertical velocity $\bar{w}$ for simulation A01. Also shown are the locations x_b^- , x_b^+ , x_w^- , x_w^+ where the quantities first turn negative and consequently turn zero again, and the location of the minimum magnitudes x_b^0 and x_w^0 . Both plots show profiles every 8s from time 48s to 112s.

inner boundary of the shell x_b^- , is observed to shift only by a very small distance, which allows us to consider it constant. The outer boundary of the shell is observed to shift outwards into the environment. Contrary to the mean buoyancy, the minimum magnitude of the velocity is not time-invariant and figure 4.4(b) clearly shows the shell accelerating downwards. Figure 4.4 hence gives a clear picture of a negatively buoyant mixture of cloudy and non-cloudy air accelerating downwards, i.e. a subsiding shell. In both figures we observe a lateral shift in the locations of the minima, x_b^0 and x_w^0 . The location of the minima moves outwards into the environment as the shell thickens.

In figure 4.5, the area in the numerical domain where $\bar{b}$ and $\bar{w}$ is negative is shown in red and blue respectively. The flow studied over 148 s (which is approximately 7 shell large-eddy turn over times) can be considered to include two phases, each consisting of negatively buoyant parcels of air, but with either positive or negative velocities. The first 'drag phase', i.e. when

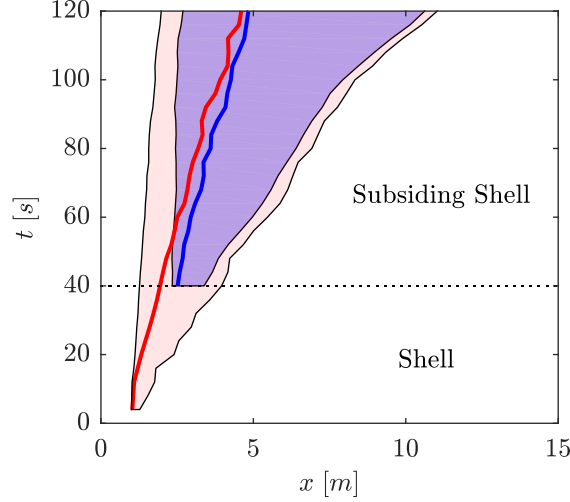


Figure 4.5: Boundaries of the subsiding shell in simulation A01. The negatively buoyant mixture is shown in red and region with negative vertical velocity is in blue. The inner and outer bounds of the red region is x_b^- and x_b^+ . Red line is x_b^0 and blue line is x_w^0 .

the cold layer is dragged up along the updraft, occurs during approximately the first 40s (which includes a flow transition period). In this phase, a negatively buoyant region is formed, but the mixed air parcels have positive vertical velocity. The second 'buoyancy phase' starts once this cold layer starts moving downwards, i.e. the buoyancy dominates. The transition from the drag phase to the buoyancy phase occurs when the shear across the shell inner boundary dominates the buoyancy in the shell, and this is analysed in detail in section 4.5.

4.4 Self-similarity and characteristic scales of the shell

In this section, we explore the self-similarity aspects of the flow. The self-similarity variable is defined as

$$\eta_b = \frac{x - x_b^0}{l_s} \quad (4.5)$$

where $l_s(t) = x_b^+(t) - x_b^-(t)$ is the thickness of the shell calculated from DNS data.

The $\bar{b}$ profiles from time 96s to 140s neatly collapse on top of each other when normalized with $\bar{b}_{\min}$ as shown in figure 4.6a. The colours indicate progress in time (from lighter to darker). Also, given that the flow does not reach an 'equilibrium' state in the sense that the shell is accelerating, $\bar{w}$ shows a very good collapse when normalized with $\bar{w}_{\min}$ (figure 4.6b). The noticeable shift in most of the figures for η_b values less than -0.25 corresponds to the cloud

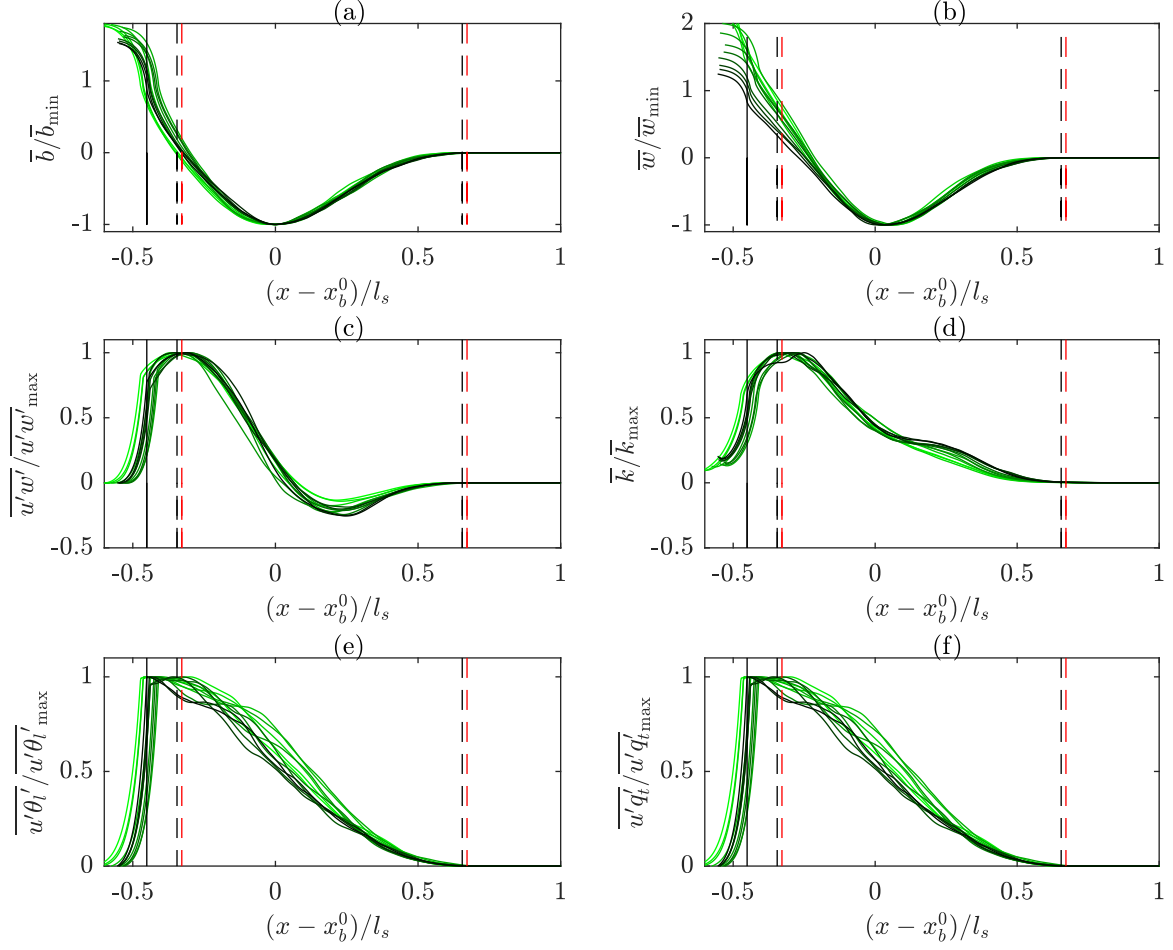


Figure 4.6: Self similarity plots for the shell in simulation A01. (a) $\bar{b}$ (b) $\bar{w}$, (c) $\overline{u'w'}$, (d) $\bar{k}$, (e) $\overline{u'\theta'_l}$, (f) $\overline{u'q'_t}$. All profiles are from time 96s to 140s. The colours indicate progress in time (from lighter to darker). The black line denotes the boundary of the nudging zone, black dashed lines are the boundaries of the shell at 96s and the red dashed lines are the boundaries of the shell at 140s.

layer in the domain where the nudging is applied.

Self similarity in the mean Turbulent Kinetic Energy (TKE) $\bar{k}$, and the turbulence fluxes $\overline{u'w'}$, $\overline{u'\theta'_l}$, and $\overline{u'q'_t}$ is investigated. The TKE is calculated as $\bar{k} = \frac{1}{2}(\overline{u'^2} + \overline{v'^2} + \overline{w'^2})$ where $\overline{u'^2}$, $\overline{v'^2}$ and $\overline{w'^2}$, are the measures of the turbulent fluctuations along x , y and z directions respectively. These quantities are normalized with their respective maxima. The results are shown in figures 4.6(c), (d), (e) and (f) where a satisfactory collapse is observed for the quantities which indicates self-similarity. All plots show profiles every 4s from 96s to 140s.

Now that self-similarity of the first and second order statistics has been demonstrated, the different possible characteristic scales for this problem are explored. This can be done in several ways; one approach would be to relate the scales used to non-dimensionalize the profiles directly to external flow parameters and to time, as is done for example in van Reeuwijk, Krug, and

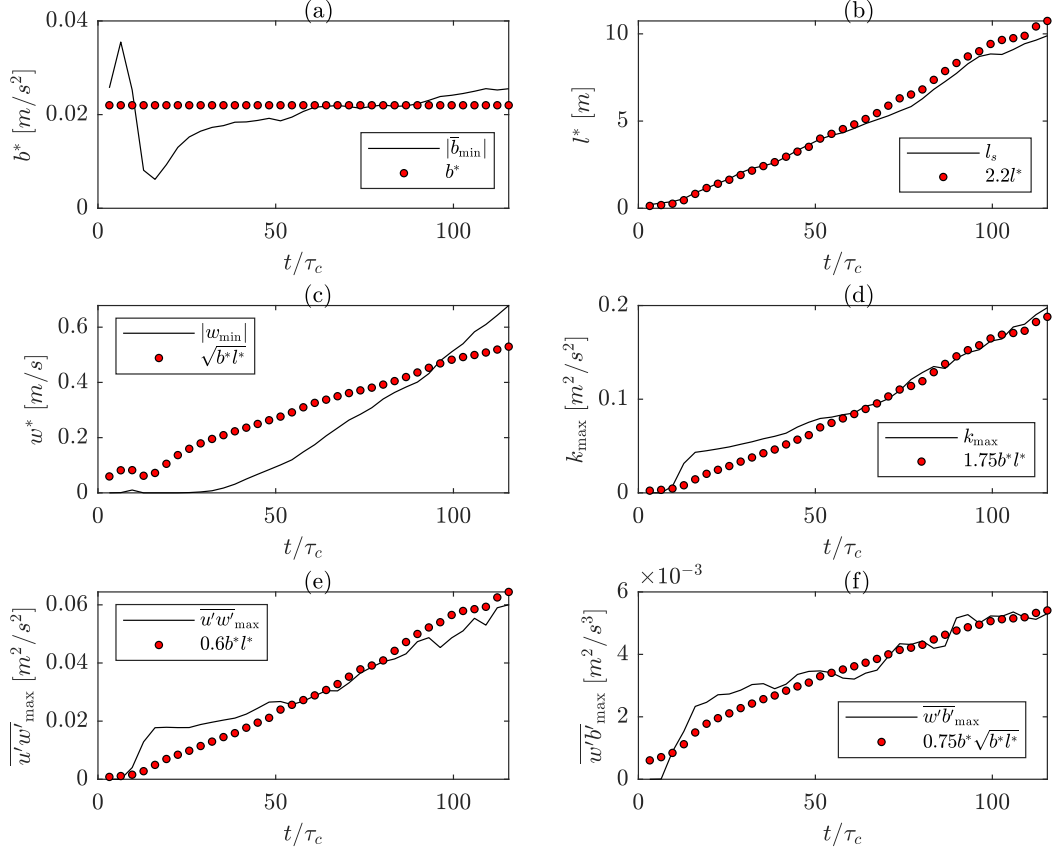


Figure 4.7: Relationship between characteristic scales and second order moments and respective maxima/minima for simulation A01. Relationship between (a) buoyancy scale b^* and $|b_{min}|$, (b) length scale l^* and l_s , (c) velocity scale w^* and $|w_{min}|$, (d) maximum total kinetic energy k_{max} and b^*l^* , (e) maximum turbulent momentum flux $\overline{u'w'}_{max}$ and b^*l^* , and (f) maximum turbulent buoyancy production $\overline{w'b'}_{max}$ and $b^*\sqrt{b^*l^*}$. The x-axis is normalized with τ_c .

Holzner (2018). This is done by using internal scales, which are derived from integral properties of the flow problem (Craske and van Reeuwijk 2015). Once the relevant internal scales are identified, the internal scales are linked to external scales.

We define characteristic scales using integral properties of the flow, namely the buoyancy integral B and the volume flux Q defined as,

$$B(t) = - \int_{x_b^-(t)}^{x_b^+(t)} \overline{b}(x, t) dx,$$

$$Q(t) = \int_{x_b^-(t)}^{x_b^+(t)} \overline{w}(x, t) dx.$$

The buoyancy integral B can be linked to the characteristic scales b^* and l^* as

$$B = b^* l^*. \quad (4.6)$$

The buoyancy of the mixture of cloudy and non-cloudy air, which were initially at two different thermodynamic states, reaches a minimum value when the mixture is critically saturated. Intuitively, the characteristic buoyancy scale b^* for this particular problem will be the saturation buoyancy b_s , i.e.

$$b^* = |b_s|. \quad (4.7)$$

The magnitude of b_s can be predicted *a priori* by using the mean values of the thermodynamic variables, i.e., $\bar{\theta}_l$ and $\bar{q}_l$. As explained in section 4.2, $\bar{q}_l = 0$ on the saturation curve shown in figure 4.2. From the definition for $\bar{\theta}_l$ (equation (2.7)), it then follows that $\bar{\theta}_{l,s} = \bar{\theta}_s$ implying that b_s can be determined from equation (4.3) as

$$b_s = g \left(\frac{\bar{\theta}_s - \theta_0}{\theta_0} - \left(1 - \frac{R_v}{R_d}\right)(\bar{q}_{t,s} - q_{t,0}) \right). \quad (4.8)$$

After an initial transient region up to $t/\tau_c \approx 60$, the values of $|b_s|$ and $|\bar{b}_{\min}|$ show a good agreement as shown in figure 4.7a. The saturation point is set by the initial thermodynamics of the cloud and the environment and we observe it to be invariant with time as we assume linear mixing.

Once the buoyancy scale b^* has been defined, the characteristic shell width l^* follows directly as

$$l^* = \frac{B}{b^*}, \quad (4.9)$$

which can be interpreted as the top-hat width of the shell (i.e. the width in case the buoyancy was constant inside the shell). Figure 4.7(b) shows that this definition is indeed appropriate, and we observe a relation $l_s = 2.2l^*$. The x axis has been normalized with τ_c . The length scale l^* , which is a measure of the shell thickness, is also observed to evolve linearly with time in figure 4.7b. Abma, Heus, and Mellado (2013) observed a quadratic growth in their idealized model. However, the current study includes factors which limit the free growth of the shell, such as the in-cloud positive buoyancy and the velocity, which could be the reason for the linear growth of the shell thickness.

A characteristic velocity scale is identified next. Since b^* and l^* are characteristic scales

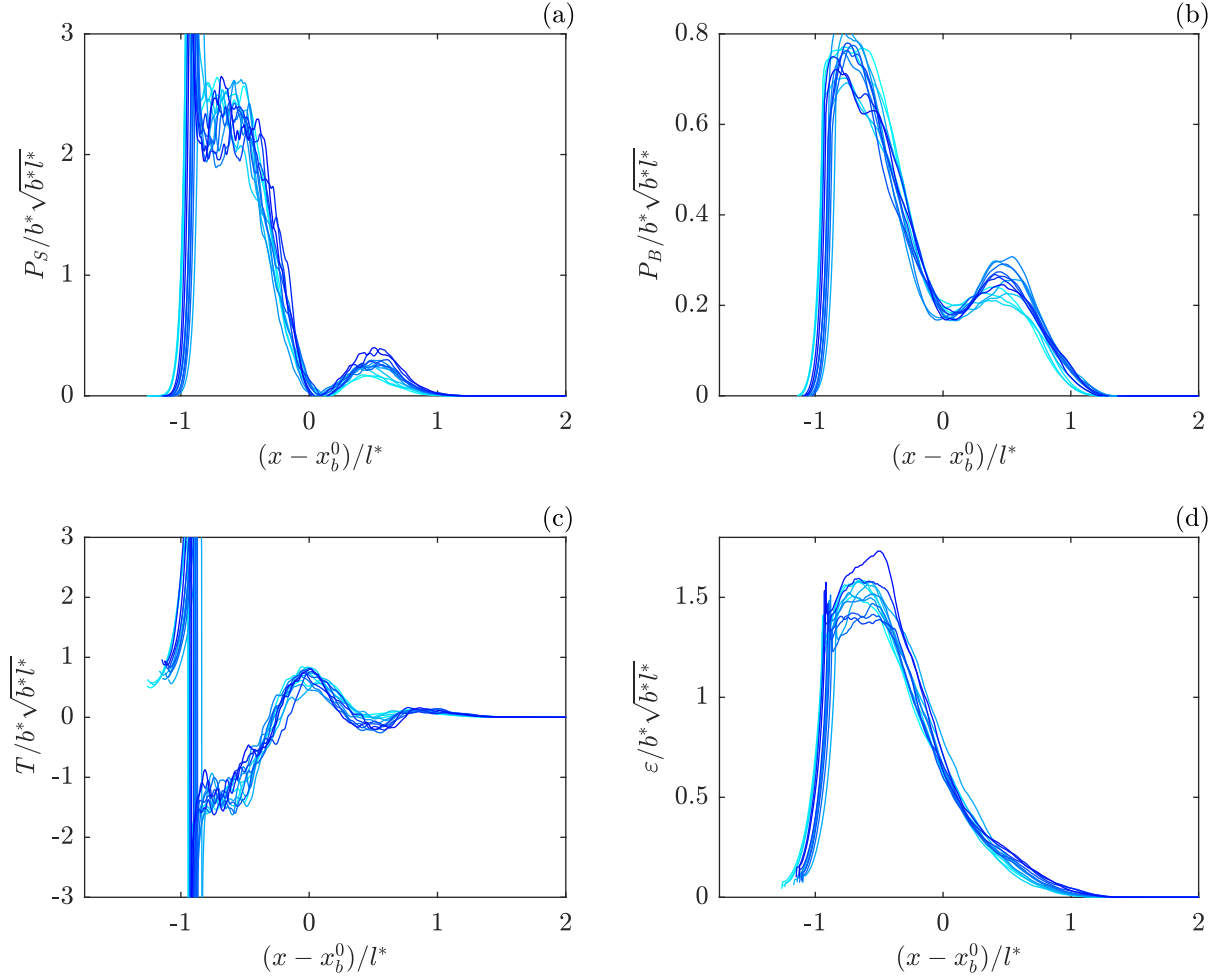


Figure 4.8: Scalings for TKE budget quantities for simulation A01. (a) P_S , the shear production, (b) P_B , the buoyancy production, (c) T , the transport term and (d) ε , the viscous dissipation rate of TKE. All profiles are from time 96s to 140s. The colours indicate progress in time (from lighter to darker).

for this problem, it would follow that the characteristic velocity $w^* = \sqrt{b^* l^*}$. This velocity scale is tested in figure 4.7c. It is clear that the velocity scale $\sqrt{b^* l^*}$ is not representative of the shell velocity. However, remarkably, the turbulence kinetic energy k and turbulent horizontal transport of vertical momentum $\overline{u'w'}$ do scale with $\sqrt{b^* l^*}$ as shown in figures 4.7d and e, and the buoyancy TKE production term $\overline{w'b'}$ scales with $b^* \sqrt{b^* l^*}$. The shell is also observed to be accelerating as is shown in the linear growth of the velocity scale w^* in figure 4.7c. A 'flow equilibrium' or a steady state is not reached, and the velocity shows a possible ballistic growth with time with an acceleration defined by b^* and hence the thermodynamics of the cloud.

The collapse of the different terms of the TKE budget are now tested to confirm the ballistic growth of the shell argument. The budget quantities are normalized with the internal characteristic scales b^* and l^* . The different components of the averaged TKE budget, i.e., the

kinetic energy production terms (gradient and buoyancy production), transport terms and the viscous dissipation are examined. The TKE budget is given by

$$\frac{\partial k}{\partial t} = \underbrace{-\overline{u'w'} \frac{\partial \bar{w}}{\partial x}}_{P_S} + \underbrace{\overline{w'b'}}_{P_B} - \underbrace{\frac{\partial \overline{u'p'}}{\partial x} - \frac{\partial \overline{u'u'_i u'_i}}{\partial x} + \nu \frac{\partial^2 k}{\partial x^2}}_T - \underbrace{\nu \frac{\partial u'_i}{\partial x_j} \frac{\partial u'_i}{\partial x_j}}_{\varepsilon}, \quad (4.10)$$

where $\bar{k} = \frac{1}{2} \overline{u'_i u'_i}$ and repeated indices in a term imply a summation for all values of the repeated index. The term P_S denotes turbulence shear production and P_B is the buoyancy production term or the buoyancy flux. The next three terms combine to form the transport term T which includes the pressure transport term, turbulent advective transport and the diffusive transport of kinetic energy. The last term ε is the viscous dissipation rate of TKE.

Good collapse of the turbulent quantities are shown in figure 4.8(a) - (d) when scaled with the buoyancy scale b^* and length scale l^* which are calculated according to equations (4.7) and (4.9). The mean flow velocity is not important in generating and driving the shell and this renders the velocity scale w^* passive. The mean velocity is slaved to the buoyancy effects and hence the turbulent quantities scale with the buoyancy scale b^* .

4.5 Theory

In this section, we carry out a theoretical analysis to identify the processes which generate the different phases observed in the flow. We also identify how the shell is fed with the buoyancy which drives the flow. We start with Reynolds averaged (over the two homogeneous axes) equations for the vertical velocity and buoyancy using equations (4.1b) and (4.1c),

$$\frac{\partial \bar{w}}{\partial t} + \frac{\partial \overline{u'w'}}{\partial x} = \bar{b} + S_1, \quad (4.11)$$

$$\frac{\partial \bar{b}}{\partial t} + \frac{\partial \overline{u'b'}}{\partial x} + g \left(\frac{A}{\theta_0} - \frac{R_v}{R_d} \right) \left(\frac{\partial \bar{q}_s}{\partial t} + \frac{\partial \overline{u'q'_s}}{\partial x} \right) = g \left[\frac{S_2}{\theta_0} + \left(\frac{A}{\theta_0} - 1 \right) S_3 \right], \quad (4.12)$$

where $A = \frac{\theta}{T} \frac{L}{c_p}$ is assumed to be a constant, and S_1, S_2, S_3 are the Reynolds averaged terms for the cloud forcing. The detailed derivation is provided in appendix B.

Integrating equation (4.11) from the shell inner boundary $x_b^-(t)$ to the shell outer boundary

$x_b^+(t)$ results in,

$$\frac{dQ}{dt} = -B + \left(\overline{w}|_{x_b^+} \frac{dx_b^+}{dt} - \overline{w}|_{x_b^-} \frac{dx_b^-}{dt} \right) + \overline{u'w'}|_{x_b^-} - \overline{u'w'}|_{x_b^+}. \quad (4.13)$$

The budget equation for the volume flux Q is vital towards explaining the presence of the drag and buoyancy flow phases in the shell. The terms at the shell outer boundary x_b^+ , along with the Leibnitz integral term at x_b^- , are observed to be small and hence neglected. These are calculated starting from an initial time of $t = 4s$ when the first statistics are obtained. The remaining terms highlight the fact that the flow inside the shell is determined by a balance between B , the buoyancy integral, and $\overline{u'w'}|_{x_b^-}$, the horizontal transport of vertical momentum at the inner boundary of the shell. The onset of the buoyancy phase happens when the negative integral buoyancy flux B in the shell overcomes the vertical momentum flux $\overline{u'w'}$ transferred horizontally into the shell at x_b^- , which results in a reversal in the direction of the shell velocity. When $\overline{u'w'}|_{x_b^-}$ dominates the budget, we have the drag phase identified in section 4.3, i.e., the cold layer is dragged up by the cloud updraft. As B increases with time and consequently overcomes the momentum flux, the negatively buoyant layer reverses its direction and we start seeing the subsiding shell.

Equation (4.12) is now integrated from $x_b^-(t)$ to $x_b^+(t)$ giving,

$$\frac{dB}{dt} = \overline{u'b'}|_{x_b^-} - \overline{u'b'}|_{x_b^+} + g \left(\frac{A}{\theta_0} - \frac{R_v}{R_d} \right) \int_{x_b^-}^{x_b^+} \left(\frac{\partial \overline{q_s}}{\partial t} + \frac{\partial \overline{u'q_s'}}{\partial x} \right) dx, \quad (4.14)$$

Analyzing the different terms in equation (4.14), the third term on the right hand side can be shown to be equal to zero in the region $x > L_c$. It is also observed that the magnitude of $\overline{u'b'}|_{x_b^-}$ (not shown) is time-invariant for a particular simulation, and that of $\overline{u'b'}|_{x_b^+}$ is negligible. Hence the dominant term in the B budget is $\overline{u'b'}|_{x_b^-}$, which is the buoyancy flux at the inner boundary of the shell. Assuming $\overline{u'b'}|_{x_b^-} \approx \text{constant}$, and neglecting all small terms, $B = \int \overline{u'b'}|_{x_b^-} dt$. This shows that the total amount of buoyancy flux $\overline{u'b'}$ fed into the shell by the cloud ultimately drives the turbulent flow and is responsible for feeding the shell buoyancy and hence increasing its thickness.

Since the magnitude of $\overline{u'b'}|_{x_b^-}$ is observed to be time-invariant, a possible parameterization

Table 4.2: Parameterization coefficients for all simulations

Sim No	Shell	b_c	w_c	$F(m^2/s^3)$	γ	$\alpha \approx \zeta/2$
A01	Yes	0.039	0.81	2.8×10^{-3}	0.09	0.14
A02	Yes	0.057	0.96	3.6×10^{-3}	0.07	0.12
A03	Yes	0.046	0.81	2.4×10^{-3}	0.06	0.17
A04	Yes	0.042	0.67	1.3×10^{-3}	0.05	0.26
A05	Yes	0.072	0.52	2.3×10^{-3}	0.06	0.5
A06	Yes	0.004	0.31	2.7×10^{-4}	0.22	0.1
A07	No	0.015	0.31	1.9×10^{-4}	0.04	0.26
A08	No	0.051	2.03	1.5×10^{-4}	0.001	0.31
A09	No	0.011	0.43	2.1×10^{-4}	0.04	0.20
A10	Yes	0.001	2.00	2.5×10^{-5}	0.01	0.002

using w_c and b_c follows as

$$\overline{u'b'}|_{x_b^-} = \gamma w_c b_c, \quad (4.15)$$

where γ is a constant whose values for the different simulations are given in table 4.2. This parameterization is used in the following section to explain the possible external factors that define the shell thickness and also to quantify entrainment. It is also worth noting that one of the possible reasons for $\overline{u'b'}|_{x_b^-}$ being time-invariant could be the effects of nudging which keeps b_c and w_c a constant.

4.6 Cloud variability

In this section we study how the shell properties depend on the initial thermodynamic properties of the cloud by studying the results from the different simulations and hence link the internal scales with external flow parameters. A comparison of the shell formation during the first 100s for different clouds is shown in figure 4.9. In simulations (a) A06, (b) A01, (c) A03 and (d) A02, there is an early onset of the buoyancy phase in the shell compared to simulations (e) A05, (f) A04 and (g) A10. In (h) A09 and (i) A07, the drag phase dominates till the end of the

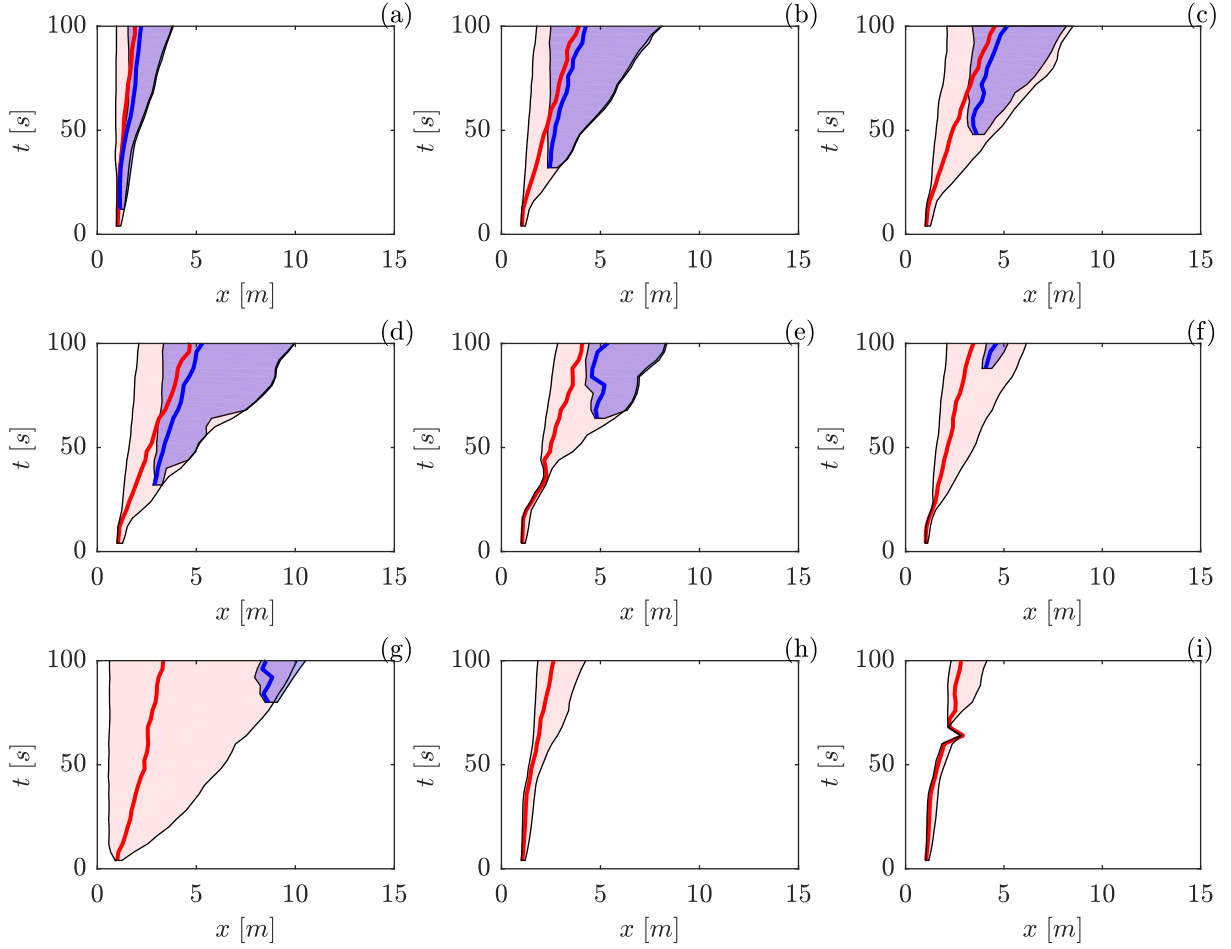


Figure 4.9: Cloud-environment mixing region for different simulations. (a) A06, (b) A01 (c) A03, (d) A02, (e) A05 (f) A04 (g) A10 (h) A09 (i) A07. Line styles and color schemes as in figure 4.5.

simulation. In simulation A08 (not shown) no shell is formed at all. It should be noted that a subsiding shell is formed in simulation A09 later on in the simulation (after 100s).

The mean buoyancy and vertical velocity are analyzed next. Figure 4.10 shows the normalized plots for $\bar{b}$ and $\bar{w}$. All the selected simulations reach a self-similar regime for buoyancy where $\bar{b}$ collapses neatly in the region where the shell is formed. The collapse for $\bar{w}$ is much less convincing, however, which is expected due to the passive nature of the mean velocity and the ballistic acceleration of the shell.

There is a distinct difference visually in the shell thickness between the different simulations as shown in figure 4.9. This can be explained by analyzing the budget for the buoyancy flux B given in equation (4.14). In equation (4.14), $\frac{dB}{dt}$, is by definition, the rate of growth of the turbulent length scale (or the shell thickness), which depends on the magnitude of the buoyancy flux $\overline{u'b'}$ pumped into the shell at its inner boundary.

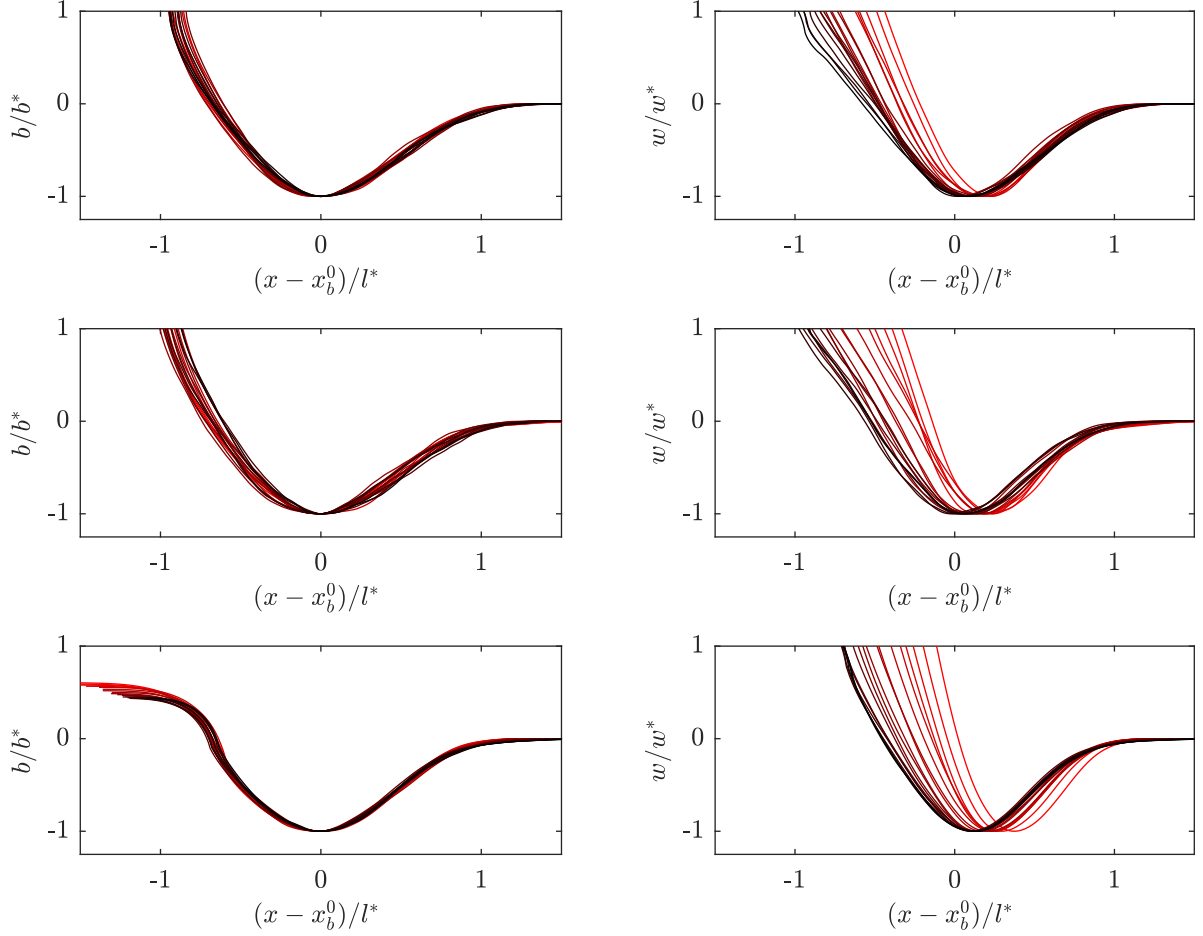


Figure 4.10: Self similarity plots for $\bar{b}$ and $\bar{w}$ for different simulations. (a),(b) A01; (c),(d) A02; (e),(f) A06.

The different simulations confirm that the buoyancy scale b^* is indeed the fundamental characteristic scale. Since the shell accelerates ballistically, it follows that a possible relation linking the internal velocity scale with external flow parameters would be $w_{\min} = b^*t$. The higher the magnitude of b^* , the lesser the time needed by the shell to descend. This relationship between $\bar{w}_{\min}$ and b^*t is checked for the simulations in which we see the formation of a subsiding shell and is shown in figure 4.11. Simulation A10 has been excluded in the figure even though a subsiding shell is generated. This is because the evaporative cooling is not strong enough to generate a negative vertical velocity comparable in magnitude to the $w_{\min}$ seen in the other simulations during the duration of the simulation. We observe a very good relationship between the two quantities (with a slope of approximately 0.25) which leads to the equation

$$\bar{w}_{\min} \approx 0.25 |b_s|(t - t_B), \quad (4.16)$$

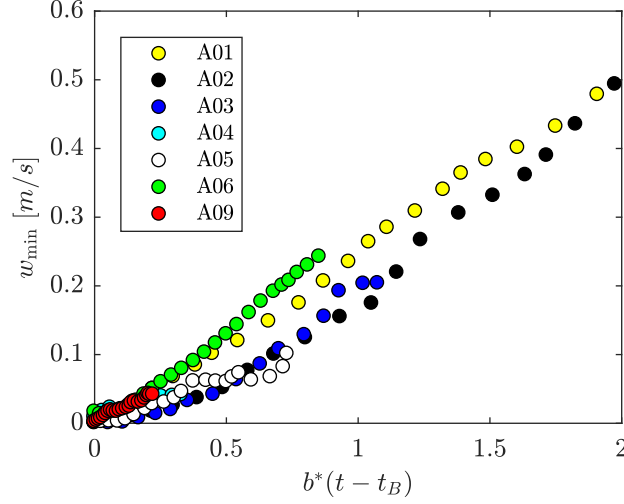


Figure 4.11: Relationship between $\bar{w}_{\min}$ and $b^*(t - t_B)$ in a subsiding shell

where t_B is the time at which the buoyancy phase starts (which is different for each of the simulations considered in figure 4.11; however no exact relation between t_B and initial cloud thermodynamics was observed using the DNS data).

The time dependence in equation (4.16) can be removed by using equations (4.9) and (4.15), thereby successfully linking the internal velocity scale with the external flow parameters,

$$\bar{w}_{\min} = 0.25|b_s| \left(\frac{|b_s|l^*}{\gamma w_c b_c} - t_B \right). \quad (4.17)$$

Shell thickness and entrainment

In this sub-section, we develop a model to study the rate of entrainment of the environment air into the cloud. The shell can be considered to be part of the cloud and it grows with the entrainment and mixing with the environmental air. Hence turbulent entrainment can be studied in terms of the rate of growth of the thickness l^* of the shell. Comparisons between the observed shell thickness l_s for the different simulations is done in figure 4.12 where l_s is normalized with the characteristic scale l^* for each simulation. In section 4.4, a relation $l_s = 2.2l^*$ was observed for simulation A01. Interestingly, this relation holds for all simulations as seen in figure 4.12 and could be useful in predicting the size of the shell thickness at a particular time given the initial cloud properties.

From this relation, an entrainment analysis can be performed by comparison with the Morton,

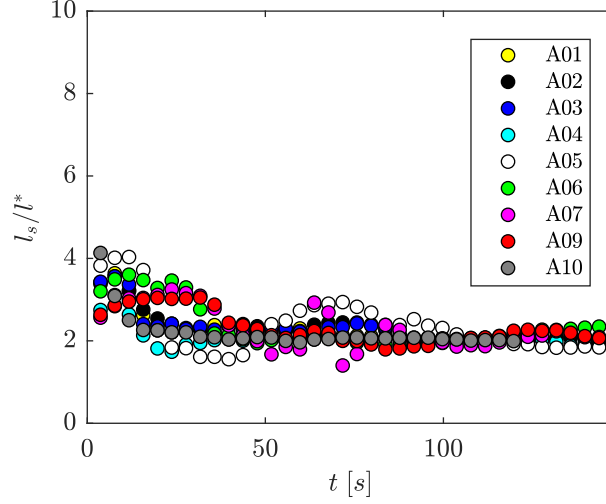


Figure 4.12: Evolution of normalized shell thickness.

Taylor and Turner model (Morton, Taylor, and Turner 1956) for the turbulent entrainment velocity which is,

$$w_e = \alpha \hat{w} \quad (4.18)$$

where w_e is the entrainment velocity, which is a fraction of a turbulent characteristic velocity $\hat{w}$. α is the entrainment coefficient. This entrainment hypothesis is the standard closure used in integral descriptions of turbulent flows like jets and plumes (van Reeuwijk and Craske 2015). We adapt this model to be used as a measure of entrainment in our current study. The model connects the velocity at which the environmental air is entrained into the shell (w_e), to a characteristic cloud velocity ($\hat{w}$), by a coefficient of proportionality α . Considering the entrainment velocity w_e as the rate of change of the characteristic thickness l^* with time, we get,

$$\frac{d}{dt}(l^*) = \alpha \hat{w} \quad (4.19)$$

Using equations (4.9), (4.15), and the relation $B \approx \overline{u'b'}|_{x_b^-} t$, l^* can be replaced in equation (4.19). Comparing the resulting relation with equation (4.18), the entrainment co-efficient α is given by,

$$\alpha = \frac{\gamma b_c}{|b_s|} \quad (4.20)$$

The coefficient is constant by definition and the values are given in table 2. The second column indicates whether a subsiding shell is formed within the first 100s of the simulation.

The entrainment co-efficient is different for different simulations and shows that entrainment is dependent on the initial thermodynamics and updraft velocities of the cloud and environment.

The entrainment coefficient α can be linked to the fractional entrainment rate ϵ used in cumulus parameterization schemes for large scale models. This fractional entrainment rate which can be expressed as the ratio of the entrainment rate E to the convective mass flux M^* is inversely proportional to the radius R^* of a cloud, i.e. $\epsilon = E/M^* \approx \zeta/R^*$, where ζ is a dimensionless proportionality constant (P. Squires and Turner 1962; Simpson and Wiggert 1969; Simpson 1971). Assuming a circular cross-section for the cloud,

$$\frac{\zeta}{R^*} = \frac{E}{M^*} = \frac{2\pi R^* w_e}{\pi R^{*2} \hat{w}} \quad (4.21)$$

Using equation (4.18) this can be rewritten as,

$$\epsilon = \frac{\zeta}{R^*} = 2 \frac{\alpha}{R^*} \quad (4.22)$$

Since our temporal simulations do not include a valid cloud radius, a fair comparison with numerical values of ϵ present in LES studies such as Siebesma and Cuijpers (1995b), Dawe and Austin (2011), Romps (2010) is not possible. However, the value of the proportionality constant ζ can be compared. For the study in Romps (2010), $\zeta/R^* = (\epsilon - \delta)/R^*$, (where δ is the fractional detrainment rate) and the values calculated for a cloud layer between 750m and 1400m are, $\epsilon = 2.2 \text{ km}^{-1}$ to 2.8 km^{-1} and $\delta = 3.5 \text{ km}^{-1}$ to 4.1 km^{-1} resulting in values of $\zeta/R^* = 1.3$. Assuming a radius $R^* = 500\text{m}$, this leads to $\zeta = 0.65$. For the current study, $\zeta = 2\alpha$ as shown in equation (4.22), giving numerical values in the range 0.2 to 0.99 which are comparable with that in Romps (2010).

4.7 Concluding remarks

A numerical case was developed to study the dynamics of the descending shell formed at the edges of actively growing shallow cumulus clouds. DNS was used to conduct a temporal study on the cloud-environment mixing and study the properties of the turbulent flow generated

by evaporative cooling. A forcing was applied on the cloud layer to maintain the in-cloud velocity and thermodynamics at pre-defined values to simulate an actively growing cloud. This introduces shear into the setup, and we end up with a buoyantly driven shell inside a shear layer. A bulk condensation scheme was used to describe cloud thermodynamics by diagnostically calculating the liquid water content in the cloud.

Two distinct flow phases were observed within a negatively buoyant turbulent cloud-environment mixture. The first is a 'drag' phase where the momentum flux transfer dominates and the negatively buoyant shell is dragged vertically upwards by the active cloud layer. The onset of the second 'buoyancy' phase occurs when the buoyancy flux within the shell dominates and consequently the shell starts descending. The time at which the onset of the buoyancy phase occurs (leading to the subsequent descending motion of the shell), depends on the dominating term in the velocity flux budget given by equation 4.13. Higher the momentum flux transfer between the cloud core and the shell, the greater the delay in the onset of the buoyancy phase.

The shell buoyancy scale is observed to be invariant with time which is consistent with what is seen by Abma, Heus, and Mellado (2013), and in our case is set entirely by the initial thermodynamic state of the cloud and the environment. However the shell thickness is observed to increase linearly with time while Abma, Heus, and Mellado (2013) observed a quadratic growth. Since the rate of change of the shell thickness has been shown to be dependent on the buoyancy flux pumped into the shell at the inner boundary ($\overline{u'b'}|_{x_b^-}$), the addition of positive buoyancy and updrafts in the cloud layer in this study could be the reason for this difference. The presence of the actively growing cloud inhibits the free growth of the shell. The velocity increases ballistically with the acceleration defined by the saturation buoyancy value b_s . The mean velocity is expected to be passive and the turbulent shell is buoyancy driven. Initial cloud conditions like the liquid water content, buoyancy of cloud core, strength of the core updraft etc. define the thickness and growth of the shell.

A self-similar regime is observed after an initial transient. However contrary to classical self similar flows, the TKE budget terms and the velocity moments scale according to the buoyancy and not with the mean velocity. The TKE terms scale with $b^*\sqrt{b^*l^*}$ and the velocity moments with b^*l^* . Internal scales based on the integral quantities of mean buoyancy and

vertical velocity were used to show self-similarity. These scales were successfully linked with external flow parameters.

The entrainment coefficient can be calculated by considering the shell as centred on the cloud edge and using the time rate of change of the shell thickness as an entrainment velocity. This coefficient will be a constant for a particular initial state of the cloud and the environment. A comparison is made with parameterization schemes used in large scale models and the numerical values of the entrainment coefficients are found to be of the same order of magnitude.

It is interesting to note here that for this case the shell thickness and the velocity continues to grow indefinitely. Since the shell is in the vicinity of an actively growing cloud, it is continuously fed with moisture from the cloud and the water droplets can evaporate leading to evaporative cooling and further fuelling the shell growth. In the presence of a more mature cloud nearing the end of its lifetime, the shell would have probably grown inward at the expense of the cloud. This could mean that the shell thickness and velocity are limited only by the cloud evolution phase and ultimately lifetime. It is also important to highlight the fact that by imposing a periodic boundary condition on a domain size of $30m$, larger eddies which could dominate flow before the end of the simulation are being suppressed. However due to the limitations of DNS and the temporal setup of the problem, this is unavoidable.

Using relations to predict the thickness and minimum vertical velocity of the shell in a standard shallow cumulus cloud like in simulation A01, the shell thickness would grow to $l_s = 99.8m$ considering a cloud updraft lifetime of $408s$. The minimum magnitude of the vertical velocity in the shell would reach values of $w_{\min} = -2.3m/s$. This is consistent with values observed in single cloud transects in Katzwinkel et al. (2014). The current experiment was considered with a non-stratified environment, but stratification in the environment could also possibly limit the velocity and thickness of the shell.

Chapter 5

A Lagrangian study of interfaces at the cloud edge

In this chapter, interfaces at the edge of an idealised, non-precipitating, warm cloud are studied using direct numerical simulations and massless particles. Different zones at the edge of a cloud are identified and particle movement across these zones are quantified. A turbulent-non turbulent interface is detected by applying thresholds on the enstrophy. Particle behaviour during entrainment and detraining across the different interfaces are investigated and a clearer picture of the mixing at a cloud edge is presented. Comparisons are made with large eddy simulations (data provided by Dr Thijs Heus from Cleveland State University). The chapter includes material that has been submitted and is currently under review in the Journal of Atmospheric Sciences (co-authored with Dr Thijs Heus and Dr Maarten van Reeuiwijk).

5.1 Introduction

Cumulus convection is one of the most important unresolved processes in weather and climate forecasting. The parameterization of different processes in convective schemes such as the representation of turbulent fluxes is a major source of uncertainty in Numerical Weather Prediction (NWP) models and Global Circulation Models (Bony et al. [2015](#)). Some of the most successful convective parameterisations employ mass-flux schemes (bulk and spectral). In such schemes a cloud model is employed to specify the upward mass flux through the cloud base. These mass flux schemes are mostly of two types: bulk schemes where a single entraining-detraining plume represents the combined effect of an ensemble of active cumuli, or spectral schemes where

multiple plumes are considered. Some examples (not an exhaustive list by any means) of the bulk mass flux models are the schemes by Tiedtke (1989), Kain and Fritsch (1990), Bechtold et al. (2001), Gregory and Rowntree (1990), Gerard (2015) and some popular spectral methods are the works of Arakawa and Schubert (1974), Johnson (1976) and Moorthi and Suarez (1992). As mentioned briefly in chapter 4, two important parameters which modify the mass flux and the vertical transport of temperature, moisture and momentum in these models are the entrainment and detrainment rates. A multitude of parameterisations exist to calculate these rates as summarized in de Rooy et al. (2013). Most of the schemes mentioned so far calculate the change of mass flux with height using entrainment and detrainment rates which have been divided into large scale dynamical rates, and smaller scale turbulent rates.

LES has become the primary tool to diagnose entrainment and detrainment rates and it has served the community well over the past years with the majority of the parameterisations arising from LES studies (de Rooy et al. (2013) and references therein). A traditional definition to diagnose bulk entrainment and detrainment rates through LES is (Siebesma 1998),

$$E_\phi = -\frac{1}{A\phi_e} \oint_{\partial\Omega_E} \rho \hat{\mathbf{n}} \cdot (\mathbf{u} - \mathbf{u}_i) \phi dl, \quad (5.1a)$$

$$D_\phi = \frac{1}{A\phi_c} \oint_{\partial\Omega_D} \rho \hat{\mathbf{n}} \cdot (\mathbf{u} - \mathbf{u}_i) \phi dl. \quad (5.1b)$$

where E_ϕ and D_ϕ are the entrainment and detrainment rates, ϕ is a conserved scalar and the subscripts c and e denote averages over the cloud and environment respectively. The path integral is taken around the edge of a cloud with area A at a constant vertical height. Here the cloud boundary $\partial\Omega$ has been decomposed into an entraining and detraining region, denoted $\partial\Omega_E$ and $\partial\Omega_D$ respectively. The regions are defined by the sign of the net entrainment velocity across the interface $\hat{\mathbf{n}} \cdot (\mathbf{u} - \mathbf{u}_i)$, and clearly $\partial\Omega = \partial\Omega_E \cup \partial\Omega_D$.

Although the definitions above are rigorous, the entrainment/detrainment rates will depend on the choice of the interface $\partial\Omega$. There are multiple interfaces that can be chosen. Most operational parameterisations use the boundary of the cloud core as the interface over which entrainment is calculated. Different definitions of the cloud core interface exist: often these are based on non-zero threshold values on liquid water content and vertical velocity (Romps 2010)

or thresholds on buoyancy and/or vertical velocity (de Roode and Bretherton 2003). Convective structures can also be identified using decaying passive tracers that are constantly emitted from the surface (Couvreur, Hourdin, and Rio 2010; Park, Gentine, et al. 2016; Park, Heus, and Gentine 2017). Siebesma and Cuijpers (1995a) approximated fractional entrainment and detrainment rates using LES and evaluated the effect of different definitions for the cloudy area. They employ a single bulk active cloudy part and a passive environmental part and define the active cloud domain in different ways: cloud (all grid cells with non-zero liquid water), updraft (non-zero liquid water with positive vertical velocity) and core (updraft with positive buoyancy). Their study reveals that the updraft sampling gives the best approximations for the turbulent fluxes of the conserved variables θ_l and q_l (for the temperature and humidity respectively). This is because the updraft sampling includes the negatively buoyant but decelerating part of the updraft rise as well. A different decomposition (as originally proposed by Tiedtke 1989) into an updraft, a downdraft and an environment was also evaluated to check the role of downdrafts. This did not prove to be better than the updraft sampling but it was stated that this would be relevant in the cases where the mass flux in the downdraft would be comparable to that in the cloud updraft. A more recent study by Gu et al. (2020) has shown that a bulk mass flux parameterization using a simple cloud-environment decomposition does not capture the correct magnitude and vertical transport of turbulent fluxes of heat and humidity. Inclusion of the downdraft significantly improved mass flux parameterizations (especially at the cloud top).

Romps (2010) recognizes the importance of defining the interface over which entrainment takes place and defines two categories, active and inactive, whereby a Lagrangian parcel can be considered to have entrained when it flips from inactive to active and vice-versa for detrainment. The atmosphere is divided into these two categories using thresholds for a condensate mixing ratio and the vertical velocity. The 'local' rates calculated in Romps (2010) revealed values twice as high as that in the particle budget calculations in bulk plume schemes. Dawe and Austin (2011) investigated the difference between the bulk (from bulk mass flux schemes) and local rates, and attributed this to the presence of the moist and negatively buoyant subsiding shells around the cloud cores and drier air at the edge of the cloud core. Bulk plume mass flux parameterisations define the properties of entrained air as the horizontal slab average over the

environment and that of the detrained air as the slab average over the cloud core as shown in equations (5.1a) and (5.1b). However, the presence of the shell means that the air entering and leaving the cloud is effectively pre-mixed.

As explained in de Rooy et al. (2013), it is important to note that the two approaches will result in the correct turbulent transport as long as the mixing coefficients ε and δ are diagnosed correctly. Smaller ε (δ) values combined with the higher difference between the entraining (detraining) air and the cloud (environment) should result in the same lateral turbulent flux as in the direct approach. Dawe and Austin (2011) also showed a preferential entrainment of parcels with average humidity and vertical velocity higher than that of the mean shell properties (thus enhancing the flux transfer). This makes it highly relevant to take a closer look at a cloud edge and focus on what effect the choice of interface has on air parcels at the cloud edge. This is the primary motivation for the present work.

A detailed study of lateral mixing at the cloud edge and the dynamics of the subsiding shell was performed in chapter 4. The DNS results for the buoyancy distribution in chapter 4 (figure 4.4) revealed the different possible interfaces over which cloud-environment mixing can occur. The formation of the shell gives rise to two interfaces which could possibly be of interest. The interface separating regions with zero and non-zero liquid water lies within the shell and this is the first interface of interest. The results in chapter 4 showed that this interface is at the point where the buoyancy in the shell is a minimum. We shall refer to this interface as the Visible Shell Boundary (VSB) since it separates the visible part of the shell (which has non-zero liquid water) from the invisible region of the shell (no liquid water). The second interface of interest is the outer boundary of the shell which separates the turbulent region at the cloud edge from the non-turbulent environment, i.e. the Turbulent-Non Turbulent Interface (TNTI). The TNTI has been extensively studied at the edges of jets, plumes, wakes, mixing layers and boundary layers as reviewed in da Silva et al. (2014). The interface layer is known to include two adjacent layers, the Viscous Super Layer (VSL) where vorticity is introduced through diffusion, and the Turbulent SubLayer (TSL) which matches the vorticity from the turbulent region to the VSL. The TNTI is considered to be a surface with zero thickness between or within these two layers. However, this interface has been rarely considered in most cloud-edge studies. LES

studies using a decaying scalar emitted from the surface to identify coherent structures in the convective boundary layer (Couvreur, Hourdin, and Rio 2010; Park, Heus, and Gentine 2017) report areas around the cloud with elevated levels of those scalars, quickly dropping off when moving further away into the environment. It is possible that these areas are a proxy for the TNTI. In this chapter we will show that, as far as this idealised flow is concerned, the TNTI represents the outer edge of the idealized cloud system.

The effectiveness of Lagrangian particle tracking in clouds was demonstrated by Heus, van Dijk, et al. (2008) who used LES and tracked massless Lagrangian particles that followed the flow to study mixing between clouds and the environment. This study settled the debate surrounding the origin of in-cloud air by tracing back cloud-air parcels, clearly revealing the absence of significant cloud top mixing and that practically all mixing occurs laterally. Yeo and Romps (2012) used Lagrangian particle tracking on an individual cumulus cloud and calculated a higher rate of entrainment compared to the Eulerian direct measurements. This was attributed to the fast re-circulation of air in and out of the core. It was also shown that almost half of the air entrained by a cloud during its lifetime had been previously detrained. These were effects which could not be captured or resolved by Eulerian measurements.

The combination of DNS and a Lagrangian particle tracking routine facilitates a study of mixing and entrainment over the different interfaces at cloud edges in detail. We will highlight the importance of the TNTI and hence the importance of including the subsiding shell in cloud edge mixing studies. By following individual particles as they entrain and detrain across the different interfaces, we show that a Lagrangian parcel can be considered to be 'entrained' when it crosses the TNTI and that the shell extends the cloud edge to this interface. We also aim to highlight the degree of pre-mixing done by the shell to the entraining and detraining air parcels. The case setup of the DNS includes important cloud characteristics such as in-cloud buoyancy and updrafts, but at the same time ignores the effects of microphysics and the larger scales. However it is intentionally designed so to avoid the complexity of a real cloud and only focus on the process of lateral mixing and entrainment at the cloud edge. In order to investigate the extent to which the findings are transferable to realistic clouds, results from an LES of a no-wind BOMEX case is analysed to explore whether we can detect the TNTI there. Using conditional

averages of the enstrophy and mass flux we show that the different interfaces can be distinctly identified and present results highlighting the net mass exchange between the different zones.

This chapter is structured as follows. In section 5.2, we explain the case setup, governing equations and the details of the simulations performed. In section 5.3, we present the interfaces and how they are identified in this study. In section 5.4, we introduce the tracers and present results. In section 5.5, we look at how the properties of the tracers change during entrainment and detrainment across the interfaces. In section 5.6, we highlight the degree of premixing done by the shell. Results showing the detection of the TNTI in LES is presented in 5.7. Section 5.8 includes a discussion of the results from the simulations and concluding remarks.

5.2 Case setup and simulation details

5.2.1 *Direct Numerical Simulations*

The case setup is identical to that used in chapter 4 (figure 4.1) with the domain divided into a cloud and environmental layer. The cloud layer is moist and positively buoyant and the environment is dry and the buoyancy is defined to be zero. A negatively buoyant shell forms due to the nudging in the cloud layer, which then develops in a self-similar fashion. Two distinct flow phases were observed in chapter 4 within a negatively buoyant turbulent cloud-environment mixture. The first is a 'drag' phase where the momentum flux transfer (between the cloud core and the shell) dominates and the negatively buoyant shell is dragged vertically upwards by the active cloud layer. The onset of the second 'buoyancy' phase occurs when the negative buoyancy within the shell overcomes the drag and consequently the shell starts descending. Another pertinent finding in chapter 4 is that the shell falls ballistically and the mean velocity inside the shell is dynamically unimportant.

The governing equations are the same as in chapter 4 (equation (4.1)) and the buoyancy is calculated according to equation (4.3). The bulk condensation scheme described in section 2.2 is again used to calculate q_l .

The simulation is performed on a domain of $30m \times 15m \times 15m$ using a grid of $1536 \times 768 \times 768$ points. The initial profiles are the same as simulation A03 in table 4.1 in chapter 4 and

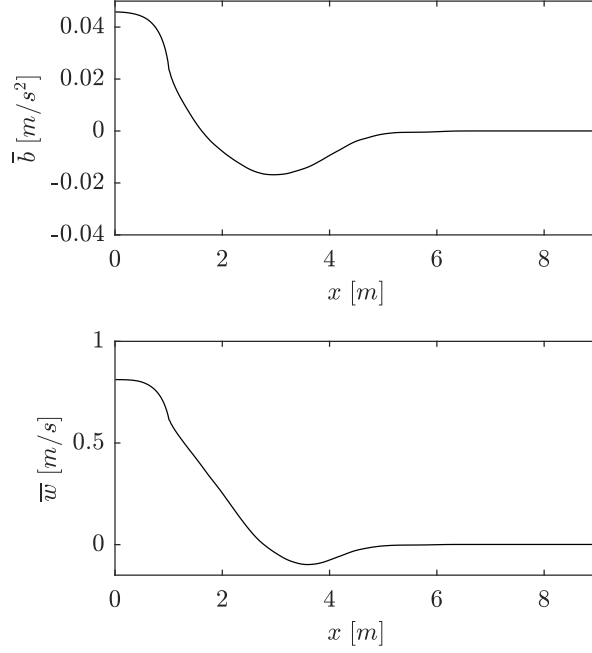


Figure 5.1: Mean buoyancy $\bar{b}$ and mean vertical velocity $\bar{w}$ at t_0 when particles are seeded.

the simulation is run for 80s. The kinematic viscosity ν is $4 \times 10^{-4} \text{ m}^2/\text{s}$. The Taylor Reynolds number (Re_λ) at the end of the simulation is 91 and the grid resolution $r_x = \frac{\Delta x}{\eta} = 1.3$ where η is the Kolmogorov length scale. The turnover time for the largest eddies in the shell, $\tau = l_e/u'$, is 14.4s and the Kolmogorov time scale $t_\eta = (\nu/\varepsilon)^{0.5}$ is 0.45s (where the length scale for the largest eddies in the shell $l_e = u'^3/\varepsilon$). Here u' is the rms velocity and ε is the dissipation rate. It is important to mention here that as in chapter 4, ε is calculated as an average over the width of the shell and not the entire cloud domain. Hence the time scales τ and t_η are representative of the characteristic time scales of the largest and smallest eddies inside the shell.

Non-inertial particles are considered in this chapter which are carried along by the flow. Hence only the particle locations are updated by solving equation (2.21b). A tricubic Hermite interpolation scheme described in section 3.3.2 is used to interpolate the particle velocities from the Eulerian flow velocity fields. A third-order Adams-Bashforth time-stepping scheme described in section 3.3.3 is used to integrate the particle locations at each time step. The particles at processor boundaries are communicated across processors after each time integration step following the flow field according to section 3.3.4.

A total of 3 million particles are seeded into the numerical domain after the flow has reached a self-similar state at $t_0 = 68\text{s}$. Importantly, by this stage, the flow is in the buoyancy regime

and there is a descending shell present in the domain (at earlier times, the shell is only visible in the turbulence but the cloud boundary is still dragged up due to the turbulence). Figure 5.1 shows the mean buoyancy and vertical velocity profiles at the time of seeding. The particles are seeded homogeneously across the x , y and z axes within a volume bounded by $[0, 9m]$, $[0, 15m]$, and $[0, 30m]$ respectively. Since the outer boundary of the shell is at approximately $7.5m$ at the end of the simulation, the particles are seeded only up to a distance of $9m$ along the x axis. The region from $9m$ to the boundary at $15m$ is the quiescent environment and the results are not affected by not seeding within this region. Data for the particles is written every $0.2s$.

5.2.2 Large Eddy Simulations

To explore the feasibility of a TNTI in more realistic set ups, the MicroHH LES (van Heerwaarden et al. 2017) is used to perform an LES of shallow cumulus convection based on the BOMEX case (Siebesma, Bretherton, et al. 2003) at an isotropic $4.1m$ grid spacing, using $800 \times 800 \times 800$ grid points and a $3.2km$ horizontal domain size. The large eddy simulations and the postprocessing were performed by Dr Thijs Heus from Cleveland State University. Note that this grid spacing is much finer than the $25m$ that Heus and Jonker (2008) found was sufficient for a converging mass flux in the subsiding shell. With this resolution, the internal dynamics of the shell are better resolved and the enstrophy approaches a meaningful value. A simulation time of $10h$ is used, of which the first $3h$ are discarded as spin-up. In order to separate shear driven turbulence from convective turbulence, we set the geostrophic wind to zero. As it turns out, shear does not seem to make a major difference to our results, other than enlarging the shell size.

5.3 Interfaces at the cloud edge

As mentioned in the introduction, multiple interfaces exist at the cloud edge over which we can consider entrainment and detrainment. In this section we clearly define and visualize the two interfaces that exist due to the presence of the shell, i.e. the Visible Shell Boundary (VSB) and the TNTI. We also include the Cloud Core Boundary (CCB) which is commonly used in most

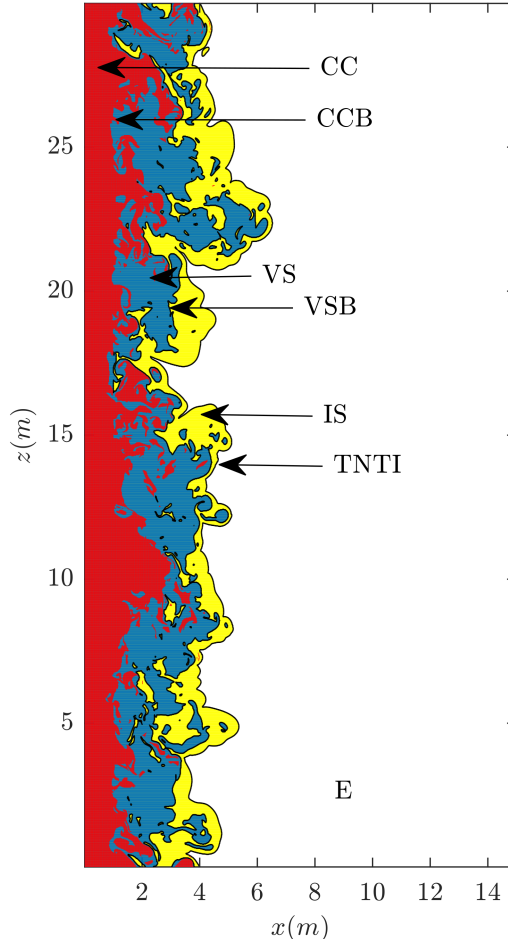


Figure 5.2: The different zones at the edge of the cloudy domain at the time of seeding (t_0) shown using contours of b . The color scheme is: red - Cloud Core (CC), blue - Visible Shell (VS), yellow - Invisible Shell (IS) and white - Environment (E). Also shown are the interfaces: Cloud Core Boundary (CCB), Visible Shell Boundary (VSB) and Turbulent Non-Turbulent Interface (TNTI).

parameterization studies. The CCB and the VSB are defined by applying thresholds on the buoyancy b and the liquid water mass fraction q_l . The TNTI is defined by applying a threshold on the enstrophy ω^2 . The enstrophy is a scalar quantity which is defined as $\omega^2 = \boldsymbol{\omega} \cdot \boldsymbol{\omega}$, where $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ is the vorticity. We apply a threshold value of $q_{l,th} = 10^{-5}$ kg/kg and $\omega_{th}^2 = 10^{-6}$ s $^{-2}$. The sensitivity of the TNTI to the threshold values has been investigated in appendix C. The three interfaces divide the domain into four different zones which can be defined as:

1. Cloud core (CC), where $b > 0$, $q_l \geq q_{l,th}$;
2. Visible Shell (VS), where $b < 0$, $q_l \geq q_{l,th}$;
3. Invisible Shell (IS), where $b < 0$, $q_l < q_{l,th}$, $\omega^2 \geq \omega_{th}^2$;
4. Environment (E), where $b = 0$ and $\omega^2 < \omega_{th}^2$.

These zones are shown in figure 5.2. The snapshot represents the flow buoyancy at t_0 and depicts the CC (red), VS (blue), IS (yellow) and the E (white). The CCB is defined on the interface between the CC and the VS, the VSB on the interface between the VS and the IS and the TNTI on the interface between the IS and E. The TNTI and CCB are contours of $b = 0$ and the VSB is given by $b = b_s$. For reference, the boundary considered by Romps (2010) would be closer to the CCB than the VSB due to the high threshold applied to the vertical velocity in that study.

Interestingly, the VSB coincides with the location where the buoyancy is minimum. Evaporation of cloud liquid water due to mixing and entrainment results in latent heat absorption. This evaporative cooling is maximum at the point where all the liquid water has evaporated, i.e. at the VSB. This can be explained using equation (4.3). When q_l drops to zero due to complete evaporation, the consequent temperature drop results in a negative value for $(\theta - \theta_0)/\theta_0$ with the buoyancy falling to a minimum as shown in chapter 4.

5.4 Lagrangian particles

Lagrangian particles are seeded uniformly across the four zones at $t = t_0$ over the interval $0 < x < 9m$, $0 < y < 15m$, $0 < z < 30m$. A total of 3 million particles were divided among the different zones with 578,964 in the CC, 502,801 in the VS, 347,348 in the IS and 1,572,052 in the E. Since the particles are passive, they follow the flow. A snapshot of the particles at a normalized time $t^* = (t - t_0)/\tau = 0.67$ is shown in figure 5.3. The particles are colored according to the zones in which they are initially seeded at t_0 : CC (red), VS (blue), IS (yellow) and E (pink). This figure provides a qualitative idea of the source and destination of entraining and detraining particles. The CC contains particles from the VS and IS, there are indications of CC particles in the IS and even indications of E particles in the VS.

Figure 5.4 quantifies the movement of the particles between the zones by showing an origin-destination matrix for the initial and final zones of all particles that leave their zone of origin. Each square in the matrix represents a particular zone. The rows represent the zone of origin and the columns represent the destination zone at $t^* = 0.67$. The colors (and the numbers)

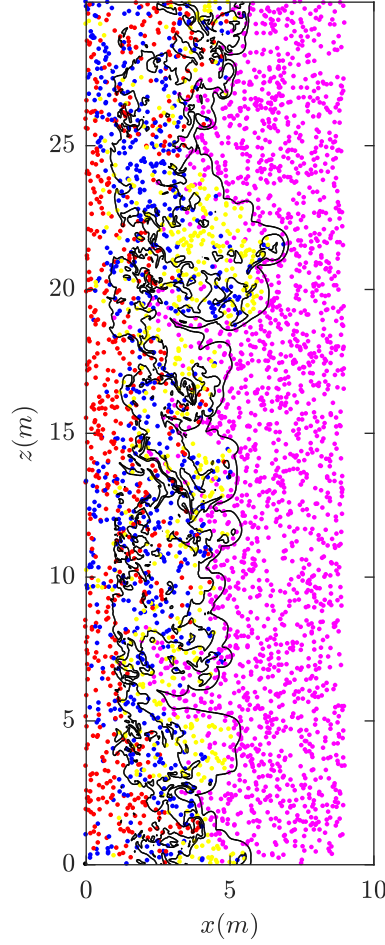


Figure 5.3: Instantaneous particle positions on a two dimensional slice of the flow at $t^* = 0.67$. Also shown are the three interfaces. Particle colors represent the zone in which they were initially seeded : red (CC), blue (VS), yellow (IS) and pink (E).

indicate the percentage of particles that originated in the zone represented by the row and has a final destination in the zone represented by the column. The percentages are calculated over the total number of particles (in all four zones) at t^* . Hence the sum of values in all the cells in the matrix is equal to 100. It is necessary to exercise caution when generating such a matrix since the percentages will be dependent on the initial seeding density and the domain size. For instance, an analysis of the particles that started and finished in their zones of origin revealed that a high percentage simply do not make any crossing at all. In the time interval from $t^* = 0$ to 0.67, the following percentage (number) of particles remain in their zones of origin without making any crossing: CC - 89% (385,146), VS - 73% (221,989), IS - 90% (163,162) and E - 99.9% (1,380,563). Hence all particles that remain in their zones of origin are excluded to give a better understanding of mixing and crossing between different zones. We still have a significant number of particles to obtain reliable statistics for figure 5.4 : CC - 193,818, VS -



Figure 5.4: Origin-destination matrix for particle final locations according to zones. Figure shows the percentage wise distribution of particles based on the zone of origin at the time of seeding and the zone where they end up at time $t^* = 0.67$.

280,812, IS - 184,186 and E - 191,489. Particles starting in the CC detrain into the VS (16.4%) and very rarely make it to the IS in the time interval considered (0.4%). particles which entrain back to the CC (5.9%) were originally detrained. Particles originating in the VS cross over to the both the CC and IS, of which 9.7% entrain back. Entrainment into the CC (17.7%) is much more dominant than detrainment into the IS (5.8%). The CC-VS mixing is nearly symmetrical, showing nearly equal transport of particles between the two layers. Conversely, VS - IS mixing is highly skewed with particles originating in the IS showing a very high preference to entrain into the VS (16.3%) compared to particles starting from the VS detraining into the IS.

Analysis of the particles that originate and finish in the IS (2.3%) reveals that these are made up almost entirely (99%) of particles that entrain and detrain back from the VS. A negligible percentage of particles detrain into the environment and entrain back. The almost one-sided crossing of particles at the TNTI is also revealed by the high percentage of particles (21.4%) that originate from the environment into the IS and the negligible percentage moving in the opposite direction. Since the shell thickness increases linearly as shown in chapter 4, we can consider the TNTI as a moving interface that would uniformly entrain particles resident in the environment, i.e. $\Delta N_e = nA\Delta h$. Here ΔN_e is the number of particles entrained when the interface moves a horizontal distance Δh covering an area A , and $n = N_p/V$ is the particle number density, with V the initial seeding volume. Therefore the number of particles entrained over a time step dt is given by $dN_e/dt = n A dh/dt$.

A comparison between the number of particles entraining across the TNTI calculated directly from the DNS data, and from the model show a very good agreement (not shown). A moving interface results in a constant number of particles entrained from the environment in our setup with negligible detrainment across the TNTI. This explains the skewness in crossings at the TNTI. Yeo and Romps (2012) have shown that a high percentage of air entrained at the cloud boundary had previously been detrained from the cloud. However, entrainment at the TNTI in our setup is almost entirely from the environment. A similar argument can be used to explain the skewness at the VSB. Since the VSB is moving as a function of time as the shell thickens, the entrainment from the IS to the VS dominates the detrainment from VS to IS.

Another striking result from figure 5.4 is that a negligible percentage of particles travel all the way from the CC to the environment and vice-versa. This will be addressed further in section 5.6 where we investigate the degree of premixing done by the shell and how it acts as a buffer layer between the CC and the environment.

A better perspective of the path followed by the particles can be obtained by looking at the average times taken by particles to travel across different zones. This quantity is determined by calculating how long a particle resides in a zone after entering it via an interface. The residence times normalized by the shell time scale τ are shown in figure 5.5. Calculating the average time after seeding to cross the nearest interface from each zone is quite deceptive since this is highly dependant on the seeding density. We will hence avoid this calculation and focus on residence times after entrainment or detrainment across an interface. For particles originating in the CC, the nearest interface will be the CCB, whilst for those originating in the VS, the CCB and the VSB are the nearest interfaces. For particles from the IS, the VSB and the TNTI are the nearest interfaces and for those from the environment, the TNTI is the sole interface of interest.

Particles originating in the CC have a mean residence time of 0.44τ in the VS after crossing the CCB and before they detrain into the IS. Since very few particles in the IS cross the TNTI the residence time in the IS is not calculated.

A majority of the particles originating from the IS cross the VSB into the VS, where they reside for 0.29τ before crossing into the CC. Particles originating in the environment cross the TNTI and remain in the IS for 0.46τ . A small percentage (5%) cross over to the VS and resides

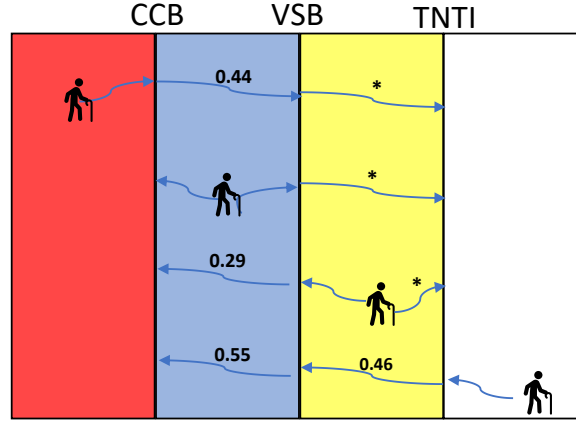


Figure 5.5: Average time taken by all entraining/detraining particles to travel across a zone. The values shown are averages of the residence times in a zone normalized with τ . Asterisk indicates insufficient number of particles travelling from interface to interface to get a reliable mean value.

there for 0.55τ .

5.5 Entrainment at the cloud edge

In this section we analyse the time histories of particles that cross the three interfaces. This will reveal particle behaviour before, at and after crossing each interface, and is information that is impossible to obtain with Eulerian statistics. For this analysis, we consider each interface individually and look at all particle crossings across it. A particle is considered to have entrained when it moves to a different zone from right to left (towards the CC) and to have detrained when it moves to a different zone from left to right (towards the environment). The time variable t_e and t_d represent the time at which a particle entrains or detrains across an interface respectively. In case of multiple entrainment events by the same particle across a particular interface, the time of occurrence of the first entrainment event is taken as the entrainment time t_e . For detrainment we follow a slightly different procedure. A detrainment event is considered to take place only if a particle moves to a different zone and resides there, i.e. detraining particles that are entrained back are not considered in the analysis while particles that detrain-entrain-detrain are counted. In short, for a particle to be considered in the detrainment analysis, the last crossing between zones should have been from right to left. The time of the last crossing from right to left is taken as the detrainment time t_d . We adopted such an approach since entraining particles show a tendency to detrain after one or two time steps immediately after entrainment, before entraining

again at the next time step. Counting such short term detrainment events contaminates the plot and are hence these are not considered in the detrainment plot.

Figure 5.6 shows box plots of the enstrophy ω^2 , and buoyancy b of all entraining particles. In box plots, groups of particle data are expressed using their quartiles. The tops and bottoms of the box are the first and third quartiles (or the 25th and 75th percentiles), and the red line is the median of the particle data group. The x -axis represents the time before and after a crossing and is normalized with the shell time scale τ . The whiskers (showing variability from the first and third quartiles) and outlier points for the box plot have been removed from the figure for the sake of clarity. A sharp jump in the enstrophy values is observed as particles cross the TNTI as shown in figure 5.6a. This is consistent with vorticity jumps that are observed across the TNTI in several flows (da Silva et al. 2014). Once entrained into the IS, the particle acquires enstrophy rapidly. The buoyancy shows a very smooth decrease for particles entraining across the TNTI as shown in figure 5.6b. As shown in section 5.3, the outer boundary of the shell where the buoyancy drops to zero coincides with the TNTI. The value of buoyancy is zero in the environment and since almost all the particles crossing the TNTI originate from the environment (as was also shown in section 5.4) there is a smooth decrease in the buoyancy as particles cross into the IS.

In order to visualize the increase in particle enstrophy as they entrain into the VS through the VSB, the enstrophy is plotted on a linear scale (figure 5.6c). However, the observed increase is significantly less than the multiple orders of magnitude seen at the TNTI. The VSB resides deep in the subsiding shell where turbulence intensities are high, and the particles are not subjected to sharp gradients across this interface. The enstrophy values before entrainment predominantly indicate particles originating from the IS and almost none from the environment. In sharp contrast to the enstrophy, there is a kink in the buoyancy as the particles entrain into the VS. This is due to the VSB coinciding with the buoyancy minimum. The majority of the particles crossing into the VS are from the IS as seen by the negative values of buoyancy before entrainment. This is also consistent with the origin-destination matrix in figure 5.4. Positive values for the buoyancy can be observed for $(t - t_e)/\tau > 0.6$ which indicates that particles cross over into the CC.

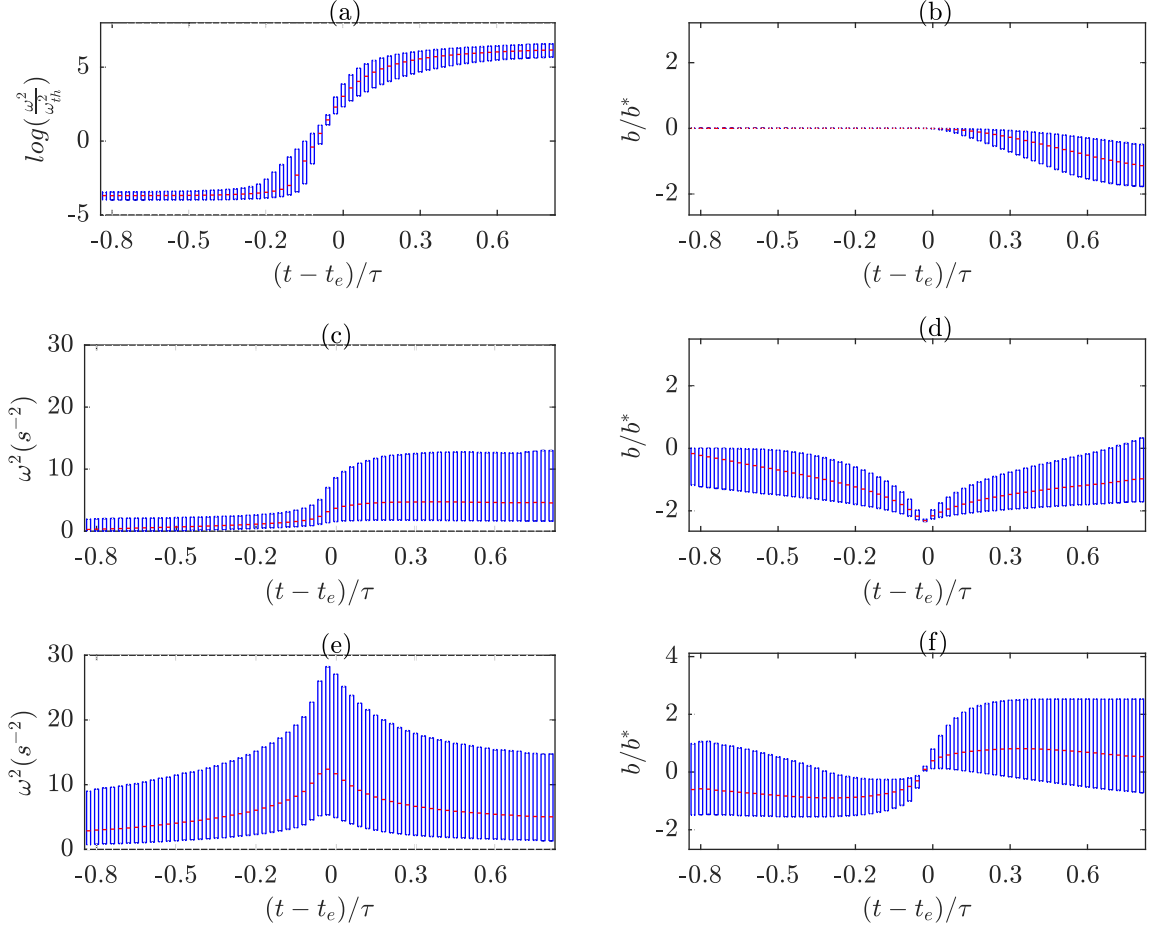


Figure 5.6: Box plot showing the time histories for ω^2 and b for entraining particles crossing the TNTI (a,b), VSB(c,d) and CCB(e,f). Outlier points and whiskers for extreme values have been removed for the sake of clarity.

Particles crossing the CCB show a similar behaviour as those crossing the VSB with the enstrophy showing an increase till the interface, after which it falls again as the particle moves into the core away from the mixing layer. The buoyancy shows a kink at the point where the particles cross over from the negatively buoyant VS into the positively buoyant CC. The positive and negative values for the buoyancy before entrainment indicate that entraining particles include those which originate from the VS as well as those which have been recently detrained from the core. At about 0.3τ before entrainment, the buoyancy is almost entirely negative indicating only particles from the VS.

The finite jump in enstrophy values at the TNTI combined with the relatively flat behaviour across the VSB and the CCB highlights the relevance of the TNTI as the entraining cloud interface. The VSB and the CCB can be considered to be a cross-over point where particle buoyancy decreases significantly (to a minimum at the VSB and zero at the CCB) as a result of

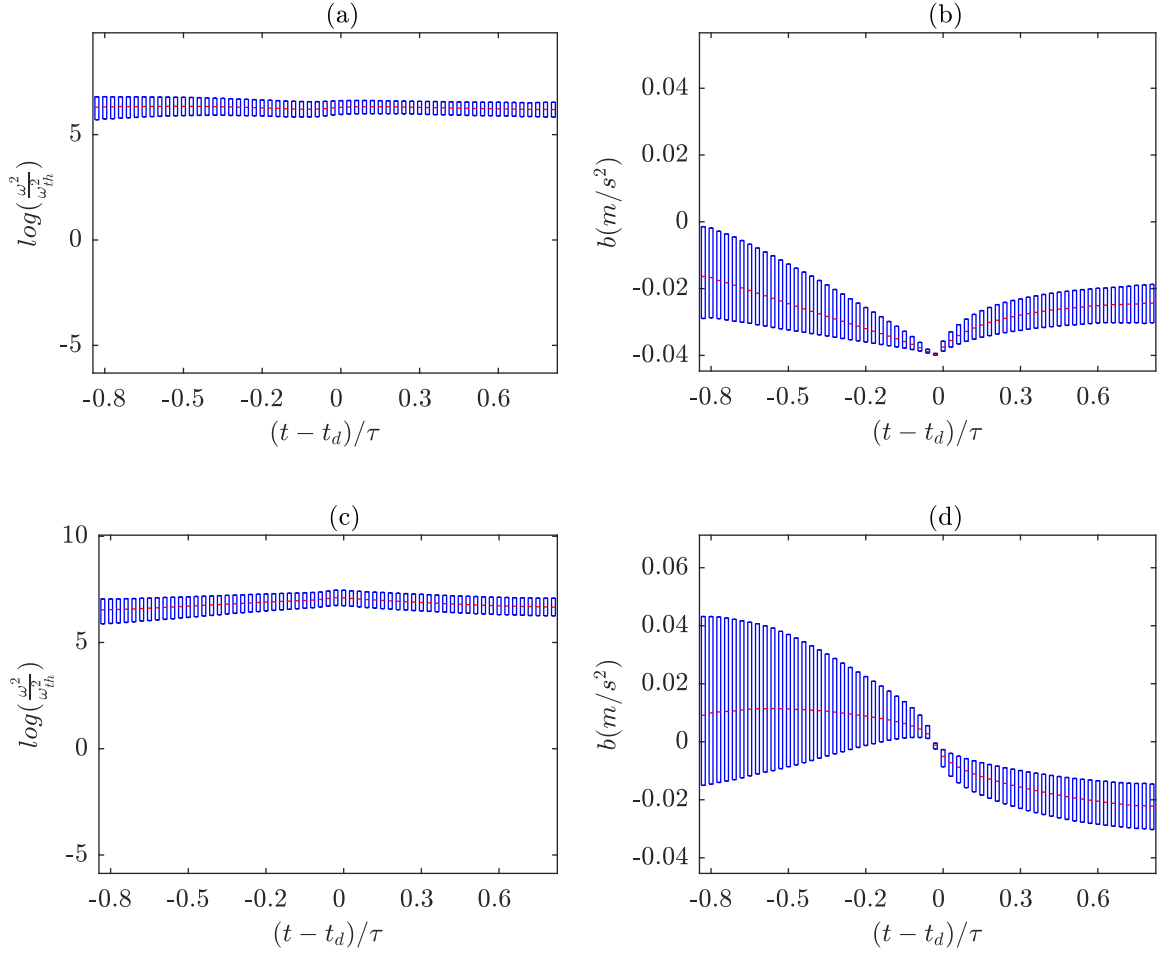


Figure 5.7: Box plot showing the time histories for ω^2 and b for detrainment particles crossing the VSB(a,b) and CCB(c,d). Outlier points and whiskers for extreme values have been removed for the sake of clarity.

evaporative cooling.

Detrainment plots show similar behaviours. We only show plots for the VSB and the CCB. This is because very few qualifying detrainment events were observed at the TNTI compared to the VSB and the CCB as shown in section 5.4. This is an indication of the pre-mixing done by the shell. Particles originating from the CC and detrainning all the way to the environment is an extremely rare event within the time scale studied (0.67τ). Similar to the entrainment plots, there are no finite jumps in enstrophy during detrainment across the VSB and the CCB. Across the VSB, the majority of detrainning particles are from the VS (entirely negative buoyancy at start of the plot). But across the CCB, there are particles that originate from both the CC and the VS. The detrainning particles that originate from the CC are probably those at the edge of the CC which mix with the negatively buoyant shell as a result of which they lose their positive buoyancy and is detrainned from the CC. A closer look at the properties of entraining

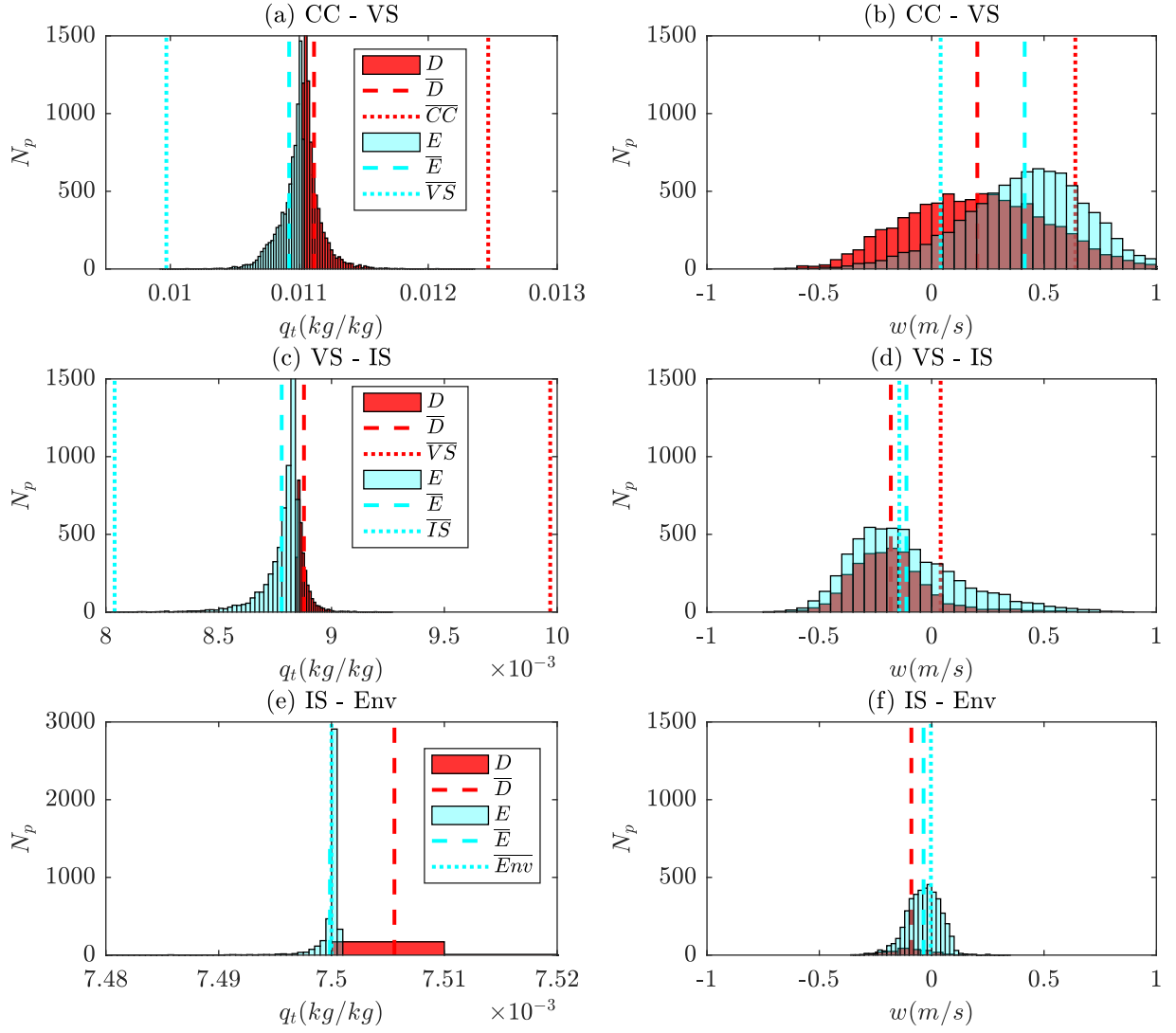


Figure 5.8: Histograms showing the properties of particles that have E- entrained (cyan) and D- detrained (red) across the CCB (a, b), VSB (c,d) and the TNTI (e,f) at time $t^* = 0.67$. The properties shown are (a,c,e) q_t , and (b,d,f) w . The dashed and dot-dashed cyan lines indicate mean magnitudes of the entrained particles and all particles in the entraining zone respectively and the red dashed and dotted line indicates the mean of detraining particles and all the particles in the detraining zone.

and detraining particles is taken in the next section.

5.6 Shell pre-mixing and preferential entrainment at interfaces

In this section we look at how effective the shell is in premixing the entraining and detraining parcels. All particles crossing the CCB, VSB and the TNTI at normalized time $t^* = 0.67$ are considered irrespective of their origin. As mentioned in the introduction, Dawe and Austin

(2011) attributed the difference between the bulk and local entrainment rates to be essentially due to the presence of the subsiding shell around the CC. This means that the properties of entraining and detraining air can no longer be the same as the mean values in the environment and the CC respectively. This is explored in figure 5.8 which shows histograms of the total water mass fraction q_t (a, c, e) and vertical velocity w (b, d, f) for all particles that have entrained and detrained across the interfaces. Figure 5.8 shows entrainment and detraining across the CCB (a,b), the VSB (c,d), and the TNTI (e,f).

The histograms in figure 5.8a and b are clearly skewed and suggest that the properties of the entraining and detraining particles do not have a mean value equal to the horizontal slab average values of the environment and CC respectively. The particles entraining (cyan) across the CCB have a mean value (cyan dashed line) closer to the inner edge of the shell. The mean is also higher than the mean for all particles in the VS (cyan dotted line), i.e. there is clear evidence for preferential entrainment of particles which have a q_t and w higher than the mean values in the shell. Dawe and Austin (2011) explained this preferential entrainment by the presence of negatively buoyant regions which still had positive vertical velocity and condensed liquid water. As these parcels rise, there is latent heat release due to further condensation, thus making the parcels positively buoyant which leads to it being entrained into the CC. This is true in the current simulation as well. In the buoyancy phase, even though the mean value of vertical velocity in the shell is negative, there still are upward moving negatively buoyant parcels with liquid water (especially in the VS). We would not expect to see this effect happen at the VSB and this is indeed true as seen in figure 5.8c and d. However, the mean values of q_t (cyan dashed line) and θ_l (not shown) of particles crossing into the VS coincides with the mean saturation value $\overline{q_s}$ and $\overline{\theta_s}$.¹ This again highlights the degree to which the shell premixes the entraining air. Entrainment across the TNTI is shown in figure 5.8e and f and involves particles only from the environment as was shown in section 5.4. The mean value of q_t of particles entraining into the IS coincides with the mean of the environment as expected. Entraining particles also have

¹As shown in chapter 4, considering a classical q_t - θ_l mixing diagram and assuming linear mixing between a saturated cloud and unsaturated environment parcel, the intermediate thermodynamic states of the cloud environment mixture can be assumed to lie on a straight line connecting the two initial states. This means that the mean properties of the saturation mixture, $\overline{q_s}$ and $\overline{\theta_s}$, are the coordinates of the point where the mixing line crosses the saturation curve (figure 4.2)

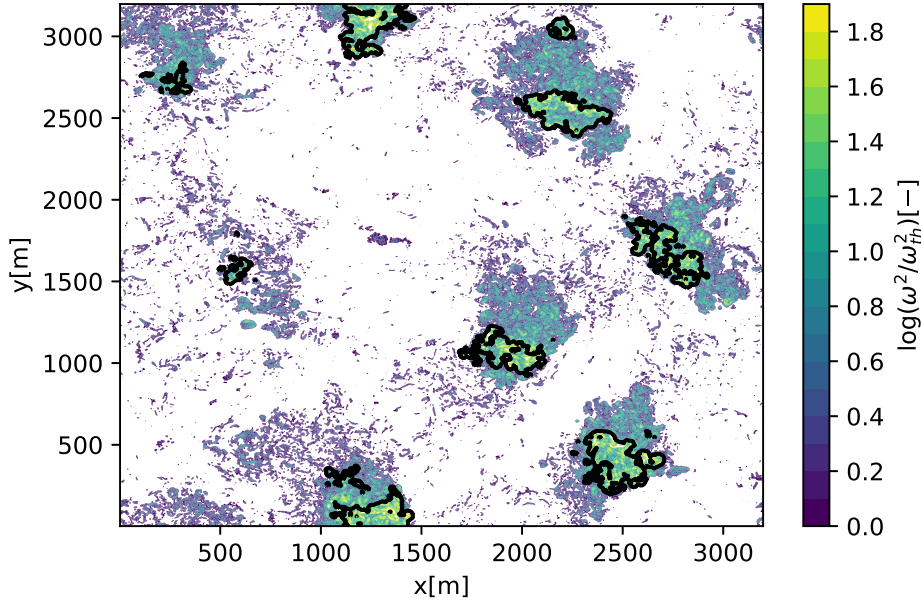


Figure 5.9: Contour plot of enstrophy at a mid-cloud layer ($z = 800\text{m}$). Black contours denote the VSB. The enstrophy is normalized using the threshold value $\omega_{th}^2 = 10^{-3}\text{s}^{-2}$.

a mean vertical velocity that is slightly negative. A possible reason for this could be the rapid entrainment of particles that were detrained from the IS and have negative velocities. Figure 5.8 also shows the properties of particles detraining across the CCB and the VSB (red). Figure 5.8a clearly shows that it is the drier air at the edges of the CC that is detraining across the CCB. For the CC, $\overline{q_t} = 12.5\text{ g/kg}$ (red dotted line) while the mean of the detraining particles is significantly lower at around 11.1 g/kg (red dashed line). Another interesting observation is that the mean vertical velocity of the detraining parcels is positive as shown in figure 5.8b. These could be the parcels that are negatively buoyant at the edges of the CC but still moving up due to the positive vertical momentum of the fluid in the CC. The vertical velocity histogram also shows a very similar behaviour to the entrainment. Detrainment across the VSB (figure 5.8c and d) shows a very small sample range for q_t . Very few particles detrain into the IS which is consistent with the percentages seen in the matrix in figure 5.4. The mean of the vertical velocity of the detraining particles is negative and is very close to that of the IS (blue dotted line). Detrainment across the TNTI is almost entirely negligible with very few particles crossing from the IS.

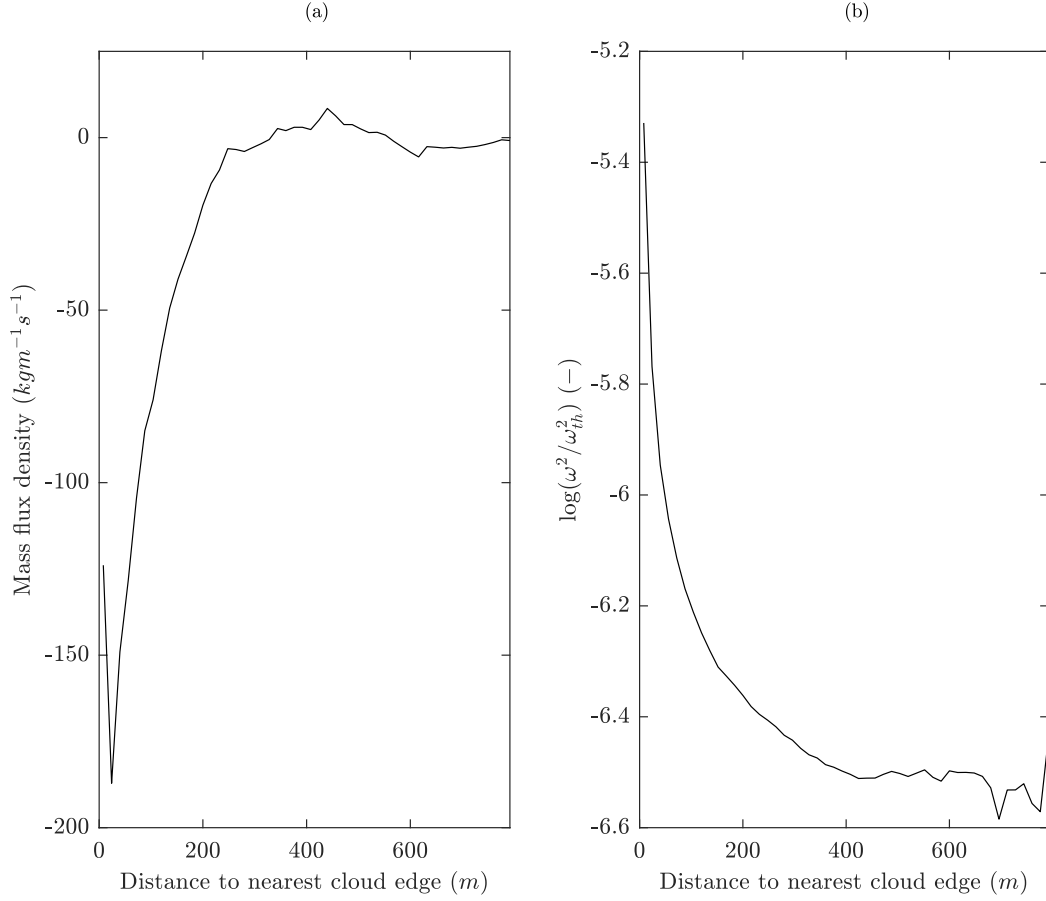


Figure 5.10: Mass flux density and enstrophy as a function of the distance to the nearest cloud edge.

5.7 Presence of the interface in LES

The DNS setup is highly idealized. In order to verify whether the results for the DNS extrapolate to situations in which the full cloud life cycle is represented, we ran a high resolution LES of shear-free BOMEX case (Holland and Rasmusson 1973) at a resolution of 4.1 m.

Figure 5.9 shows a contour plot of the horizontal cross-section of enstrophy at a mid-cloud layer ($z = 1000$ m). A visual inspection suggests that most of the IS is indeed localized, and usually centered around the clouds (denoted in black contours). Typical values of enstrophy drop from 10^{-1} in the clouds to below 10^{-3} in the environment.

Figure 5.10 shows the mass flux density (a) and enstrophy (b) plotted as a function of the distance to the nearest cloud edge. The plots clearly show that the shell itself is confined to within less than 200m from the nearest cloud edge.

The additional empty IS areas at plot locations (2000m, 1250m) and (2250m,2750m), are

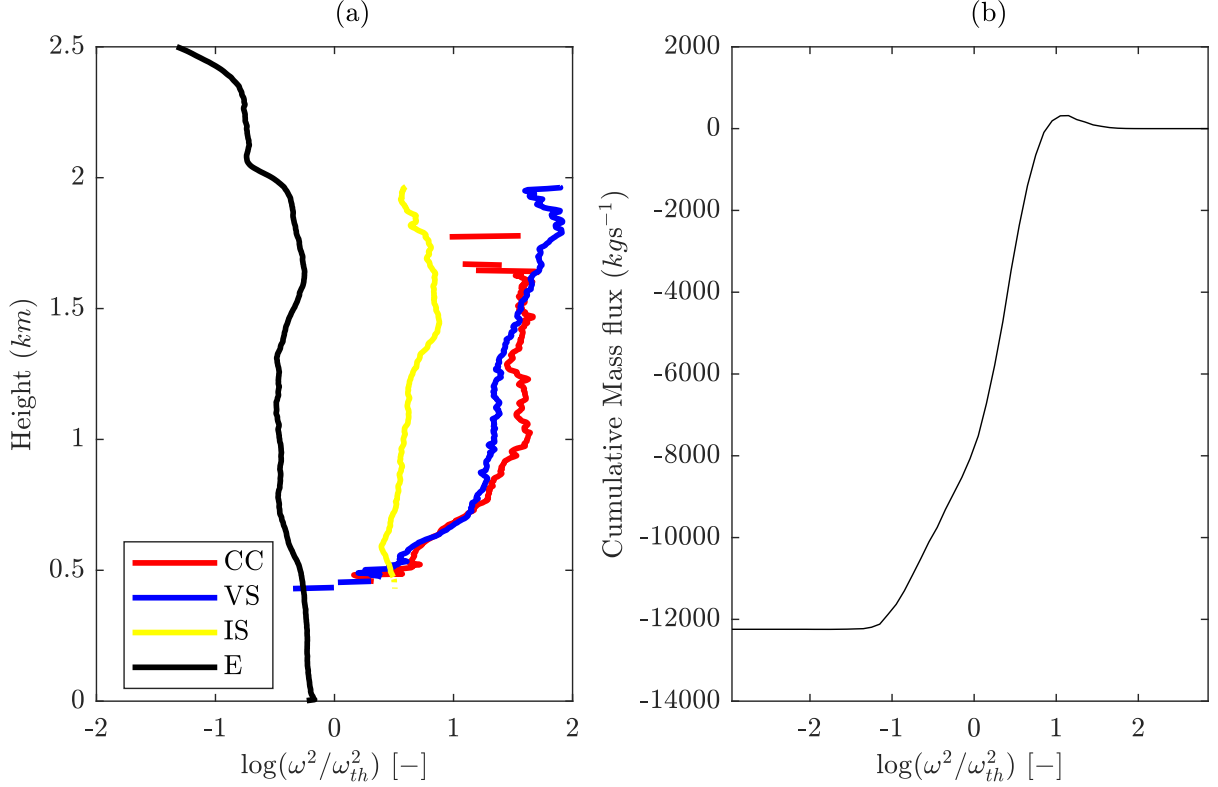


Figure 5.11: (a) Conditionally sampled enstrophy in each of the zones, averaged between hour 4-10 of the simulation, with a sample time of 0.5hr. Red: Cloud core, Blue: Visible shell, Yellow: Invisible shell, Black: Environment. (b) Cumulative mass flux vs enstrophy for non-cloudy regions, averaged between hour 4-10 of the simulation, with a sample time of 0.5hr.

likely related to a recently-dissipated cloud and do not necessarily contribute to the negative mass flux. Clouds will also generate internal waves which in turn produce vorticity in the environment (Fodor and Mellado 2020). However, disentangling both is subtle and is beyond the scope of this work.

Figure 5.11(a) shows the conditionally sampled enstrophy over the cloud layer, with each layer defined similar to the definitions in section 5.3, but with the adjusted thresholds $q_{l,th} = 0$ and $\omega_{th}^2 = 10^{-3} s^{-2}$. For these and the consecutive graphs, we have used the LES output between the 3rd and 10th hour, with a sample time of 0.5hr. The IS is defined with $\omega_{th}^2 = 10^{-3} s^{-2}$ and with no threshold on the buoyancy. Throughout the cloud layer, the enstrophy in the cloud and its immediate surroundings is an order of magnitude higher than the enstrophy in the environment. This enstrophy jump across the two zones shows that similar to the TNTI observed in the DNS, we can observe a clear interface between the IS and the environment as well. Because the ambient fluid is still turbulent, this is now actually a Turbulent-Turbulent Interface (TTI). According to Kankanwadi and Buxton (2020), the adjustment in enstrophy

across the TTI is analogous to the TNTI.

The choice of the enstrophy threshold $\omega_{th}^2 = 10^{-3} \text{ s}^{-2}$ can be justified by looking at the cumulative mass flux for all non-cloudy grid cells plotted against the enstrophy as shown in figure 5.11(b). Starting from zero at high enstrophy (clouds), there is a small bump (perhaps evaporating cloud tops), after which a steep decrease in mass flux and an inflection point at $\omega^2 = 10^{-3} \text{ s}^{-2}$ is seen. In other words, the mass flux per unit enstrophy is the highest in the IS which is centered around the clouds (see figure 5.11). Finally, figure 5.12 shows the conditionally sampled mass flux profile. In the middle of the cloud layer, far away from the lifting condensation level and the level of neutral buoyancy, the IS is responsible for the majority of the negative mass flux which remains almost constant from the cloud base at 0.5 km up to 1.1 km. Highly negative values of mass flux in the environment at around 1.2 km to 1.5 km are observed. One possible reason could be that the cloud top generates internal waves with a net negative mass flux because the initial upward motion is still part of the high enstrophy region. However, between the height range of 0.75 km to 1.1 km, the mass flux in the environment is close to zero. The mass flux in the VS is small but positive and this is possibly due to the effect of the CC which drags the negatively buoyant shell upwards. Overall, the results suggest that, in the mid layer of the cloud (for the conditions considered in this simulation), the upwards mass flux in the cloud core is balanced by the negative mass flux in the IS with no lateral mass exchange at the TTI, or, the net exchange rate across the TTI is zero. This is consistent with the results in Jonker, Heus, and Sullivan (2008b) where the mass flux in the shell (within 200 m of the cloud edge) was shown to compensate for about 80% of the in-cloud mass flux.

Our DNS study can be considered to correspond to the LES results between 0.5 km and 0.8 km. In this region, the gradient of the mass flux in the environment shows a negative slope which represents air being entrained from the environment. The DNS study reveals a similar net entrainment at the TNTI as mentioned in section 5.4.

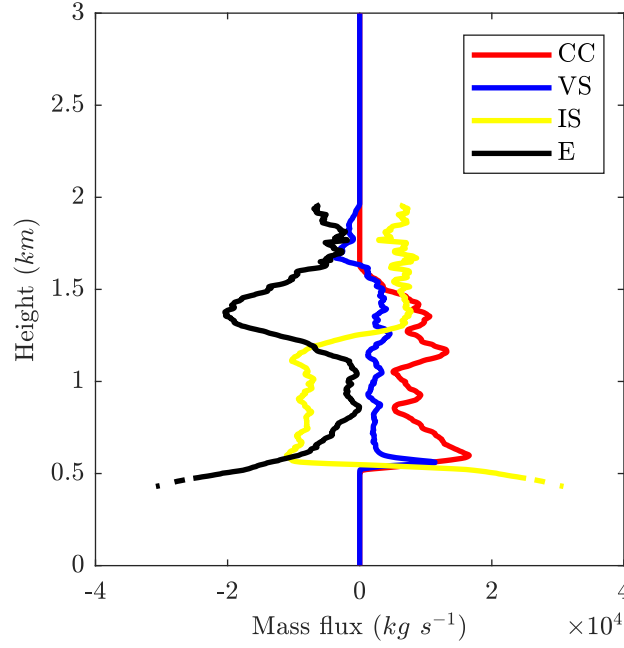


Figure 5.12: Conditionally sampled mass flux in each zone, averaged between hour 4-10 of the simulation, with a sample time of 0.5hr. Red: Cloud core, Blue: Visible shell, Yellow: Invisible shell, Black: Environment.

5.8 Discussion and Concluding remarks

A numerical study of the different interfaces at the edge of a cumulus cloud was performed using DNS and LES. The study reveals the presence of four distinct zones which can be detected by applying thresholds on the enstrophy and q_t . The four zones have been defined as the Cloud Core, a Visible and Invisible Shell and the environment layer. The different zones give rise to three distinct interfaces: the Cloud Core Boundary, Visible Shell Boundary (traditionally considered the cloud edge in parameterization studies) and a Turbulent Non-Turbulent interface. Massless Lagrangian particles were introduced at the cloud edge and their trajectories and properties were tracked. We show that the presence of the shell extends the cloud edge to the TNTI and a Lagrangian particle experiences finite jumps in its enstrophy and a smooth increase in buoyancy when it crosses this interface. The VSB is essentially a cross-over station which does not significantly affect entraining or detraining parcels. It coincides with the location of minimum buoyancy within the shell and parcels entraining across this boundary have saturation values that can be predicted from the mixing diagram.

We also observe preferential entrainment across the CCB as shown by Dawe and Austin (2011), where particles with total humidity q_t and vertical velocity w higher than the mean of

all parcels in the shell more likely to entrain. Also, drier air that is close to the CCB is more likely to detrain. This drier air is also likely to be negatively buoyant but moving with a positive vertical velocity in the cloud core.

The DNS study is performed using a highly idealized setup. The simplifications include an infinitely long cloud interface, a lack of stratification and no other sources of turbulence such as wind shear for the environment. It is also important to highlight the fact that by imposing a periodic boundary condition on a domain size of $30m$, larger eddies which could dominate flow before the end of the simulation are being suppressed. However, the LES simulations are performed using a more realistic setup and was able to detect the TNTI using the same thresholds as in the DNS which shows that it is possible to extend the notion of a TNTI to turbulent environments. Indeed, da Silva et al. (2014) describes the interface layer as a thin region with a finite thickness that separates either (a) regions with different turbulent intensity or (b) turbulent and (external) irrotational flow regions. Conditionally averaged mass flux in the different zones in the LES results reveal that within the mid cloud layer, there is no net exchange across the TNTI. The upward mass flux in the cloud core is compensated by the mass flux in the IS with negligible mass flux in the environment.

While we do not observe any detrainment across the TNTI, this does not mean that no air can be transported from the cloud into the environment. The cloud will eventually dissipate, and so will the IS. During this process, the humid air of the cloud will moisten the environment. However, this is an entirely different mechanism than any direct mixing between the cloud and the environment, with different results. For instance, the more tiered detrainment ensures that the cloud remains less diluted, which results in stronger updrafts. We also speculate that a slowly dissipating IS may allow for preconditioning certain regions for subsequent convection; further research is needed to confirm or reject such speculation.

Chapter 6

Preferential concentration of sedimenting droplets in decaying turbulence

In this chapter, an analysis of the effect of gravity on the preferential concentration of droplets in decaying homogeneous isotropic turbulence is performed. The radial distribution functions calculated from direct numerical simulations of a polydisperse distribution of non-sedimenting and sedimenting droplets are compared with theoretical predictions. The effect of gravity on the geometric collision kernel is also investigated.

6.1 Introduction

The preferential concentration of inertial particles has been extensively studied in numerical and experimental studies (Maxey [1987](#); K. D. Squires and Eaton [1991](#); L.-P. Wang and Maxey [1993](#); Eaton and Fessler [1994](#); Fessler, Kulick, and Eaton [1994](#)). In turbulent flows, inertial particles are centrifuged away from vortex cores or regions of high vorticity and tend to accumulate in regions of low vorticity and high strain rate. The resulting regions of high or low local particle concentrations has significant implications in particle laden flows such as clouds, fuel droplet combustion, aerosol settling and modulation of turbulence by particles. Different methods have been used to quantify and characterize the preferential concentration: including bin counting (L.-P. Wang and Maxey [1993](#); Eaton and Fessler [1994](#)), Radial Distribution Functions (RDF) (Sundaram and Collins [1997](#); Reade and Collins [2000b](#); Salazar et al. [2008](#); Bateson and Aliseda [2012](#)) and Voronoi analysis (Monchaux, Bourgoin, and Cartellier [2010](#); Huck et al. [2018](#)).

In clouds, the implications of particle clustering is significant; it has been shown that clustering can lead to enhanced collision of water droplets. This helps explain the fast broadening of cloud droplet size distributions which could be a reason for the observed warm-rain formation in cumulus clouds within half an hour (Pinsky and Khain 1997; Falkovich, Fouxon, and Stepanov 2002; Shaw 2003). Sundaram and Collins (1997) quantified this effect by multiplying the collision kernel calculated by Saffman and Turner (1956) with the RDF calculated at the point of collision for a monodisperse distribution of particles in homogeneous isotropic turbulence. DNS studies have shown that turbulence can enhance the collision kernel relative to stagnant flow through an increase in both the relative velocities of the colliding droplets as well as the increase in the RDF (Franklin, Vaillancourt, Yau, and Bartello 2005; Franklin, Vaillancourt, and Yau 2007; Ayala, Rosa, L.-P. Wang, and Grabowski 2008). Reade and Collins (2000b) showed that the RDF can have values up to a 100 at separation distances equal to the collision radius further highlighting the importance of clustering towards the collision process.

There have been numerous DNS studies focusing on particle clustering which have resulted in various empirical formulas for the RDF. Reade and Collins (2000b) modelled the RDF using a series of DNS data (at $Re_\lambda = 54.5$) of monodisperse non-sedimenting particles in homogeneous isotropic turbulence and suggested the following function:

$$g(\hat{r}, St) = 1 + c_0 \hat{r}^{-c_1} \exp[-c_2 \hat{r}]. \quad (6.1)$$

Here $\hat{r} = r/\eta$ where r is the inter-particle separation distance and η is the Kolmogorov length scale. The coefficients c_0 , c_1 and c_2 are all in principle, functions of St . The study reveals an inverse power-law of the form $\hat{r}^{-c_1}$ at small $\hat{r} = r/\eta$, and transitions into an exponentially decaying tail at higher $\hat{r}$.

However, since this relation suggests that a high level of particle clustering occurs at $r \ll \eta$, the mechanism governing this phenomenon cannot be just limited to a simple ejection of particles from vortex cores. Various theoretical studies have focused on the mechanism behind the clustering of particles at sub-Kolmogorov scales (Balkovsky, Falkovich, and Fouxon 2001; Zaichik and Alipchenkov 2003; Chun et al. 2005). Analytical expressions have also been developed to predict the power-law behaviour of the RDF in the limit of small non-zero St in

these studies. In this chapter, we focus more on clustering at sub-Kolmogorov scales.

Chun et al. (2005) studied the mechanism governing the clustering phenomenon at length scales smaller than η and in the limit of $St \ll 1$. An analytical theory was developed for particle pairs with an inter-particle radial separation distance falling between η and the particle diameter D , i.e. $\eta \gg r \gg D$. The solution was derived assuming Stokes flow around each droplet sphere, $Re_p < 1$, $D/\eta \ll 1$, a dilute particle loading and neglecting the effect of settling. In a frame of reference moving along with a particle, the turbulent flow is approximated as a locally linear flow field and the variation in the local fluid velocity is approximated based on the velocity gradient tensor defined along the particle path. They showed that in a monodisperse distribution, the power-law dependence arises from a balance between an inward drift velocity caused by the particle inertia (inertial particles sample more strain than rotation giving rise to a net inward drift velocity) and a diffusion due to the random nature of the flow. The coefficient c_1 was observed to scale quadratically with St . For particles with different Stokes numbers, an additional diffusion arises due to the different particle response times to the local turbulent accelerations. This tends to homogenise the particle pair concentration leading to a reduction in the RDF. The additional acceleration diffusion term is independent of r and the resulting behaviour of the RDF is a power law dependence ($\hat{r}^{-c_1}$) at larger scales and a transition to a plateau (independent of $\hat{r}$) at smaller scales. An expression is also derived for the cross over length scale r_c at which this transition occurs.

The presence of gravity breaks the spherical symmetry in particle pair concentration as well as relative velocities between two neighbouring droplets. Ayala, Rosa, and L.-P. Wang (2008) extended the relations from Chun et al. (2005) for monodisperse sedimenting droplets in a turbulent flow. The power law coefficients were assumed to be functions of a non-dimensional parameter for gravity $g/(u_\eta/t_\eta)$ (where u_η and t_η are the Kolmogorov velocity and time scales respectively) in addition to St and the Taylor Reynolds number Re_λ , and empirical expressions were generated by curve-fitting DNS data. A similar procedure was followed to obtain expressions for the bidisperse distribution and the cross over length scale r_c . The addition of gravity tends to enhance the effect of the acceleration diffusion term from the theory of Chun et al. (2005), causing a further reduction in RDF. By comparing the model with DNS results,

Ayala, Rosa, and L.-P. Wang (2008) showed that the effect of acceleration-driven diffusion is very strong for bidisperse pairs under the effect of gravity. The effect of gravity on the relative velocities and preferential concentration of colliding particles was explored by Woittiez, Jonker, and Portela (2009) using a series of DNS simulations. The rate of collision of sedimenting droplets was found to be lower than non-sedimenting droplets for a monodisperse distribution due to decreased interaction times between droplets and turbulent structures. For a bidisperse distribution, the higher relative velocities due to different sedimenting velocities for the droplets of unequal sizes resulted in a higher collision kernel.

In this study, particle clustering and collisions are analysed in decaying turbulence. Yong Zhou, Wexler, and L.-P. Wang (1998) showed that using frozen turbulent flow fields in DNS to study particle-turbulence interactions can result in an overestimation of the collision kernel by up to 20% for a monodisperse system of droplets. Franklin, Vaillancourt, Yau, and Bartello (2005) also showed an overestimation of the collision kernel by 31% for the case of sedimenting droplets. In the setup adopted here, turbulent flow structures are evolving in both time and space and accordingly particles interact with evolving flow scales rather than a frozen field. The setup also allows a direct comparison with data and statistics from wind tunnel experiments. The setup simulates a polydisperse distribution of droplets in grid-generated isotropic turbulence. The objective of this chapter is to study the effect of gravity on the preferential concentration of inertial particles in a slowly decaying turbulent flow. The RDF is used to quantify the degree of particle clustering and the values of the RDF at scales up to 4η are compared for simulations with non-sedimenting and sedimenting droplets respectively. The numerical results are compared with the theoretical models of Chun et al. (2005) and Ayala, Rosa, L.-P. Wang, and Grabowski (2008) for non-sedimenting and sedimenting droplets. We also analyze the effect of gravity on the geometric collision kernel.

The chapter is structured as follows. In section 6.2, the case setup is presented along with the characteristics of the turbulence and the relevant droplet parameters. In section 6.3, the results for both monodisperse and bidisperse RDFs are presented with comparisons to theoretical predictions. In section 6.4, the effect of gravity on the geometric collision kernel is presented. Section 6.5 includes a discussion of the results along with concluding remarks.

6.2 Case setup and Numerical model

6.2.1 Flow field

A novel case setup is developed where the numerical simulation closely resembles the flow in wind tunnel experiments. The wind tunnel setup used by Bateson and Aliseda (2012) is taken as a reference for flow characteristics and grid dimensions. The test section of the wind tunnel has a cross-section $1.2m \times 1.2m$, and is $3m$ long. The grid is a 9×9 biplanar array formed by aluminum tubes of $2.54cm$ diameter. The grid spacing $G = 10.16cm$ and the grid solidity which is the ratio of the obstructed area to the total area of the grid is equal to 0.44. The wind tunnel has a flow rate of $1.9 m^3/s$ which produces a droplet volume fraction of 2.5×10^{-5} in the test section. Measurements are taken at five downstream locations downstream of the grid at $x/G = 6.4, 14, 17, 22, 29$. In wind tunnel experiments, grid generated turbulence decays as the fluid moves downstream. The numerical case setup in this study aims to simulate the decaying turbulence by capturing the temporal evolution of a fluid section exiting the grid. Hence the simulations are temporal flow experiments and is similar to observing and following a fluid section exiting the grid through a camera which is being translated along an axis $\tilde{x}$.

Simulating the motion of an active grid is difficult to achieve numerically. We circumvent this by simulating the turbulent flow just downstream of a passive grid. As the first step, we assume the average fluid velocity $\tilde{u}$ just downstream of the grid is given by,

$$\tilde{u} = \begin{cases} 0 & \text{at grid} \\ U_g & \text{otherwise} \end{cases}$$

where $U_g = Q_w / (A_w - A_{obs})$. Here Q_w and A_w are the flow rate and the area of the wind tunnel cross-section, respectively, and A_{obs} is the obstructed area of the grid which is related to A_w through the solidity A_{obs}/A_w . The velocity distribution is shown in figure 6.1a.

The frame of reference for the numerical simulation is obtained by applying a Galilean transformation to the axes $\tilde{x}$ and $\tilde{t}$, i.e. $x = \tilde{x} - U\tilde{t}$ and $t = \tilde{t}$. The velocity with which the translating axis x moves relative to $\tilde{x}$ is given by $U = Q_w / A_w$. In the moving frame of reference,

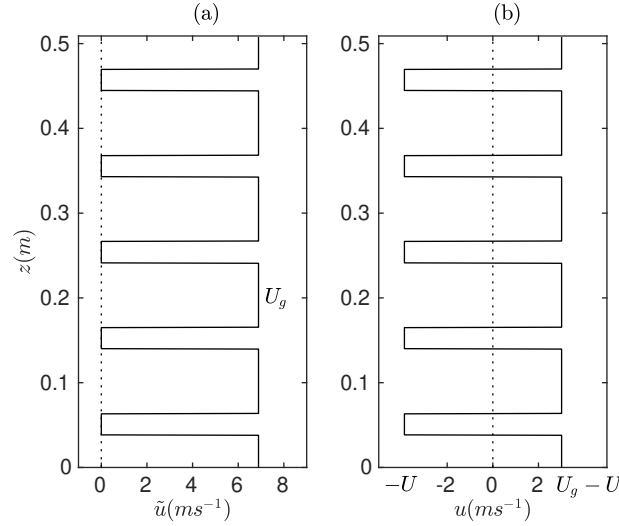


Figure 6.1: (a) Velocity distribution generated by active grid in the experiment. (b) Initial velocity in the frame of reference for the numerical simulation.

the initial condition u becomes

$$u = \begin{cases} -U & \text{at grid} \\ U_g - U & \text{otherwise.} \end{cases}$$

This velocity distribution is shown in figure 6.1b. The flow is then perturbed with random noise and allowed to transition with time into isotropic, homogeneous turbulence.

The governing equations of the flow are given by equations (4.1a) and (4.1b). Note that there are no active scalars and the buoyancy $b = 0$. The number of particles required to reach a target droplet volume fraction of $\mathcal{O}(10^{-5})$ in a numerical domain whose sizes matches that of the wind-tunnel test section would be very prohibitive (in terms of computational cost). Hence we calculate the two-point spatial correlation using the normalized autocorrelation function $R_{ij}(r) = \frac{\overline{u'_i(\mathbf{x})u'_j(\mathbf{x}+r)}}{(\overline{u'^2_i u'^2_j})^{1/2}}$, where u'_i is the fluctuation from the mean for the instantaneous velocity field u . A length scale L_{11} indicative of the size of the largest eddies in the flow can then be calculated by $L_{11} = \int_0^L R_{11} dr$, hence allowing us to reduce domain sizes accordingly. The value of L_{11} calculated in a simulation with no particles and a numerical domain of size $1.2m \times 1.2m \times 1.2m$ is $0.06m$ at $t = 1s$. Accordingly, a numerical domain of size $0.509m \times 0.509m \times 0.509m$ was selected and this allows us to reach the target volume fraction with a manageable number of droplets.

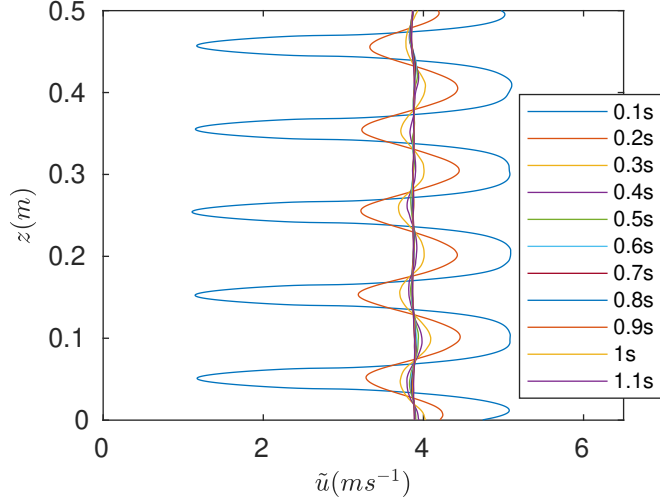


Figure 6.2: Averaged velocity profiles $\tilde{u} = u + U$ at different times.

A cubic domain is discretized using 1024^3 grid cells. Time-steps are dynamically calculated with a Courant-Friedrichs-Lewy (CFL) number of 0.4. Periodic boundary conditions are imposed along the $\hat{x}$ and $\hat{z}$ axes. A free slip condition is imposed along the $\hat{y}$ axis analogous to the side walls of a wind tunnel. The simulation was run for $1.1s$. The computational domain is parallelized in the $\hat{y}$ and $\hat{z}$ directions using 4096 processors.

Turbulence characterization

The velocity profiles averaged over the $\hat{y} - \hat{z}$ plane and over a time interval $\Delta t = 0.1s$ are shown in fig 6.2. The velocity $\tilde{u} = u + U$ is shown in the experimental frame $(\tilde{x}, \tilde{t})$. The evolving velocity profiles at different times show the effects of the grid slowly fading with time. After $t = 0.6s$, the flow can be considered to be isotropic.

The mean turbulent kinetic energy in the domain can be characterized as $\langle k \rangle_v = \frac{1}{2} \langle u'_i u'_i \rangle_v$, where summation is implied over repeated indices and $\langle \cdot \rangle_v = \frac{1}{t_{stat}} \int_0^{t_{stat}} \left[\frac{1}{V} \int_V \cdot dV \right]$. The large-scale eddies of the flow are characterized by the integral velocity (u_e) and length (L_e) scales. The integral velocity scale is given by the root-mean square value of the velocity fluctuations, $u_e = \left\langle \frac{2}{3} k \right\rangle_v^{1/2}$. The integral length scale is given by $L_e = \langle k \rangle_v^{3/2} / \langle \varepsilon \rangle_v$ where ε is the mean kinetic energy dissipation rate, and the large-eddy turnover time $T_e = u_e / L_e$.

The small-scale turbulence can be characterized by the Kolmogorov length (η), velocity

Table 6.1: Turbulence parameters

	t = 0.5s	t = 0.6s	t = 0.7s	t = 0.8s	t = 0.9s	t = 1.0s	t = 1.1s
$x(m)$	1.9375	2.325	2.7125	3.1	3.4875	3.875	4.2625
$\epsilon (m^2/s^3)$	0.2503	0.1245	0.0712	0.0448	0.0302	0.0215	0.0159
$t_\eta (ms)$	7.7	11.0	14.5	18.3	22.3	26.4	30.7
$u_\eta (m/s)$	0.044	0.037	0.032	0.029	0.026	0.024	0.022
$\lambda (mm)$	5.5	6.3	7.0	7.7	8.4	9.0	9.5
$\Delta x/\eta$	1.46	1.22	1.06	0.95	0.86	0.79	0.73
Re_λ	67.14	61.8	58.17	55.58	53.62	52.08	50.78

(u_η) and time (t_η) scales which are given by

$$\eta = (\nu^3 / \langle \epsilon \rangle_v)^{1/4}, \quad u_\eta = (\nu \langle \epsilon \rangle_v)^{1/4}, \quad t_\eta = (\nu / \langle \epsilon \rangle_v)^{1/2},$$

where $\nu = 1 \times 10^{-5} m^2 s^{-1}$ is the kinematic viscosity of air. These values are presented in table 6.1. Also shown is the Taylor Reynolds number $Re_\lambda = u_{rms} \lambda / \nu$ with the Taylor micro-scale $\lambda = \sqrt{15 \nu u_{rms}^2 / \epsilon}$ where u_{rms} is the root-mean square value of the turbulence velocity fluctuations.

The evolution of the velocity variances $\langle u_i'^2 \rangle_v$ with time is plotted in figure 6.3a. For isotropic homogeneous turbulence, these variances are equal to each other. The figure shows that the values for $\langle u'^2 \rangle_v$, $\langle v'^2 \rangle_v$, and $\langle w'^2 \rangle_v$ are very close to each other after $t = 0.5s$ thus attesting to the isotropy of the flow at this time. The initial high values for u' compared to v' and w' is due to the effects of the grid.

Figure 6.3b shows $\langle \epsilon \rangle_v$, the dissipation rate of turbulent kinetic energy averaged over the volume of the numerical domain, and normalized with the classical scaling u_e^3 / L_e . This value has been shown to be constant for decaying grid-turbulence in experiments (Sreenivasan 1984) and in forced as well as decaying DNS simulations of turbulence (Sreenivasan 1998). The magnitude of the constant $C_E = \epsilon L_e / u_e^3$ shown in figure 6.3b is comparable with those from other DNS data (figure 1 in the review by Vassilicos 2015).

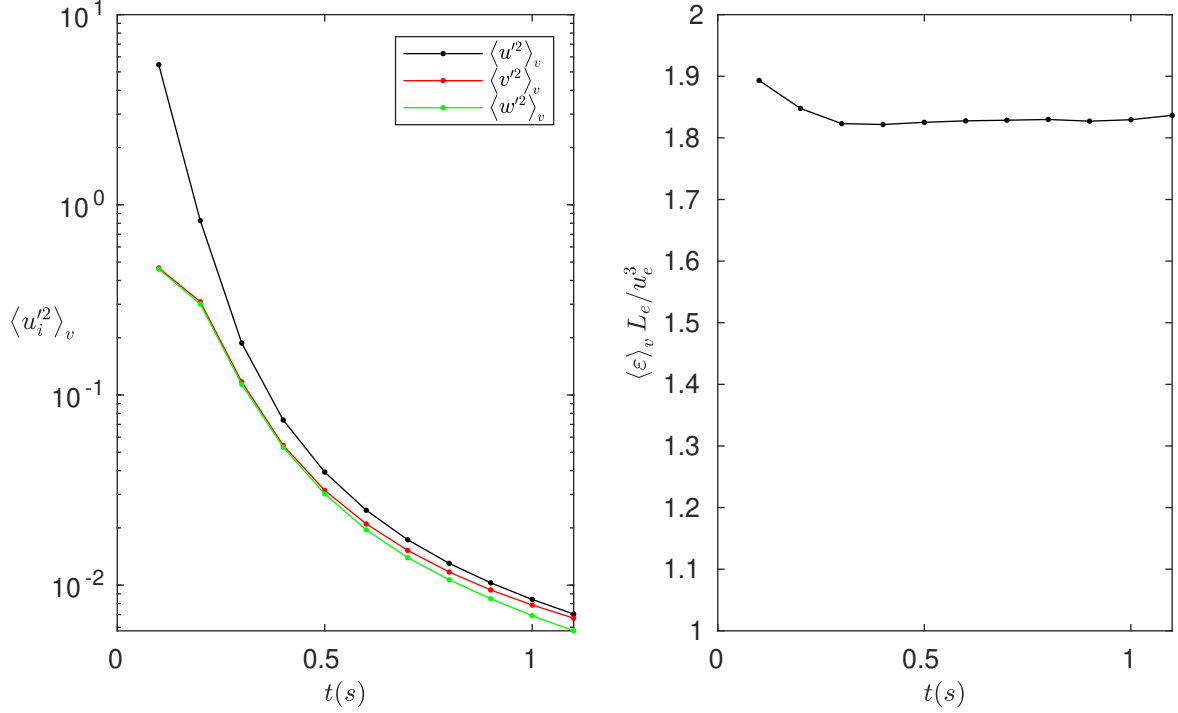


Figure 6.3: (a) Volume averaged values for the velocity fluctuations and (b) Normalized dissipation rates for the turbulence in the numerical domain.

6.2.2 Droplet dynamics

Particle motion is governed by the simplified Maxey-Riley equations (Maxey and Riley 1983) given by equations 2.21. The simplified form of the Maxey-Riley equations is valid only in the case where $R/\eta \ll 1$ where R is the particle radius. Table 6.2 shows the values of R/η of six radius categories in the polydisperse system at $\varepsilon = 215 \text{ cm}^2 \text{ s}^{-3}$ and $t = 1 \text{ s}$. The values for all the categories are well within this limit. The added-mass, Basset history force and pressure forces are neglected under the assumption that $\rho_p/\rho_f \gg 1$ where ρ_p and ρ_f are the densities of the particle and fluid. Since we are considering water droplets ($\rho_p = 1000 \text{ kg/m}^3$) dispersed in air ($\rho_f = 1.1436 \text{ kg/m}^3$), $\rho_p/\rho_f \sim 1000$. Another important assumption is the Stokes-drag approximation for the viscous drag forces. This assumption is valid in the range where the particle Reynolds number $Re_p \ll 1$. Ayala, Rosa, L.-P. Wang, and Grabowski (2008) showed that for $R > 30 \mu\text{m}$, Re_p is large enough to warrant the inclusion of a non-linear factor to model the departure from Stokes drag law. However, as was done in both Ayala, Rosa, L.-P. Wang, and Grabowski (2008) and Woittiez, Jonker, and Portela (2009), we employ the linear Stokes drag formulation to focus on the effects of gravity. We have performed simulations using a non-linear

drag formulation and not observed any qualitative difference in the results. As mentioned in Woittiez, Jonker, and Portela (2009), these non-linear drag formulas are empirical fits based on experiments for large spheres in situations different from droplets dispersed in turbulent flow.

A tricubic Hermite interpolation scheme is used to interpolate the Eulerian flow velocities to the particle locations ($\mathbf{u}(\mathbf{X}(t), t)$) as explained in section 3.3.2. A third order Adams-Bashforth time-stepping scheme is used to advance the particle locations and velocities at each time step (section 3.3.3). The particles on processor boundaries are communicated across processors after each time integration step following the flow field as detailed in section 3.3.4.

A polydisperse distribution of particles with 36 different discrete radii between $10\mu m$ and $55\mu m$ are randomly distributed across the whole computational domain at $t = 0.4s$. This range is selected since these are the most important sizes in the problem of the size-gap bottleneck in warm rain initiation. The number of particles in each size category is decided by a volume-weighted distribution (such that the total volume of particles in each size category is the same). Using such a distribution, a target volume fraction of 5×10^{-5} is achieved by introducing a total of 62.5 million particles. The target volume fraction is chosen such that the system is well within the dilute limit and any modulation of fluid turbulence due to two-way coupling with the particles can be neglected. We also neglect particle-particle aerodynamic interactions. The ghost collision approach is adopted, whereby particles are allowed to overlap after they collide. The calculation of the RDF and collision statistics is started at $t = 0.5s$ and averaged over every $0.1s$ thereafter. The very high number of particles ensures that converged particle statistics are obtained with this low averaging time. Two simulations with the same flow characteristics and droplet parameters, but one with non-sedimenting droplets and another with sedimenting droplets, are performed.

Droplet - turbulence interactions are characterised using a series of non-dimensional parameters. The most common parameter is the particle Stokes number which is defined as

$$St = \frac{\tau_p}{t_\eta}. \quad (6.2)$$

In the limit of $St \rightarrow 0$, particles behave as tracers and follow the fluid streamlines closely while in the limit $St \rightarrow \infty$, particles are not influenced by changes in the flow. The interaction

Table 6.2: Parameters for particle turbulence interaction at $\varepsilon = 215 \text{ cm}^2 \text{ s}^{-3}$ ($t = 1 \text{ s}$)

R	R/η	τ_p	$St = \tau_p/\tau_\eta$	$Sv = v_t/u_\eta$	$V_T = w_t/u_e$	τ_p/T_e	Fr
10	0.0159	0.0013	0.049	0.5336	0.1459	0.0020	0
19	0.0302	0.0047	0.1768	1.9263	0.5266	0.0072	0.002
28	0.0445	0.0102	0.3841	4.1834	1.1437	0.0156	0.0204
37	0.0587	0.0177	0.6707	7.3049	1.9970	0.0273	0.1088
46	0.0730	0.0274	1.0366	11.2908	3.0867	0.0422	0.4018
55	0.0873	0.0392	1.4819	16.1411	4.4127	0.0603	1.174

between droplets and the larger turbulent flow scales can be characterized using the parameter τ_p/T_e . The interaction between droplet turbulence and gravity can be characterised using the non-dimensional settling parameter Sv given by,

$$Sv = \frac{w_T}{u_\eta} \quad (6.3)$$

where w_t is the droplet terminal velocity as introduced in chapter 2. The interaction between sedimenting droplets and the larger scales of turbulence is characterised by

$$V_T = \frac{w_T}{u_e} \quad (6.4)$$

The values of these parameters for six different radius categories are shown in table 6.2 at $t = 1 \text{ s}$.

The details of the collision algorithm are described in section 3.5. Only droplets that can collide within one time step are considered as prospective colliding pairs. Only binary collisions are considered and colliding droplets are allowed to geometrically overlap post-collision (ghost collisions), i.e. no post-collision dynamics are calculated for the droplets. Since we only look at geometric collisions, the effects of collision efficiencies are ignored. The average geometric collision rate per unit volume $\dot{N}_c$ is calculated using equations (2.34) and (2.35) for bidisperse and monodisperse distributions respectively. The kinematic collision kernel is calculated using

equation (2.40).

The RDF $g_{12}(r; t)$ is calculated using equation 2.41. The value of δ is taken as a small fraction of the separation distance r , i.e. $\delta = 0.02r$. $g_{12}(r; t)$ is further averaged over time to obtain $g_{12}(r)$ as used in equation (2.40). In this study, the maximum value of the inter-particle separation distance r over which the RDF is calculated is $4\Delta x$. Considering particles at larger distances (beyond 4 cells in a direction) is restricted by the fact that the computational domain is parallelized in the $\hat{y}$ and $\hat{z}$ directions. Calculating particle separations at the processor boundaries requires exchange of data in the corresponding boundary cells of the neighbouring processor(s) which is a memory- and time-intensive procedure.

6.3 Radial Distribution Function

6.3.1 Monodisperse RDFs

As mentioned in the introduction, the RDF for same-sized particles can be expressed in terms of a power law. Equation (6.1) proposed by Reade and Collins (2000b) was modelled using a series of DNS data at $Re_\lambda = 54.5$ of monodisperse non-sedimenting particles. In this equation, the coefficients c_0 , c_1 and c_2 are all in principle, functions of St .

Chun et al. (2005) derived an analytical expression for the RDF of a monodisperse collection of particles with $St \ll 1$ as

$$g(r) = c_0 \left[\frac{\eta}{r} \right]^{c_1}, \quad (6.5)$$

which is similar to equation (6.1). The study does not specify a relation for the coefficient c_0 which has a physical meaning only when the locally-linear flow transitions to fully turbulent flow which happens at larger values of r . The coefficient c_1 was shown to be proportional to St^2 for $St < 0.3$.

Figure 6.4 shows three dimensional RDFs for particles of the same sizes (g_{11}) for non-sedimenting (figure 6.4a) and sedimenting particles (figure 6.4b). The plots are for the RDF at $t = 1s$ when the mean dissipation rate is $\varepsilon = 215 \text{ cm}^2 \text{ s}^{-3}$. We observe a clear power law scaling for both cases, especially at $r/\eta < 1$. The RDF at $r/\eta < 1$ remains the same up to $SV \approx 2$ after

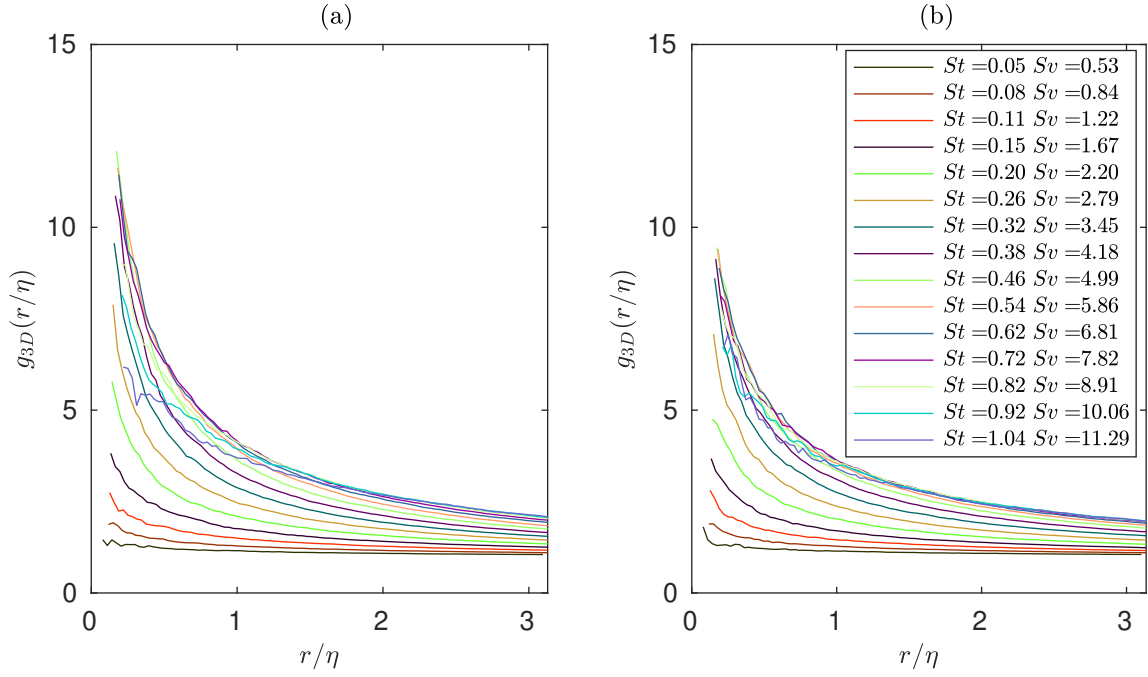


Figure 6.4: Monodisperse RDF for (a) non-sedimenting particles and (b) sedimenting particles at $t = 1s$ and $\varepsilon = 215cm^2s^{-3}$.

which sedimenting particles show a lower RDF. Gravity clearly suppresses particle clustering owing to the reduced time particles have to interact with the turbulent eddies resulting in them settling out of low vorticity regions. Both non-sedimenting and sedimenting particles exhibit a maximum RDF for $r/\eta < 1$ at $St = 0.46$, however the magnitude of the maximum is higher in the absence of gravity. For $r/\eta > 1.5$, the RDF of sedimenting droplets reaches a saturation at around $St = 0.62$ whereas for non-sedimenting particles saturation is delayed till $St = 0.92$.

The coefficients of the power law from equation (6.5) for the RDF values from $t = 0.7s$ to $t = 1.0s$ are shown in figure 6.5 for non-sedimenting (a,b) and sedimenting (c,d) particles. These are obtained by fitting the DNS data to equation (6.5). The behaviours of the coefficients c_0 and c_1 are similar to that shown in Reade and Collins (2000b). At low Stokes numbers, the coefficients are similar for both sedimenting and non-sedimenting particles. This is expected since Sv is low at these Stokes numbers and low dissipation rates. However it is interesting to note that for the coefficient c_0 , the peaks decrease with time for sedimenting particles (figure 6.5(b)), i.e. particles with the same Stokes number cluster to a lesser degree. With time, the dissipation rate decreases, and for the same Stokes number, Sv becomes more dominant. This leads to the reduction in clustering due to gravity becoming more prominent.

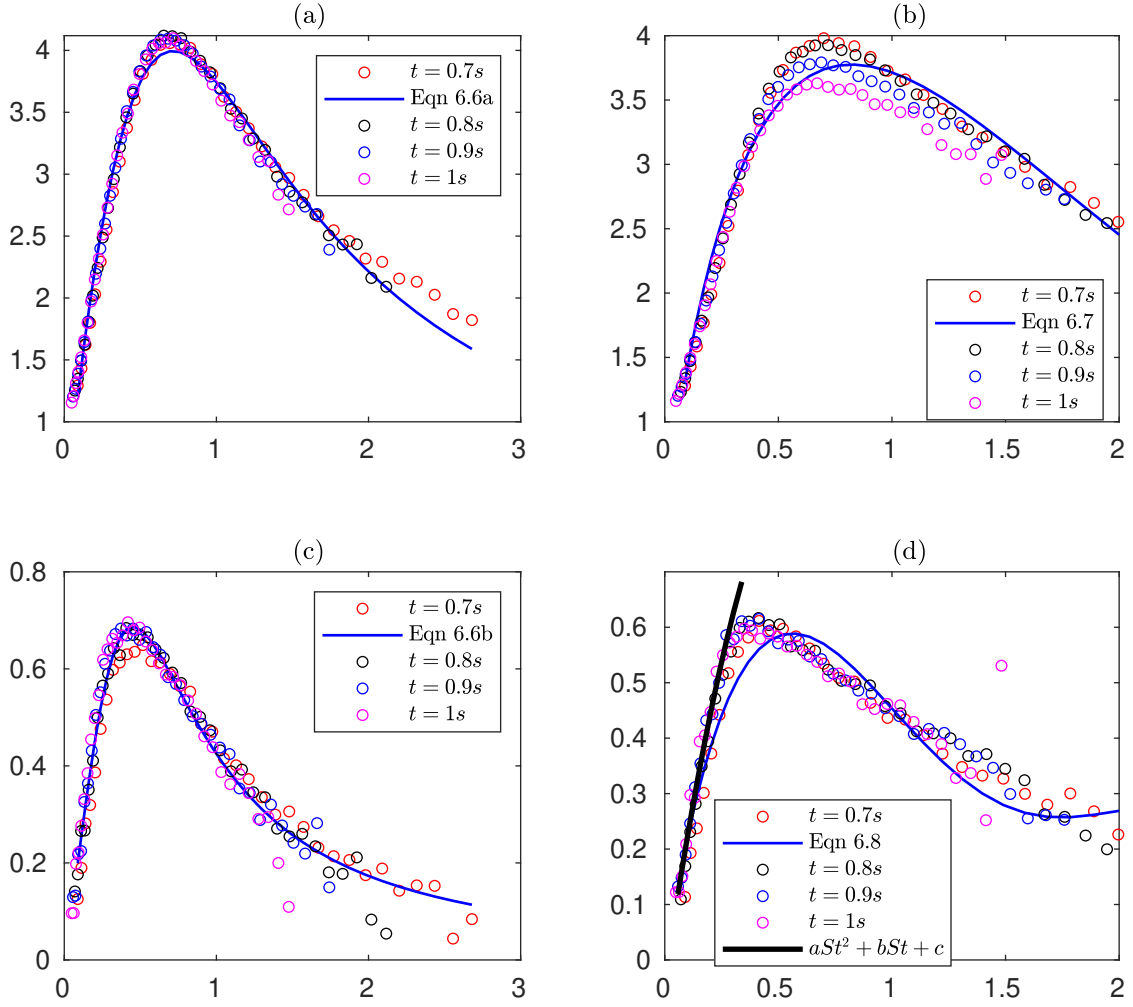


Figure 6.5: Coefficients for monodisperse RDF: (a,b) pre-factor c_0 , (c,d) clustering exponent c_1 . Left column represents non-sedimenting particles and right column represents sedimenting particles. The circles show the coefficients obtained by fitting DNS data from $t = 0.7s$ to $t = 1s$ to equation 6.1. The blue lines are the predicted values using the empirical formulas (equation (6.6) for (a) and (c), equation (6.7) for (b), and equation (6.8) for (d)). The black line in figure (d) is the fit of the DNS data to a quadratic polynomial in the range $St \ll 1$.

An empirical fit for the coefficients c_0 and c_1 was performed by Reade and Collins (2000b) by curve fitting their DNS data to the following functions

$$c_0 = \frac{d_0 St^{d_1}}{d_2 + St^{d_3}}, \quad c_1 = \frac{d_4 St^{d_5}}{d_6 + St^{d_7}}, \quad (6.6)$$

with $c_2 = 0.25$ assumed to be a constant. We use the same functions to curve fit c_0 and c_1 (the data shown in 6.5 (a) and (c)). A very good fit was obtained as shown by the blue line in figures 6.5 (a) and (c) with the following coefficients: $d_0 = 6.9650$, $d_1 = 0.7832$, $d_2 = 0.8603$, and $d_3 = 2.1867$ for c_0 and, $d_4 = 0.5$, $d_5 = 1.0890$, $d_6 = 0.1774$, and $d_7 = 2.5768$ for c_1 .

The analytical solution developed by Chun et al. (2005) was extended to sedimenting droplets

by Ayala, Rosa, and L.-P. Wang (2008) who developed an empirical model using DNS results to quantify the RDF. In order to account for the effects of gravity, they assumed the coefficients c_0 and c_1 to be a function of St , Re_λ and a dimensionless gravity parameter $|g|/(u_\eta/\tau_\eta)$. An empirical expressions for c_1 was then obtained by curve-fitting the DNS data with $c_0 = 1$. However, figure 6.5 clearly shows that c_0 is a function of St . Even though the range of Re_λ is small in our simulations, there is a clear change in the maxima for c_0 (figure 6.5b) as the simulation progresses. So we propose the following function for c_0

$$c_0 = f_1(Re_\lambda)St^{b_2} \exp(-b_3St), \quad (6.7)$$

where

$$f_1(Re_\lambda) = b_0 \exp\left(\frac{b_1}{Re_\lambda}\right),$$

Curve-fitting this function with the data plotted in figure 6.5(b) gives the following coefficients: $b_0 = 11.5915$, $b_1 = -10.0$, $b_2 = 0.7948$ and $b_3 = 0.9659$. For c_1 , the function proposed by Ayala, Rosa, and L.-P. Wang (2008) is used

$$c_1 = \frac{f_2(St)}{(|g|/(v_k/\tau_k))^{f_3(Re_\lambda)}}, \quad (6.8)$$

where

$$\begin{aligned} f_2(St) &= b_4St^4 + b_5St^3 + b_6St^2 + b_7St, \\ f_3(Re_\lambda) &= b_8 \exp\left(\frac{b_9}{Re_\lambda}\right). \end{aligned}$$

The proposed functions for c_1 is fit to the data shown in figure 6.5(d) to obtain the following coefficients: $b_4 = -0.2817$, $b_5 = 1.6703$, $b_6 = -3.3334$, $b_7 = 2.3639$, $b_8 = -0.0632$ and $b_9 = -9.9914$. These empirical formulas for c_0 and c_1 will be used to predict the RDF of colliding droplets in section 6.4.

We also check the scaling for the clustering coefficient c_1 in the range $St \ll 1$. A curve

obtained by linearly fitting a quadratic polynomial of the form $p(St) = aSt^2 + bSt + c$ to the DNS data gives very good agreement in the range $St \ll 1$ with $a = -1.9687$, $b = 2.7869$, $c = -0.0364$. A linear fit to a first order polynomial of the form $p(St) = aSt + c$ in the range $St \ll 1$ resulted in non-physical negative values of the intercept c as was shown in Saw et al. (2012) for non-sedimenting particles. Hence, a linear scaling is highly unlikely and all evidence points towards a quadratic scaling as was predicted by the analytic relation in Chun et al. (2005).

6.3.2 Bidisperse RDFs

Figure 6.6 shows RDFs of droplets of different sizes. These bidisperse RDFs are calculated by fixing the size of one droplet at $St_1 = 0.11$ and varying the size of the second droplet from $St_2 = 0.05$ to $St_2 = 0.23$. Figures 6.6 (a) and (c) shows RDFs for non-sedimenting droplets with $St_2 \leq St_1$ and $St_2 \geq St_1$ respectively. Figures 6.6 (b) and (d) shows the same for sedimenting droplets. The bidisperse RDFs exhibit a power law at relatively larger scales which taper off to a plateau at smaller scales. We observe a similar asymmetry for non-sedimenting droplets when St_2 is increased or decreased relative to the fixed St_1 as was shown by Saw et al. (2012). Interestingly, a symmetry is observed for sedimenting droplets. This can be explained by analyzing the coefficient c_1 for the RDF of unequal-sized droplets. In the absence of gravity, when St_1 is fixed and St_2 is varied, the power-law coefficient c_1 increases with St_2 , reaches a maximum at $St_1 = St_2$ and thereafter reduces gradually at a rate where we can consider it to have saturated. This is what was observed in Saw et al. (2012) as well. This explains the slope of the RDF plots in figure 6.6(a) increasing until $St_1 = St_2$ and thereafter remaining almost a constant for $St_2 > St_1$. In the presence of gravity, the behaviour of c_1 is quite different. The values increase with St_2 , reaches a maximum at $St_1 = St_2$ and thereafter drops sharply again for $St_2 > St_1$. This is reflected in the slopes of the RDFs in figures 6.6(c) and (d). Any small deviation from a monodisperse distribution results in a sharp change in the RDF slope due to the difference in settling velocities for droplets with different sizes (or for a small $\Delta St = St_2 - St_1$). This is explored in detail for colliding droplets in section 6.4. The analytical theory of Chun et al. (2005) predicts the RDF for inertial particles of different sizes using the following expression

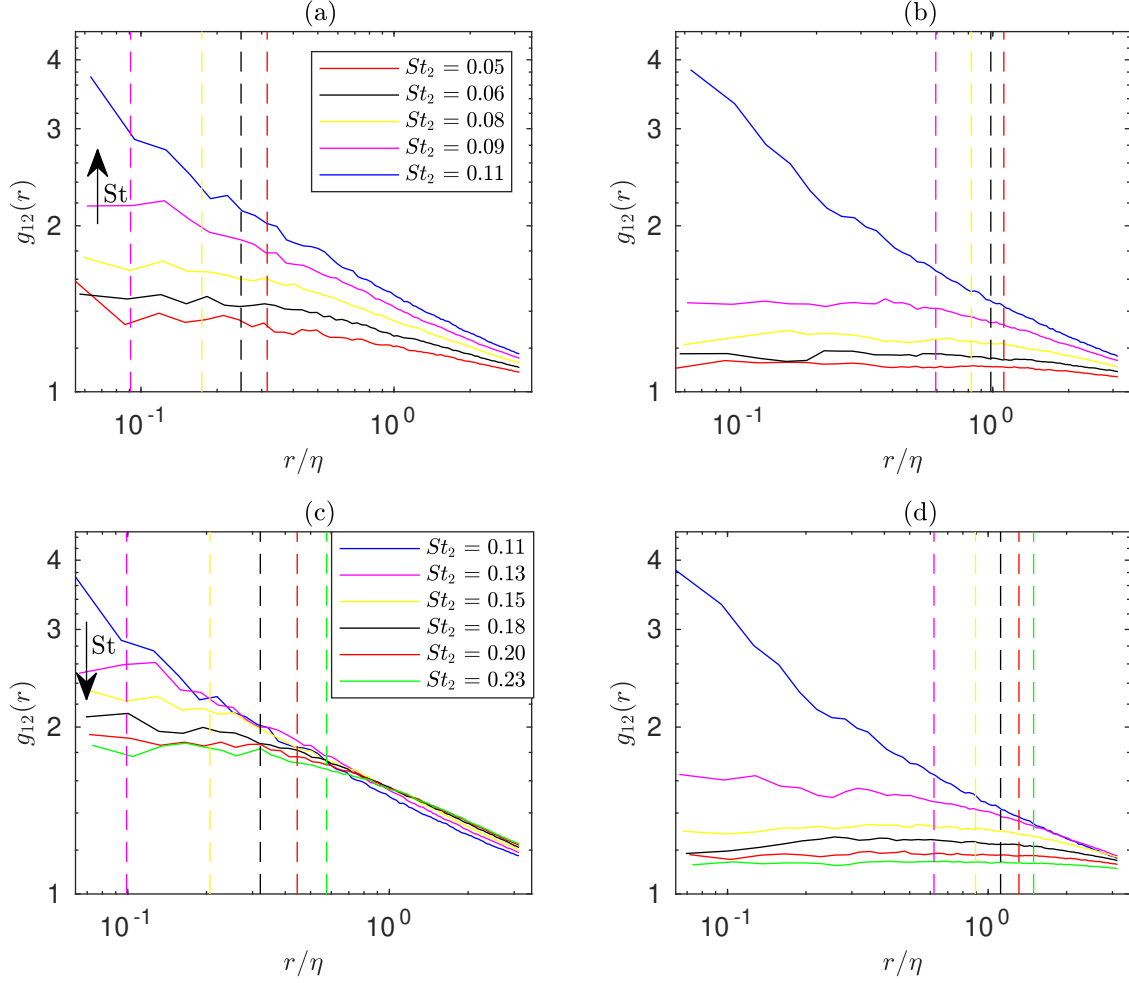


Figure 6.6: Bidisperse RDF with $St_1 = 0.11$ (fixed) and (a,b) $St_2 < St_1$ (c,d) $St_2 > St_1$ at $t = 1s$ and $= 215cm^2/s^{-3}$. The left column represents non-sedimenting particles and right column represents sedimenting particles. The dashed lines represent the value of the cross-over scale r_c for the given combination of St_1 and St_2 .

at $r \ll \eta$

$$g(r) = c_0 \left[\frac{\eta^2 + r_c^2}{r^2 + r_c^2} \right]^{c_1/2}, \quad (6.9)$$

where c_0 and c_1 are coefficients similar to equation (6.1) and r_c is a cross-over length scale. Chun et al. (2005) shows that shear-driven diffusion dominates for $r > r_c$ with the resulting RDF exhibiting a power law behaviour, while an acceleration-driven diffusion dominates for $r < r_c$ resulting in an RDF which is independent of r . Hence r_c can be considered to be a cross-over length scale at which the RDF stops exhibiting a power-law behaviour and switches to a plateau. A relation for r_c is given in Chun et al. (2005) (for $Re_\lambda = 47.1$) as

$$\frac{r_c}{\eta} \approx 5.0 |St_2 - St_1|. \quad (6.10)$$

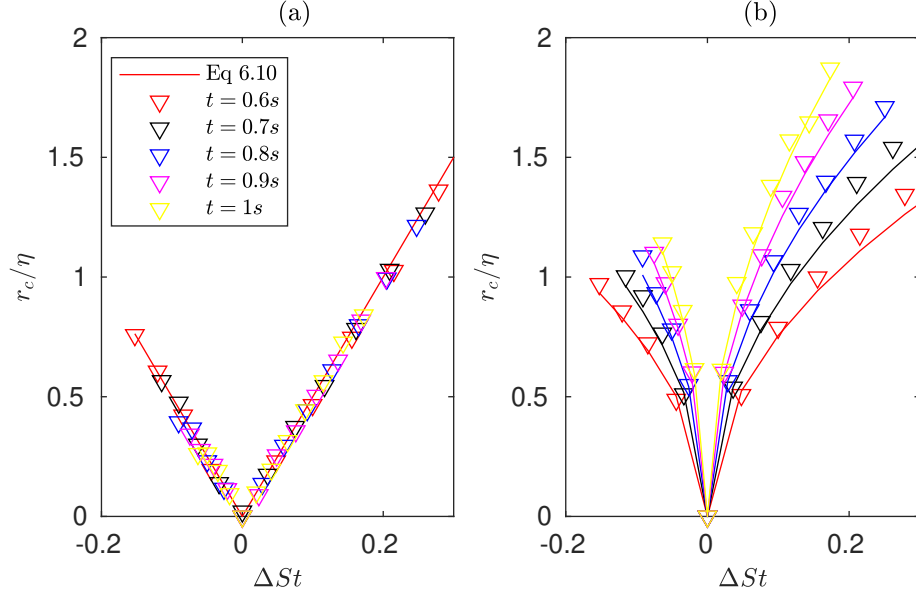


Figure 6.7: Cross-over scale r_c for (a) non-sedimenting and (b) sedimenting particles as a function of ΔSt . The red line in (a) is the analytical solution given by equation (6.10) and the lines in (b) are the solutions using equation (6.11) for different output times (and different Re_λ). $\Delta St = St_2 - St_1$ where $St_1 = [0.27, 0.20, 0.16, 0.13, 0.11]$ for different t .

For a monodisperse case, $r_c = 0$ and equation 6.9 reduces to 6.5.

Figure 6.6 also shows the cross-over scales r_c (dashed lines) calculated from equation (6.10) for the different St_2 considered. Clearly the transition from the power-law to a plateau where RDF is independent of r happens at much larger scales for sedimenting droplets.

Ayala, Rosa, and L.-P. Wang (2008) modified the expression for r_c for sedimenting droplets to

$$\left(\frac{r_c}{\eta}\right) = |St_2 - St_1| F(a_{0g}, Re_\lambda), \quad (6.11)$$

where

$$a_{0g} = a_0 + \frac{\pi}{8} \left(\frac{g}{u_\eta/t_\eta} \right)^2, \quad (6.12)$$

$$a_0 = \frac{11 + 7Re_\lambda}{205 + Re_\lambda}, \quad (6.13)$$

$$F(a_{0g}, Re_\lambda) = 20.115 \left(\frac{a_{0g}}{Re_\lambda} \right)^{1/2}. \quad (6.14)$$

We compare the cross-over scale r_c for non-sedimenting and sedimenting droplets in figure 6.7. The values of r_c are obtained by fitting the RDF to equation (6.9). This is done in two

steps. We first perform a non-linear regression of equation (6.5) to fit c_0 and c_1 . Equation (6.10) is used to predict r_c for this regression. Using these values of c_0 and c_1 , we perform another non-linear regression to equation 6.9 to calculate the value of r_c . A similar two-step procedure is adopted to calculate r_c for sedimenting droplets as well where c_0 and c_1 are determined in the first step and a non-linear regression is used to determine r_c . However, equation (6.11) is used to predict the value of r_c in the first step for this case.

The value of r_c obtained from the regression is compared with the theoretical values from equations (6.10) and (6.11) for non-sedimenting and sedimenting droplets respectively and the results are shown in figure 6.7. Saw et al. (2012) describes r_c as the measure of the offset distance between the cluster sites of particles with different Stokes numbers which tend to concentrate in the vicinity of each other. They presume these offsets to be isotropic in the absence of gravity and hence r_c can be considered to be the isotropic average of these offsets. An excellent agreement is observed for the non-sedimenting case between the DNS data from our study and equation (6.10) in figure 6.7(a). Figure 6.7(b) also shows very good agreement between the empirical formula given by equation (6.11) and the DNS data for sedimenting droplets from the current study. An explicit Reynolds number dependence is built into the empirical model of Ayala, Rosa, and L.-P. Wang (2008) and hence a good agreement is observed for all times. We observe a similar symmetry in the values of r_c for $St_2 > St_1$ and $St_2 < St_1$. The value of r_c depends only on ΔSt and the effect of gravity is the same for both heavier and lighter particles with respect to a fixed St .

6.4 Geometric Collision kernel results

In this section, we analyse the effect of gravity on the collision kernel. Figure 6.8 shows a contour plot for the collision kernel $\Gamma^K(a,d)$, RDF $g(R_1 + R_2)$ (b,e) and the magnitude of the mean radial relative velocities $\langle |w_r| \rangle$ (c,f) for all colliding droplets in the polydisperse distribution. The statistics are shown for $t = 1s$. All the figures show striking symmetry which confirms the fact that the statistics for collisions between droplets of radii R_1 and R_2 are the same as those between R_2 and R_1 .

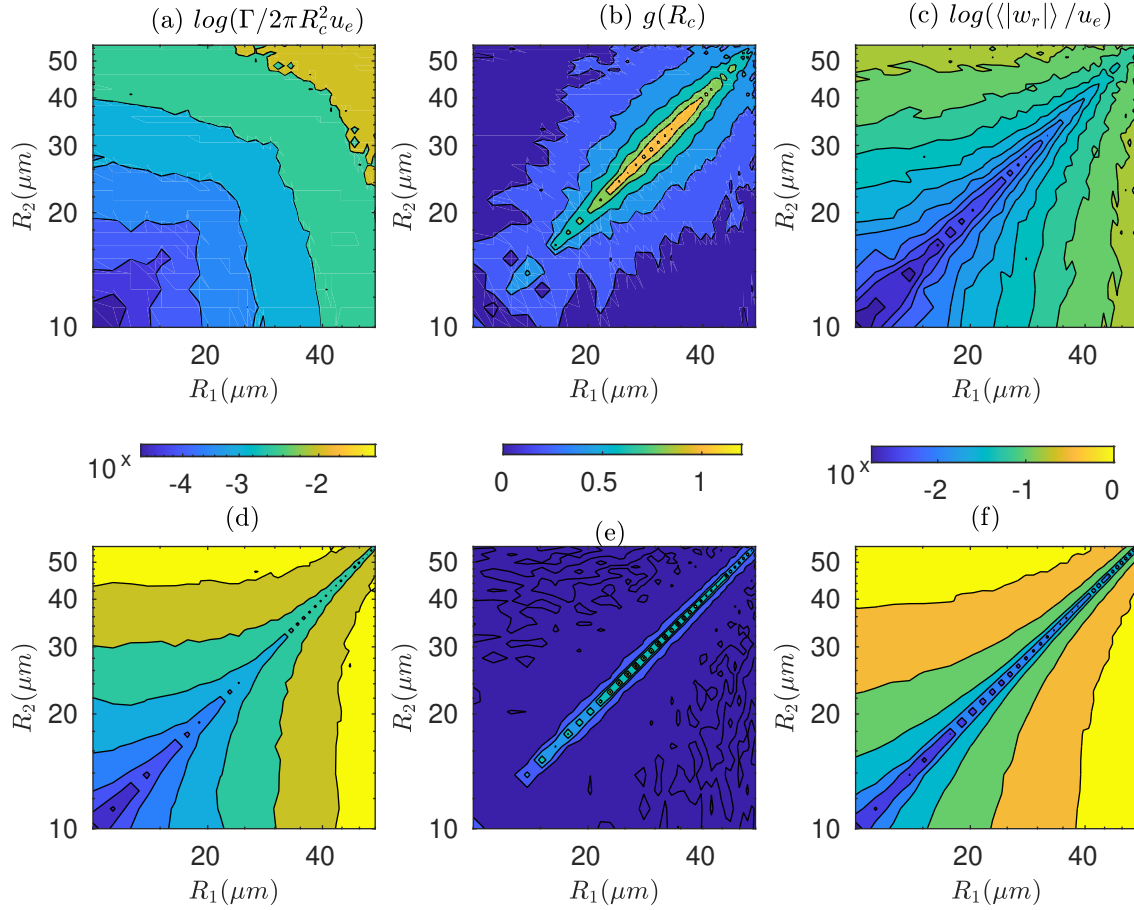


Figure 6.8: Comparisons between the polydisperse distribution of non-sedimenting droplets (top row) and sedimenting droplets (bottom row) for the (a,d) kinematic collision kernel Γ^K , (b,e) RDF and (c,f) radial relative velocity $\langle |w_r| \rangle$.

Figures 6.8(a) and (d) show that sedimentation enhances the collision kernel except when collisions are between droplets of the same size. For collisions between same-sized particles (along the leading diagonal), the kernel is higher for non-sedimenting droplets compared to sedimenting droplets, noticeably so for $R > 25\mu m$. For collisions between unequal-sized droplets (either side of the leading diagonal), the enhancement observed in the collision kernel in figure 6.8(d) due to sedimentation is obvious for colliding droplets of size $R_1 > 25\mu m, R_2 > 25\mu m$. This is because the higher velocity decorrelation due to the differential settling velocities for droplets with different sizes becomes significant at sizes greater than $25\mu m$. This can be verified by comparing figures 6.8(c) and (f) in the same size range, revealing a difference of at least an order of magnitude between $\langle |w_r| \rangle$ for non-sedimenting and sedimenting colliding droplets. For non-sedimenting droplets, bands are observed within which the collision kernels have a similar order of magnitude compared to a 'butterfly' pattern for sedimenting droplets.

Detailed analysis of the kernels are done later in the section using a cross-section from the contour plot.

A detailed analysis of the RDF at scales extending up to 4η was performed in section 6.3. In figures 6.8(b) and (e), we look at the effect of gravity on the RDF of colliding droplets. For both non-sedimenting and sedimenting droplets, the magnitude of the RDF for colliding unequal-sized droplets g_{12} is bound by that of colliding same-sized droplets g_{11} as was originally shown by Y. Zhou, Wexler, and L.-P. Wang (2001). Figure 6.8(b) suggests that the gradient from the monodisperse peak is much more gradual for non-sedimenting colliding droplets when compared to sedimenting colliding droplets. In figure 6.8(e) the RDF of sedimenting droplets falls rapidly from the monodisperse value for even a small $\Delta R = R_2 - R_1$. This is due to the rapid decorrelation of the droplet concentrations for different droplet sizes (Y. Zhou, Wexler, and L.-P. Wang 2001). The decorrelation arises from the fact that particles with different inertia tend to cluster in different (slightly-offset) regions with respect to the flow. Differential sedimentation enhances this decorrelation leading to a very sharp diagonal with high values of RDF and the values dropping to one even for a small ΔR .

In figures 6.8(c) and (f), the plots are symmetric indicating that $\langle |w_r| \rangle$ depends on ΔR (or ΔSt), the difference in inertia, rather than R_1 or R_2 . The radial relative velocity reaches a minimum for same-sized droplets and increases as ΔR is increased for both cases. Focusing on the upper quadrant, for unequal sized droplets, the magnitude of $\langle |w_r| \rangle$ increases as the droplet size increases. The effect of gravity is an overall increase in $\langle |w_r| \rangle$ of almost an order of magnitude for unequal sized droplets.

To obtain a clearer picture, the kinematic collision kernel Γ_{11}^K , the RDF g_{11} and the radial relative velocities $\langle |w_r| \rangle$ for the colliding droplets of the same size are plotted in 6.9 (a), (b) and (c). These plots correspond to the leading diagonals of figures 6.8 (a), (b) and (c). Figures 6.9(d), (e) and (f) show the collision statistics Γ_{11}^K , the RDF g_{11} and $\langle |w_r| \rangle$ for unequal sized droplets where $R_1 = 33.1\mu m$ and R_2 is varied over the entire 36 different droplet radius categories considered in the study. This corresponds to a slice in the contour plots at $R_1 = 33.1\mu m$. For all the sub-figures in figure 6.9, the red line corresponds to non-sedimenting droplets and the black line corresponds to sedimenting droplets.

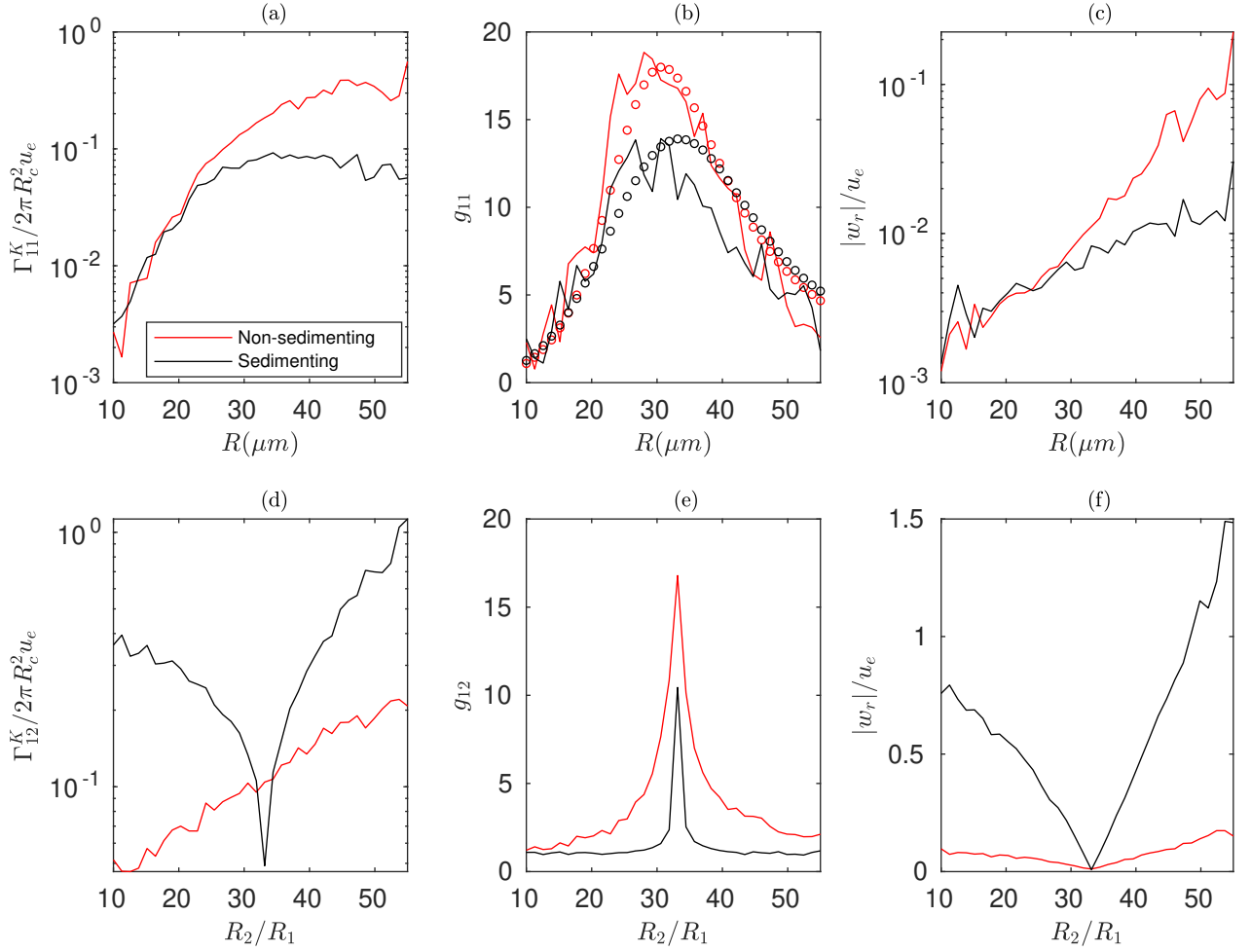


Figure 6.9: Monodisperse (top row) and bidisperse (bottom row) values of the (a,d) kinematic collision kernel Γ^K , (b,e) RDF and (c,f) radial relative velocity $\langle |w_r| \rangle$. Red lines represent non-sedimenting and black lines sedimenting colliding particles. The red and black circles in figure (b) are the RDF predicted from the empirical formulas for non-sedimenting and sedimenting droplets respectively.

Gravity clearly decreases the monodisperse collision kernel for droplets of size greater than $25\mu m$ as shown in figure 6.9(a). At these sizes, the interaction time of the droplets with both the small scale and large scale turbulent eddies decreases due to the increased settling velocities. This is evident in the values of the corresponding dimensionless numbers $S_v \approx 3.5$ and $V_T \approx 1$. For colliding droplets of unequal sizes, gravity enhances the collision kernel as shown in figure 6.9(c).

Figure 6.9(b) shows that for same-sized colliding droplets, the RDF does not monotonically increase up to $St = 1$ (for both non-sedimenting and sedimenting droplets). Instead, there is a steady increase in the RDF until it reaches a maximum at around $R = 28\mu m$. It then remains steady until $R = 35\mu m$, after which the RDF reduces steadily. The RDF maximum corresponds to a Stokes number range of 0.4 - 0.6. At higher Stokes numbers ($R > 35\mu m$),

higher particle inertia means that particles are less likely to follow the flow streamlines resulting in less clustering and reduced values of the RDF. The presence of gravity reduces the RDF magnitude of same-sized particles as a result of reduced interaction time with the smaller turbulent scales. This is prominently seen in the range $R = 22\mu m$ to $R = 42\mu m$ ($St = 0.28$ to $St = 0.86$). Also plotted are the predicted RDFs from the empirical formulas proposed in section 6.3.1. The function for the non-sedimenting droplets (red circles) give a very good agreement. For sedimenting droplets, there is good agreement till the RDF peaks, after which the function seems to over-predict the RDF values. Woittiez, Jonker, and Portela (2009) observed an increase in monodisperse RDF for droplets of radius $R > 40\mu m$ which peaks at around 70 to $80\mu m$ for a mean dissipation rate $\varepsilon = 425 cm^2 s^{-3}$. The reason for the increase was explained as the interaction between large sedimenting droplets and the large scale energetic eddies when τ_p/T_e is not negligible (~ 0.5). We do not observe a similar increase as the values of τ_p/T_e are always $\ll 1$ suggesting no significant interaction between the larger droplets and the large scale eddies. Figure 6.9(e) shows the RDFs for the bidisperse case for $R_1 = 33.1\mu m$. The sharp fall of the RDF values from a maximum to one is clearly visible for sedimenting droplets when compared with the more gradual fall for non-sedimenting droplets.

Sedimenting droplets of the same size have a lower radial relative velocity than their non-sedimenting counterparts as shown in figure 6.9(c). In the absence of gravity, droplets are subject only to turbulent accelerations. Colliding droplets experience similar turbulent accelerations just before collision and therefore a relative velocity between two colliding droplets is due to the difference in droplet inertial responses (Franklin, Vaillancourt, and Yau 2007). This is apparent in figure 6.9(c) where the average radial relative velocities of the non-sedimenting droplets increase monotonically with droplet size. In the presence of gravity, the relative velocity is a result of the effects of both droplet inertia and gravitational acceleration. At small St , droplets tend to follow the fluid streamlines and the inertial effects tend to dominate the effects of gravity. At higher St , the particle settling velocity increases, resulting in the relative velocity being dominated by the effects of sedimentation. In figure 6.9(c), the average radial velocities for sedimenting droplets deviate from that for non-sedimenting droplets at $R \sim 25\mu m$. As the colliding droplets are of the same size and hence the same settling velocity, the droplet

velocities are highly correlated resulting in a reduction in relative velocities as compared to non-sedimenting droplets. Additionally it has been shown by Woittiez, Jonker, and Portela (2009) that compared to non-sedimenting droplets, sedimenting droplets are unable to pick up as much turbulent kinetic energy from the flow.

Figure 6.9(f) clearly shows that the relative velocities of unequal-sized colliding sedimenting droplets (black lines) are significantly higher than non-sedimenting droplets (red lines). Relative velocities between non-sedimenting colliding droplets are entirely due to differential inertia. However, sedimentation significantly enhances the velocity decorrelation due to the differential terminal velocities. When $R_1 = R_2$, there is a conspicuous dip for both lines, but the relative velocities of sedimenting droplets are highly correlated as seen in fig 6.9(c) compared to non-sedimenting droplets resulting in a higher magnitude for the latter (the black line dipping below the red line).

So at St closer to 1, we would expect the geometric collision kernel to be dominated by the effect of particle clustering even if the radial relative velocities are large. A similar observation was made by Franklin, Vaillancourt, and Yau (2007). For larger St , as clustering reduces, the effect of radial relative velocities plays a major role in the monodisperse collision kernel.

The enhancement of the geometric collision kernel due to air turbulence relative to the gravitational kernel is shown in figure 6.10a. The figure shows the ratio Γ^K/Γ^g where Γ^g is the gravitational collision kernel. Also shown are the RDF (figure 6.10b) and the enhancement of the average radial relative velocity with respect to the purely gravitational case (figure 6.10c). Turbulence-induced enhancements of up to a factor of 3 are observed, especially for collisions between droplets with a small size difference.

The value of Γ^K/Γ^g is not defined for particles of the same size (since $\Gamma_g = 0$), however figure 6.10b shows that particle clustering can lead to enhancement in collisions up to 12 times that in the purely gravitational case. For larger droplets, as particle inertia increases, the effect of radial relative velocity is the significant contributor to the turbulence enhancement of the collision process. A difference in radial relative velocities between colliding particles can lead to enhancements of up to a factor of 2 for droplets of unequal size as shown in figure 6.10c.

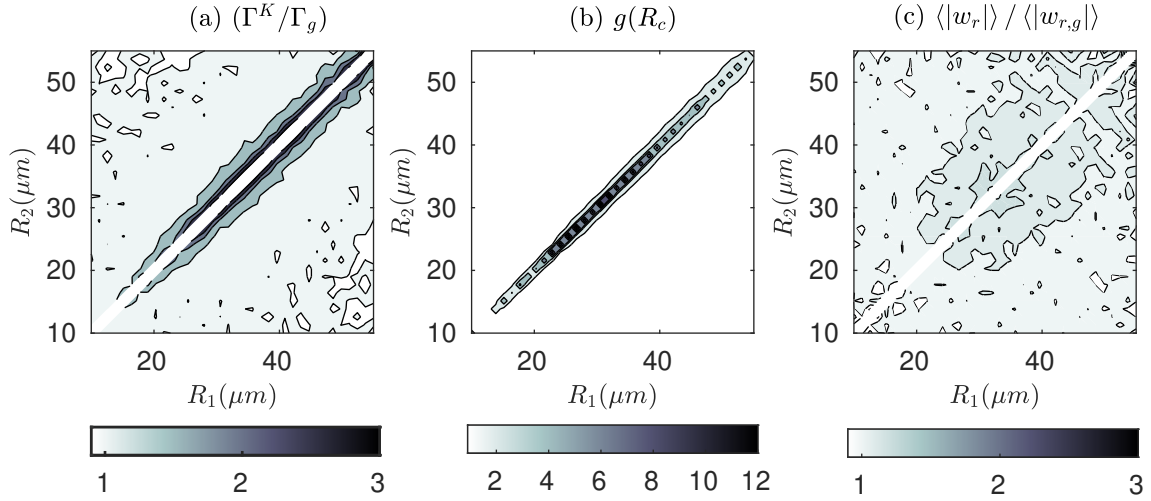


Figure 6.10: (a) Turbulence enhancement of the geometric collision kernel Γ^K , (b) RDF and (c) Turbulence enhancement of the radial relative velocity $\langle |w_r| \rangle$.

6.5 Concluding remarks

In this chapter, we investigated the effect of gravity on the preferential concentration and geometric collisions of a polydisperse distribution of water droplets in decaying homogeneous isotropic turbulence. We presented a numerical setup which simulates grid generated decaying turbulence akin to flow in a wind tunnel. The setup simulates the temporal evolution of a fluid section exiting an active grid as an analogy to following a fluid section as it moves downstream in a wind tunnel. A polydisperse distribution of water droplets with radii ranging from $R = 10\mu m$ to $R = 55\mu m$ was randomly distributed once the flow had become isotropic and the effects of the initial grid velocity distribution is forgotten. The Radial Distribution Function (RDF) was used to quantify particle clustering and simulations were performed with both non-sedimenting and sedimenting droplets.

The effect of gravity on the RDF has been studied before for colliding droplets, i.e. $g(r = R_1 + R_2)$. In this study, we perform an analysis for the effect of gravity on the RDF at separation distances up to 4η . Analysis of the RDF for same-sized droplets revealed that gravity suppresses particle clustering due to reduced particle-turbulence interaction times. The RDF for both cases increases with St for $r/\eta < 1$ and reaches a maximum at around $St = 0.45$ for $\varepsilon = 215 cm^2 s^{-3}$. For separation distance $r/\eta > 1$, the RDF reaches a maximum or a saturation value at around $St = 0.9$ for non-sedimenting droplets. The presence of gravity hastens this saturation to

$St = 0.6$. The saturation refers to the fact that the RDF magnitude will not increase even with a further increase in particle St . The DNS data reveals that the power law form of the RDF holds for sedimenting droplets as well.

For preferential concentration in droplets of unequal sizes, theory predicts that within the limit $\eta \gg r \gg d$, the RDF exhibits a power law behaviour tapering to a plateau. The cross-over scale at which the RDF tapers to a plateau, is calculated from theoretical predictions for both non-sedimenting and sedimenting droplets. For sedimenting droplets, we show that the cross-over occurs at much larger scales compared to non-sedimenting droplets. Excellent agreement is shown when the theoretical formula for non-sedimenting droplets is fit to the DNS data. The DNS data show excellent agreement with the empirical formula for predicting the cross-over scales developed by Ayala, Rosa, and L.-P. Wang (2008) for sedimenting droplets.

Contrary to non-sedimenting droplets, we show that sedimenting droplets of unequal sizes exhibit a symmetric behaviour in RDF with droplets smaller and larger in size. The asymmetry in non-sedimenting droplets is due to the 'saturation' of the coefficient c_1 . For sedimenting droplets, c_1 increases to a maximum and thereafter drops sharply. Differential sedimenting velocities for particles of unequal sizes can explain this sharp drop from the maximum.

The effect of gravity on geometric collision is analysed by looking at the kinematic collision kernel, the RDF and relative velocity of colliding droplets. For same-sized droplets, gravity reduces the collision kernel for bigger droplets. This is mainly due to a reduction in relative velocity once the effects of droplet settling velocities dominate the particle inertial effects resulting in the droplet velocities being increasingly correlated. In the case of collisions between droplets of unequal sizes, gravity results in a significant increase in the kernel magnitude.

Numerical studies involving a polydisperse distribution of droplets in homogeneous isotropic turbulence are quite rare. The contour plots for the geometric collision kernel show how gravity plays an important role in enhancing collision between unequal sized droplets with radii greater than $30\mu m$. The results of this study can help in developing models of the collision kernel based on actual cloud conditions where gravity plays an important role. However, the simulations are at a much lower Reynolds number than in actual clouds. The Reynolds number dependence of the collision kernel for sedimenting droplets needs to be evaluated. We also plan to compare the

DNS data with data from wind tunnel experiments for similar turbulence and droplet parameters.

Chapter 7

Cloud-aerosol interactions

7.1 Introduction

The quantification of the radiative forcing due to cloud interactions with anthropogenic aerosols is a significant source of uncertainty in predicting climate sensitivities (Boucher et al. [2013](#)). Aerosols influence cloud formation as they act as Cloud Condensation Nuclei (CCN) and Ice Nuclei (IN), on which cloud droplets or ice crystals form respectively. In addition to initiating formation of clouds, aerosol perturbations can also change the properties of existing clouds. This happens mainly through two effects: the cloud *albedo effect* (modification of the cloud albedo) and the *lifetime effect* (modification of the cloud vertical thickness and horizontal extent). For the same liquid water content, an increase in aerosol loading (natural or man-made) leads to higher cloud droplet number concentration (due to higher number of CCN) and a reduction in the mean droplet radius, thus increasing the optical thickness and hence the cloud albedo (Warner and Twomey [1967](#); Twomey [1974](#), [1977](#)). This is also referred to as the Twomey effect or the first indirect effect.

The second consequence of aerosol-cloud interaction is the lifetime effect. An increase in aerosol concentration can result in the suppression of precipitation (Warner [1968](#)). This stems from the reasoning that an increase in CCN reduces the mean droplet size and hence hampers the collision-coalescence process necessary for raindrop formation. The suppressed precipitation is

expected to result in an increase in cloud Liquid Water Path (LWP)¹, cloud fraction (horizontal extent), cloud vertical thickness and possibly increased lifetime (Albrecht 1989; Pincus and Baker 1994). The associated increase in the cloud reflectivity due to the presence of more smaller droplets is in addition to that by the Twomey effect and would contribute to an overall cooling effect. This effect is also called the second indirect effect and involves a broad range of possible effects of cloud-aerosol interactions.

In recent years, the traditional hypothesis behind the lifetime effect has been questioned. Ackerman et al. (2004) showed that in a marine stratocumulus environment, the competing effects of drying due to increased cloud-top entrainment and the moistening due to suppressed precipitation decide the overall response of cloud LWP to aerosol perturbations. They showed that there is a decrease in LWP with increasing aerosols when dry air resides above the boundary layer and an increase in LWP under moister conditions at the boundary layer. High resolution simulations (Jiang and Feingold 2006; Jiang, H. Xue, et al. 2006; H. Xue and Feingold 2006; H. Xue, Feingold, and Stevens 2008) have suggested that the different collective effects which make up the lifetime effect do not always happen in unison: the LWP and the cloud fraction may increase or decrease based on meteorological conditions, and there are uncertainties in the effect of aerosol perturbations on cloud lifetime. The studies reveal the possibility of two regimes, one where the traditional hypothesis holds and aerosol increase suppresses precipitation and leads to an increase in LWP and cloud fraction, and a second regime (non-precipitating regime) where increases in aerosol concentration leads to a lower cloud fraction due to enhanced entrainment of subsaturated environmental air. This is primarily due to increased evaporation rate of the smaller droplets formed due to the increased CCN.

H. Xue and Feingold (2006) studied small trade cumuli and showed that an increase in aerosol concentration results in more efficient droplet evaporation and entrainment accompanied by a suppression of drizzle. In polluted clouds (clouds with increased aerosols/CCN), faster and stronger evaporation rates and stronger downdrafts lead to enhanced horizontal buoyancy gradients and vortical circulations (and hence the turbulent kinetic energy). This enhancement further drives droplet evaporation and a dynamic positive feedback is established which would

¹A measure of the weight of liquid water droplets in the atmosphere over a unit surface area of the earth, i.e. $\int \rho r_L dz$ where r_L is the liquid water mixing ratio (AMS Glossary)

decrease the cloud liquid water more than is possible with just the enhanced evaporation alone. The study suggests that this important effect has to be considered while studying the indirect aerosol effects in trade cumulus clouds. These results were also reinforced by numerical simulations by Jiang, H. Xue, et al. (2006) and observations by Small et al. (2009).

In this chapter, we aim to investigate this feedback mechanism using direct numerical simulations on an idealized model of the cloud edge. As mentioned in chapter 1, the complexity of the multi-scale dynamics at the cloud edges, coupled with the nonlinear thermodynamics of phase changes and droplet-turbulence/ droplet-droplet interactions, makes high resolution numerical studies quite difficult. Hence, we use a setup similar to chapters 4 and 5 where only a small region at the edge of a cloud is considered. However, in order to make the system more representative of real clouds, the growth of droplets through condensation as well as through collision-coalescence are included. Aerosol activation is not considered, but by varying the droplet radius and number density, we study the effect of initial Droplet Size Distributions (DSD) on the horizontal buoyancy gradient across the cloud edge.

A series of experimental (Good, Gerashchenko, and Warhaft 2012; Gerashchenko and Warhaft 2013) and numerical (Ireland and Collins 2012) studies have focused on the dynamics of inertial particles entrained across shearless mixing layers (which is considered as a paradigm for the cloud edge). However, these studies ignored the thermodynamic processes including phase changes between droplets and ambient air in order to focus on the effects of turbulence, Reynolds number, particle inertia and gravity on the entrainment. Turbulent mixing and entrainment at cloud edges can cause strong spatial and temporal fluctuations in both temperature and humidity. The supersaturation, which is responsible for the activation and condensational growth of cloud droplets, are affected by these scalar fluctuations. Additionally vertical air velocity fluctuations can also affect the local supersaturation. Each droplet then experiences different local supersaturation which results in differences in the droplet growth histories (Cooper 1989; Srivastava 1989).

Condensation is an important process in the early stages of the cloud evolution when the droplet sizes are of the order of a few microns and droplet growth through collision-coalescence is still not effective. Droplet growth through collision-coalescence becomes important once

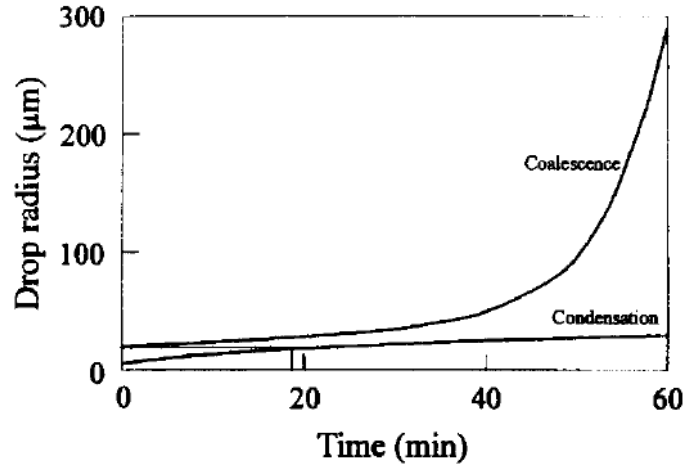


Figure 7.1: Calculated droplet growth by condensation and collision-coalescence in still air in a small cumulus with water content 1 gm^{-3} . A supersaturation of 0.2% and a collection efficiency of 1 is assumed. Figure reproduced from Jonas (1996) with permission.

droplets reach a radius of $30\mu\text{m}$. A classical problem in cloud microphysics is the condensation-collision size gap which refers to the growth of droplets in the size range $15 - 30\mu\text{m}$, where growth through neither condensation nor collision-coalescence is effective. Understanding this is important to help explain warm-rain initiation in 15-30 minutes (Szumowski et al. 1997; Knight, Vivekanandan, and Lasher-Trapp 2002). Figure 7.1 (reproduced from Jonas 1996) shows the calculated droplet growth by only condensation and only coalescence in a moderate cumulus cloud. Still air is assumed along with a supersaturation of 0.2% and a LWC of 1 g cm^{-3} . Droplet growth from a radius of $10\mu\text{m}$ to $20\mu\text{m}$ by condensation alone would take almost 20 minutes while growth from $20\mu\text{m}$ to approximately $100\mu\text{m}$ (drizzle drop size) would take around 1h. The combined growth time is much greater than the standard lifetime of a small cumulus cloud of around 30 minutes. A faster initiation of coalescence is necessary to explain observed values and it is also obvious that droplets cannot grow to drizzle size only by condensation.

Classical models involving adiabatic parcels gives a very narrow droplet size distribution since droplet growth through condensation is inversely proportional to radius. Such narrow distributions takes a long time to produce rain. However, a broad droplet size distribution such as that observed in both cumulus and stratocumulus clouds (Warner 1969a,b; Jonas 1996) could explain the fast growth of cloud droplets as it favours collision-coalescence. Multiple mechanisms have been proposed to explain the DSD broadening and the differences between models and observations: mainly the effect of small-scale turbulence which enhances collision

rates, the effect of giant CCNs at cloud base, and the entrainment and subsequent mixing of unsaturated air into the cloud core which can shrink or completely evaporate droplets and also introduce more CCN into the cloud. Using a large-eddy simulation model coupled with a sophisticated Lagrangian microphysical parcel model, Lasher-trapp, Cooper, and Blyth (2005) demonstrated that entrainment can produce differences in the supersaturation experienced by droplets and can lead to broadening of the droplet size distributions. A broad droplet size distribution was also demonstrated by Sidin, IJzermans, and Reeks (2009) using kinematic simulations of the velocity field coupled with a Lagrangian droplet growth model which accounts for the effects of latent heating and water vapor depletion. In addition to studying the effect of initial DSD on entrainment, the case setup to be used in this chapter provides the opportunity to study the evolution and possible broadening of the droplet size distribution with time due to entrainment. This is the second objective of this chapter.

Since the pioneering works of Vaillancourt, Yau, and Grabowski (2001) and Vaillancourt, Yau, Bartello, et al. (2002), DNS has been used to study the broadening of DSD by condensational growth of droplets. Studies have revealed the importance of large-scale turbulent eddies, small-scale fluctuations and the coupling between the supersaturation fluctuation and cloud droplet growth in isotropic homogeneous turbulence (Celani, Falkovich, et al. 2005; Celani, Mazzino, et al. 2007; Lanotte, Seminara, and Toschi 2009; Paoli and Shariff 2009) as well as at the cloud-environment interface (Kumar, Schumacher, and Shaw 2013, 2014; Götzfried et al. 2017; Kumar, Götzfried, et al. 2018). The studies also reveal a narrow droplet size distribution when droplets grow under condensation alone. There has been numerous studies on the effect of small-scale turbulence on collision rates (Franklin, Vaillancourt, Yau, and Bartello 2005; Franklin, Vaillancourt, and Yau 2007; Ayala, Rosa, L.-P. Wang, and Grabowski 2008; Rosa et al. 2013; S. Chen, Bartello, et al. 2016) and collision efficiencies (L.-P. Wang, Ayala, Kasprzak, et al. 2005; L.-P. Wang, Ayala, Rosa, et al. 2008; S. Chen, Yau, and Bartello 2018) as has been discussed in chapter 6. In most previous DNS studies of cloud droplet growth, condensational growth and collision-coalescence growth were treated separately. However, small-scale turbulence enhances collision rates even at sizes when droplet growth is dominated by condensation. This makes it necessary to consider the continuous growth of droplets as has been done by

Perrin and Jonker (2015), Gotoh, Suehiro, and Saito (2016), S. Chen, Yau, Bartello, and L. Xue (2018), and Saito and Gotoh (2018).

In this chapter, we combine the condensational growth of cloud droplets with collision-coalescence growth. Rather than an adiabatic cloud, we model the mixing at the cloud-edge and study the effect of the initial distribution on lateral entrainment and mixing. As droplets evaporate at the cloud-edge, the evolution of the DSD is also studied.

7.2 Simulations

7.2.1 Case setup

The case setup is similar to chapter 4 (figure 4.1) and simulates the temporal evolution of the mixing at the lateral edge of a cloud. The numerical domain is a two-layer cloud-environment system and the gravity vector is aligned in the vertical direction $\hat{z}$. Previous studies of cloud-edge mixing using DNS mainly included two types of setups: shearless mixing layers (Kumar, Schumacher, and Shaw 2013, 2014; Götzfried et al. 2017; Kumar, Bera, et al. 2017) and temporal plumes (Abma, Heus, and Mellado 2013; Perrin and Jonker 2015). Götzfried et al. (2017) considered two variants of the shearless mixing layers: one with background turbulence in both the cloud and environment layers (turbulence - turbulence systems) and the second with background turbulence in only the cloud layer (turbulence - non-turbulence systems). The cloud layer is negatively buoyant (dissipating cloud) in both cases. The temporal plume models in Perrin and Jonker (2015) and Abma, Heus, and Mellado (2013) consists of a quiescent environment layer. The cloud layer is neutrally buoyant in Perrin and Jonker (2015) and positively buoyant in Abma, Heus, and Mellado (2013). In this chapter, two types of temporal plume setups are considered : the first has a quiescent environment (as in Perrin and Jonker (2015) and chapter 4) and the second has background turbulence in both the cloud and environment layers. In both setups, the cloud layer is positively buoyant and has a positive updraft vertical velocity (actively growing), while the buoyancy is defined to be zero in the environment. The scalars used to represent the cloud-environment thermodynamics are the potential temperature θ (equation (2.3)), and the specific humidity q_v (equation (2.4)). Water droplets are initially

Table 7.1: Parameters for different turbulent-non turbulent and turbulent-turbulent simulations.

Sim No	k_2/k_1	$R(\mu m)$	N_p	Re_λ
TNT20	0/0	20	40×10^6	74.2
TT20	0.5	20	40×10^6	83.2
TNT15	0/0	15	95×10^6	71.3
TT15	0.5	15	95×10^6	93.4

seeded into the cloud layer and tracked in a Lagrangian frame of reference while allowed to grow or shrink depending on the background supersaturation. The liquid water mass fraction q_l can then be calculated by counting the number of droplets in each grid cell.

The governing equations include the incompressible conservation equations of mass (equation (4.1a)) and momentum (equation (4.1b)), coupled with the transport equations for temperature (equation (3.17a)) and moisture (equation (3.17b)) are solved. The condensation rate C_d is calculated using equation (3.16). The buoyancy is calculated by expressing equation 4.3 in terms of q_v

$$b = \frac{\theta - \theta_0}{\theta_0} + \left(\frac{R_v}{R_d} - 1 \right) (q_v - q_{v,0}) - q_l, \quad (7.1)$$

where θ_0 and $q_{v,0}$ are the environmental temperature and specific humidity respectively.

The equations of motion of inertial particles given by equation 2.21 are solved to advance the droplet positions and velocities in time. The droplet growth (shrinking) through condensation (evaporation) is governed by equation 2.22. The numerical details of solving these equations have been given in section 3.4. The collision algorithm described in section 3.5 is used to detect collisions. Once a collision is detected between a droplet pair within a particle time-step, coalescence is implemented using equations 2.31, 2.32 and 2.33.

7.2.2 Simulation Details

The system with background turbulence in the cloud and environment will be referred to as the Turbulence-Turbulence (T-T) simulations, and the temporal plume setup with a quiescent environment is referred to as the Turbulence-Non-Turbulence (T-NT) simulations. Four different

simulations are performed as shown in table 7.1. The velocity fields in the cloud and environment layers are initialized with velocity fields of isotropic homogeneous turbulence of two different intensities. The isotropic homogeneous turbulence is generated using the wind-tunnel grid setup in chapter 6. A bigger domain (than that considered in chapter 6) of dimensions $2m \times 1.016m \times 0.508m$ is used, and a simulation for $t = 1.5s$ is performed without inertial particles to generate three-dimensional fields of the three velocity components at different times. Since the grid-generated turbulence decays, the magnitude of the TKE and dissipation rate reduces with time. The velocity fields at $0.6s$ and $0.9s$ are used as the initial velocity fields for the cloud and environment layers for the T-T simulations. A top-hat profile for the cloud vertical velocity component $w_c = 0.4ms^{-1}$ is then superimposed on this velocity field. For the T-NT simulations, the initial condition for the velocities includes setting $w_c = 0.4ms^{-1}$. The temperature and water vapor fields are initialized with similar top-hat profiles with values shown in figure 7.2a. The diagnosed profiles of the resulting initial buoyancy b and supersaturation S is shown in figure 7.2b. The ratios of the turbulence intensities in the cloud layer (k_1) and the environment layer (k_2) for the T-T simulations are shown in table 7.1. The initial mean dissipation rate $\bar{\epsilon}$ is $5 \times 10^{-2}m^2s^{-3}$ in the cloud layer and $9 \times 10^{-3}m^2s^{-3}$ in the environment layer.

The simulations are performed on a domain $2m \times 1.016m \times 1.016m$. The cloud layer extends up to $L_c = 0.508m$ in the cross-stream direction $\hat{x}$. A monodisperse distribution of droplets of radius, $R = 15\mu m$ and $R = 20\mu m$, are considered in this chapter. The Taylor Reynolds number Re_λ at the end of the simulation is also given in table 7.1. Also shown are the number of particles N_p initially seeded homogeneously in the cloud layer across the $\hat{x}$, $\hat{y}$ and $\hat{z}$ directions, i.e. within a volume bounded by $[0, 0.508m]$, $[0, 1.016m]$ and $[0, 2m]$ respectively. The resulting droplet density N_d is $58cm^{-3}$ for $R = 20\mu m$ and $93.5cm^{-3}$ for $R = 15\mu m$. To put these numbers in perspective, the usual cloud droplet concentrations are of the order of $40 cm^{-3}$ in clean marine clouds and $320 cm^{-3}$ in continental clouds. The kinematic viscosity ν is $1.5 \times 10^{-5}m^2s^{-1}$.

The initial distributions are homogeneous in the $\hat{y}$ and $\hat{z}$ directions and periodic boundary conditions are imposed along these directions. All simulations are performed for $8s$. All statistics are performed over $t_{stat} = 2s$.

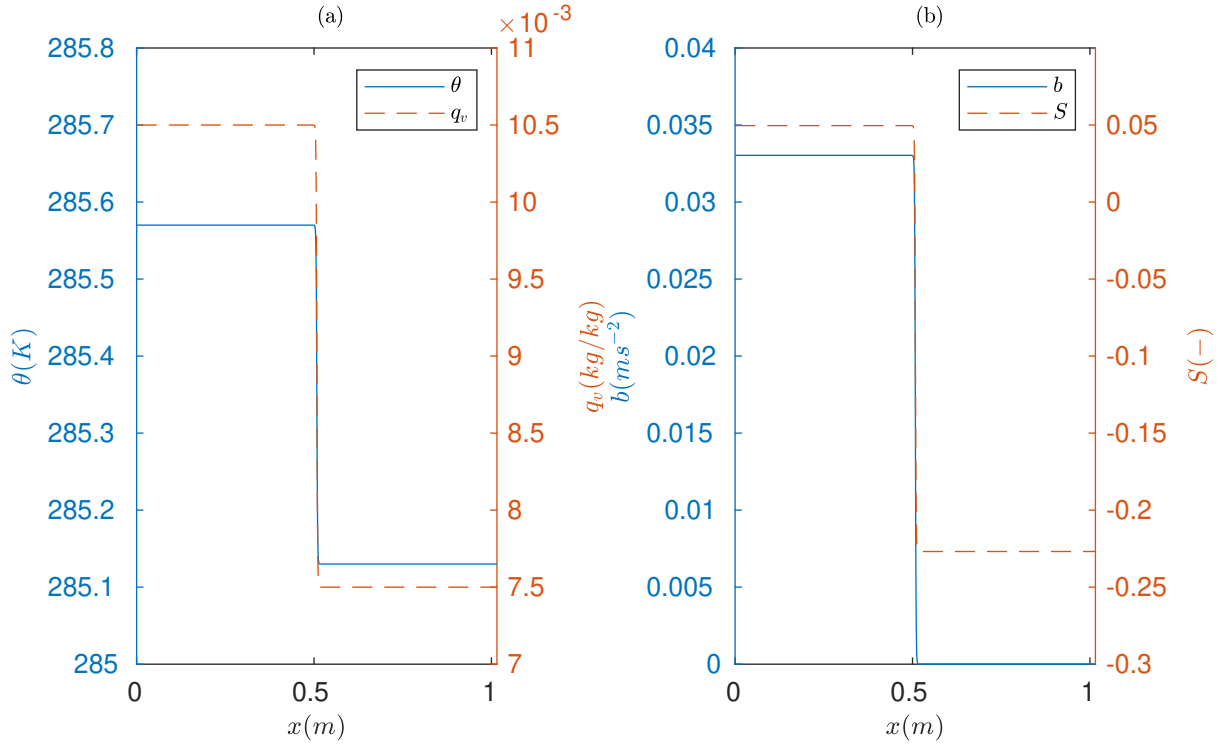


Figure 7.2: Initial profiles for TNT simulations. (a) Prognostic variables θ and q_v , (b) diagnosed profiles of buoyancy b and Supersaturation S .

7.3 Results

7.3.1 Cloud-edge mixing

In this section, we analyse the mixing at a cloud-environment interface focusing on the effect of the turbulence in the environment layer and the effect of initial droplet size distributions. Figure 7.3 shows the instantaneous buoyancy at $t = 8s$ for simulations TT20 and TNT20. Simulations TNT20 and TT20 have the same number density and droplet diameter, but differ in the background turbulence intensities in the cloud and environment. The slices for the buoyancy are taken at a span-wise distance $\hat{y} = 1m$. Entrainment and mixing of the environmental air results in the droplets at the interface being subjected to sub-saturated air. These droplets shrink and the resulting evaporative cooling leads to the formation of a negatively buoyant shell as was explored in detail in chapters 4 and 5. Overall, both plots are visually representative of inhomogeneous mixing where a subset of droplets at the cloud edge evaporate while those in

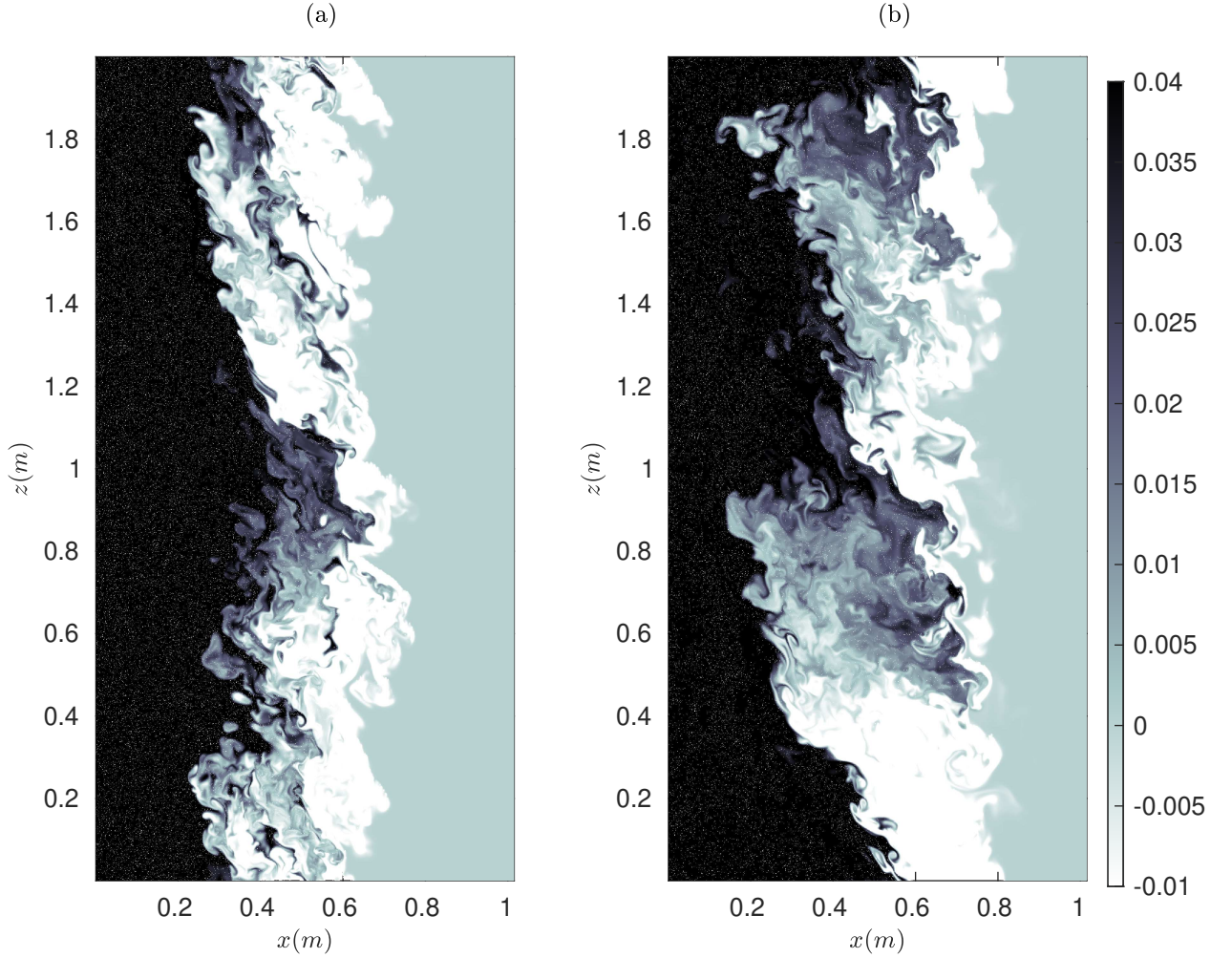


Figure 7.3: Instantaneous buoyancy b at $y = 1m$ at $t = 8s$ for (a) TNT20 and (b) TT20.

the adiabatic cloud core are untouched ² (Lehmann, Siebert, and Shaw 2009).

The shell formation and growth is significantly faster for TT20 compared to TNT20 as seen in figure 7.3. The shell has extended to almost the end of the domain for TT20 at $t = 8s$. The turbulent nature of the environment can help explain this difference. As mentioned in Götzfried et al. (2017), detrained droplets decelerate quite suddenly in a quiescent environment (as in TNT20) due to the high Turbulent Kinetic Energy (TKE) gradient across the interface. Gravity takes over and droplets are decoupled from the underlying flow and fall freely vertically downwards through the unsaturated environment. In TT20, turbulent fluctuations in the environment perturbs the vertically straight trajectories of sedimenting droplets. The droplets are horizontally advected further in the environment and they also decelerate much slower due

²The alternative is homogeneous mixing where all the droplets experience nearly the same sub-saturation and shrinks towards smaller sizes until equilibrium is reached. In this case the entire DSD shifts towards smaller diameters.

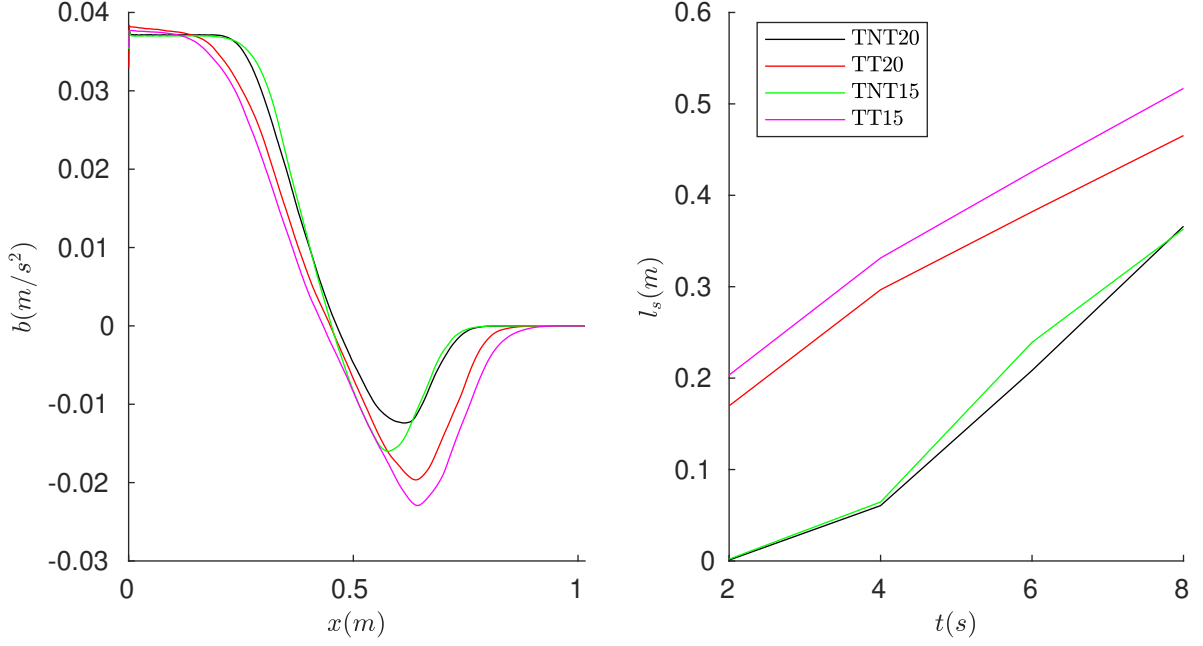


Figure 7.4: (a) Mean buoyancy at $t = 8s$ for simulations TNT20 (black), TT20 (red), TNT15 (green) and TT15 (magenta). (b) Shell thickness l_s for the same simulations.

to the smaller gradient in the velocity fluctuations.

7.3.2 Effect of initial droplet distribution

The mean buoyancy ($\bar{b}$) profiles at $t = 8s$, and the time evolution of the mean shell thickness $l_s = x_b^+ - x_b^-$ are plotted for the four simulations: TNT20 (black), TT20 (red), TNT15 (green) and TT15 (magenta), in figure 7.4. Simulation TT15, with droplets of radius $R = 15\mu m$ and $N_d = 93.5cm^{-3}$ has the strongest shell in terms of the minimum magnitude of $\bar{b}$ as shown in figure 7.4a. This is consistent with the hypothesis that increased evaporation of a larger number of smaller droplets at the cloud edge results in a stronger horizontal buoyancy gradient (Jiang, H. Xue, et al. 2006; Small et al. 2009). The shell in TT15 also has the maximum thickness across the duration of the simulation as shown in figure 7.4b where it has grown to almost $0.55m$ in $8s$. The lowest value of the magnitudes of the shell buoyancy minimum and thickness is in simulation TNT20.

The two simulations with a non-turbulent environment, TNT20 and TNT15, have a similar shell thickness with TNT15 exhibiting a slightly thicker shell between $t = 4 - 8s$. However, TNT15 does show a stronger negative shell buoyancy than TNT20. The T-T simulations have a consistently wider shell than the T-NT simulations. The rate at which the shell grows is

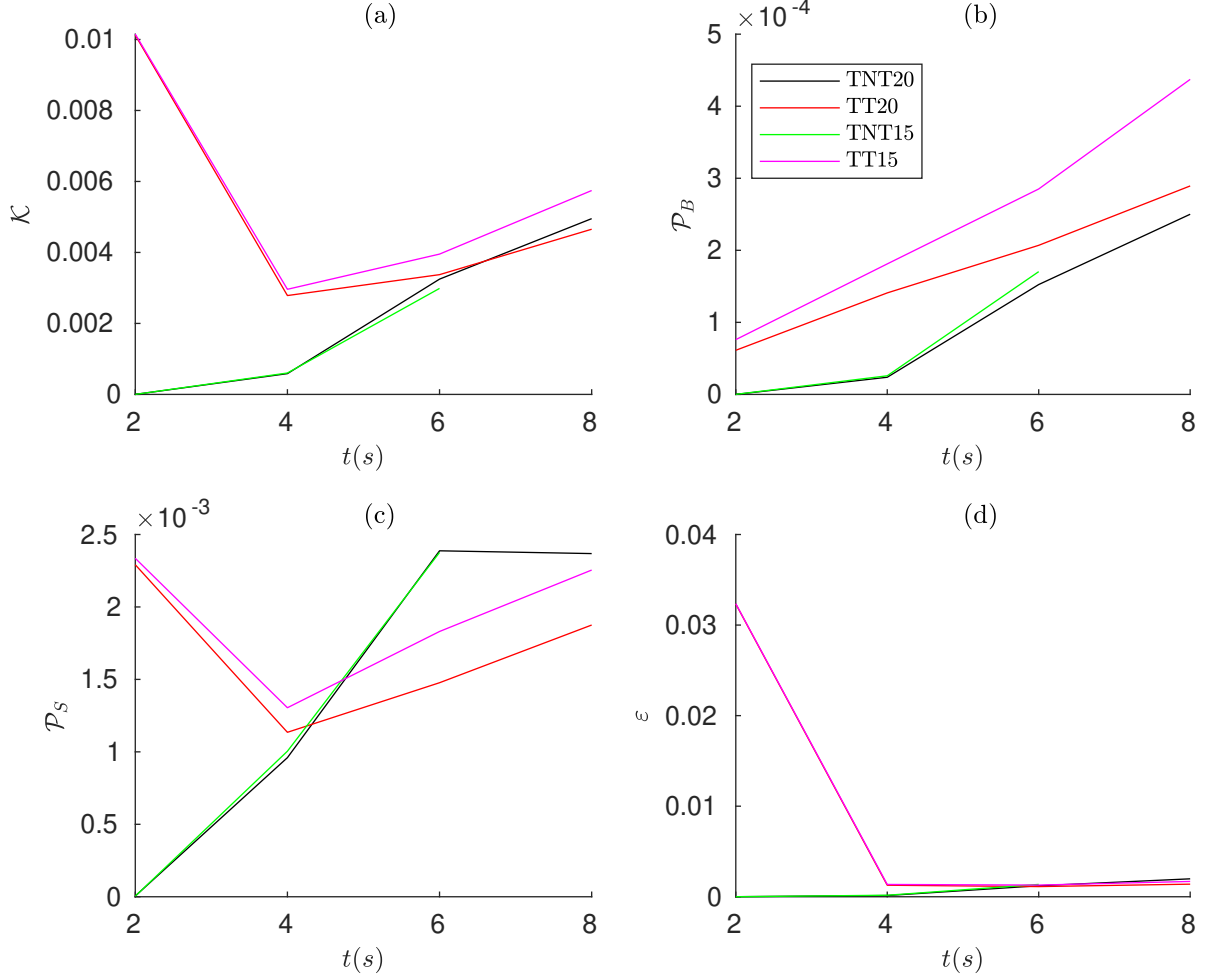


Figure 7.5: TKE budget terms for simulations TNT20 (black), TT20 (red) and TT15 (magenta). (a) turbulent kinetic energy ($\overline{K}$) (b) Buoyancy production: $\mathcal{P}_B$, (c) shear production: $\mathcal{P}_S$ and (d) dissipation rate: ε .

similar for both the T-T simulations and both the T-NT simulations irrespective of the droplet radius. However the growth rate is slower for the T-T case after 4s following an initial growth spurt. The reverse is true for the T-NT simulations with a initial slow growth rate, followed by a linear growth rate which is larger than the growth rate for T-T cases. This points to a higher entrainment rate for the T-NT case compared to the T-T case and is consistent with the results in Kankanwadi and Buxton (2020). An analysis of the mean turbulence shear production P_S shows a high and very steep gradient at the interface at $t = 4s$ time for T-NT simulations. More energetic Kelvin-Helmholtz vortices are formed at the interface resulting in more aggressive transition and mixing, causing more droplet evaporation and a higher rate of shell growth. Compared to T-NT simulations, the T-T simulations have a higher value of P_S at $t = 2s$ after which the gradients are much more gradual.

To explore the dynamical feedback, the budget for the integral Turbulent Kinetic Energy

(TKE) $\mathcal{K}$ is analysed next (figure 7.5). The integral TKE budget is obtained by integrating equation 4.10 over L_x and is given by

$$\frac{\partial \mathcal{K}}{\partial t} = \mathcal{P}_S + \mathcal{P}_B - \varepsilon \quad (7.2)$$

where $\mathcal{K} = \int_0^{L_x} k \, dx$, $\mathcal{P}_S = \int_0^{L_x} P_S \, dx$, $\mathcal{P}_B = \int_0^{L_x} P_B \, dx$ and $\varepsilon = \int_0^{L_x} \varepsilon \, dx$ is analysed next to explore the dynamical feedback (figure 7.5). At $t = 2s$, the TKE in TT20 and TT15 (figure 7.5a) is significantly higher than TNT20 and TNT15 due to the initial background turbulence. The high initial values of ε (figure 7.5d) leads to the background turbulence in the cloud layer dissipating quickly as seen by the initial rapid decay of $\mathcal{K}$ (figure 7.5a) for TT20 and TT15. There is a steady increase in $\mathcal{K}$ from $2s$ to $8s$ from turbulence shear and buoyancy productions which will be analysed next.

The effect of evaporative cooling on the TKE ($\mathcal{K}$) is captured by the buoyancy production term $\mathcal{P}_B = \overline{w'b'}$ as shown in figure 7.5b. The negative buoyancy and the resulting downdrafts lead to a net positive contribution of $\mathcal{P}_B$ to $\mathcal{K}$ ($b' < 0, w' < 0$). The turbulence in the environment is responsible for the difference in $\mathcal{P}_B$ between T-T and T-NT simulations since droplets tend to remain in the environment longer. Comparing TT20 and TT15, $\mathcal{P}_B$ is maximum for TT15 which reinforces the fact that more droplets of $R = 15\mu m$ evaporate due to mixing, compared to the droplets of $R = 20\mu m$ in TNT20. This also helps explain the strongest shell (in terms of negative buoyancy) in TT15 and the weakest in TNT20.

The downdrafts formed due to the negatively buoyant shell results in the generation of a shear layer at the interface, and this is reflected in the upward trend of the shear production term $\mathcal{P}_S$ for TNT20 from $t = 2s$. The initial downward trend for the T-T simulations points to the reduction in the gradients of the vertical velocity across the two layers as the turbulence decays. Once the downdrafts are established in the T-T simulations after approximately $4s$, there is a steady increase in $\mathcal{P}_S$ till the end of the simulation. Consistent with higher values of $\mathcal{P}_B$, the magnitude of $\mathcal{P}_S$ is higher for TT15 compared to TT20.

The integral dissipation rate of the velocity fluctuations ε is shown in figure 7.5d. For the T-T simulations, the high values of ε decrease as the TKE decays. As the simulations

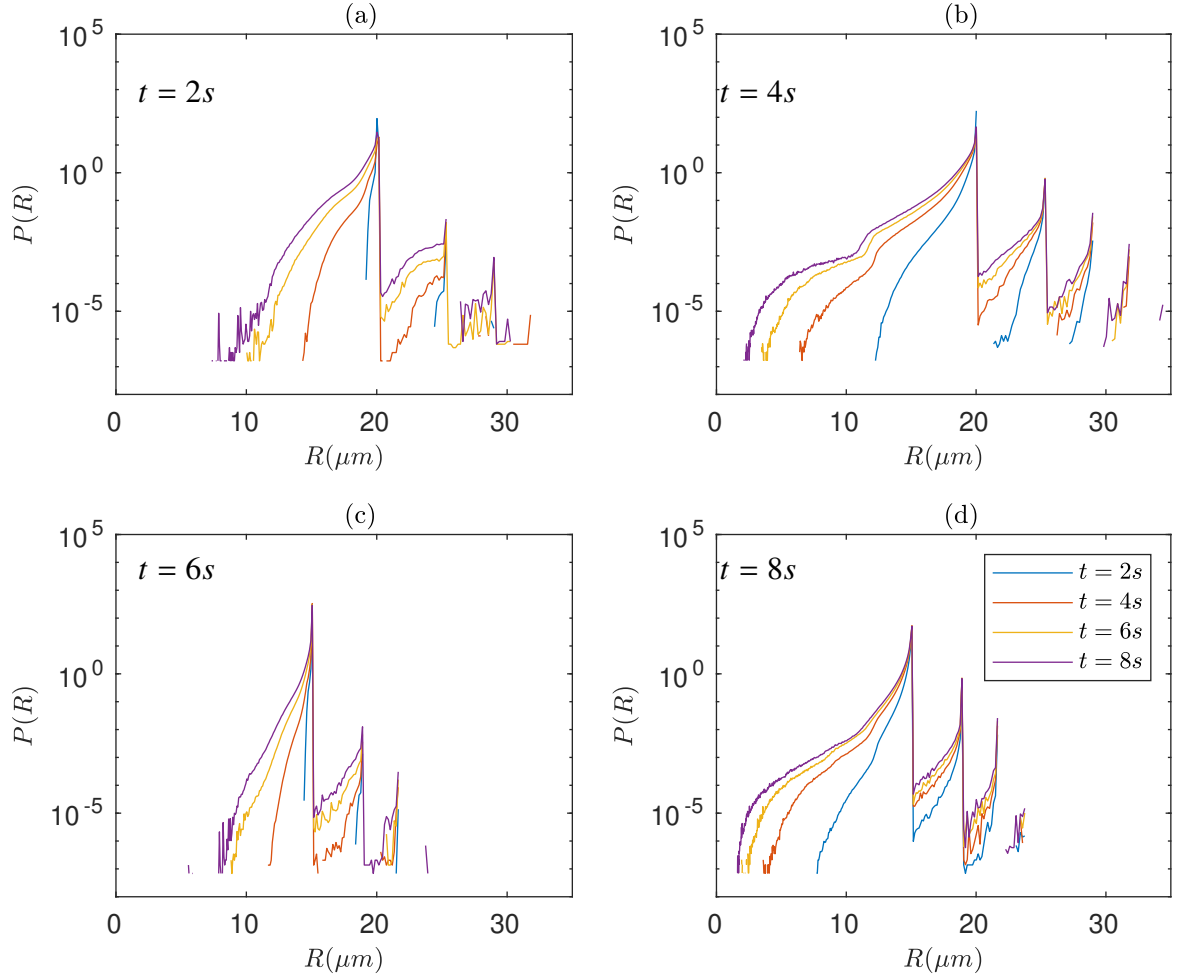


Figure 7.6: (a) Time evolution of the droplet size distributions for simulations (a) TNT20, (b) TT20, (c) TNT15 and (d) TT15.

progress, higher gradients in the velocity fluctuations result in the ε for TNT20 overtaking those for the T-T simulations. There is a steady increase in the ε for the T-NT simulations as seen in Perrin and Jonker (2015) while the values remain steady and almost a constant for the T-T simulations. TT15 has a slightly higher value than TT20 which points towards increased small-scale fluctuations due to more droplets evaporating.

The dynamic feedback can be seen when figures 7.5a, b, c and d are analysed together. Greater evaporation of droplets in TT15 results in an increase in $\mathcal{P}_B$ and a horizontal buoyancy gradient is established. This gradient and the resulting downdrafts leads to an increased shear contribution $\mathcal{P}_S$. The steadily increasing production terms with an almost constant values for ε leads to a steady increase in TKE which further enhances entrainment leading to further evaporation. The positive dynamic feedback is hence established in both T-NT and T-T simulations.

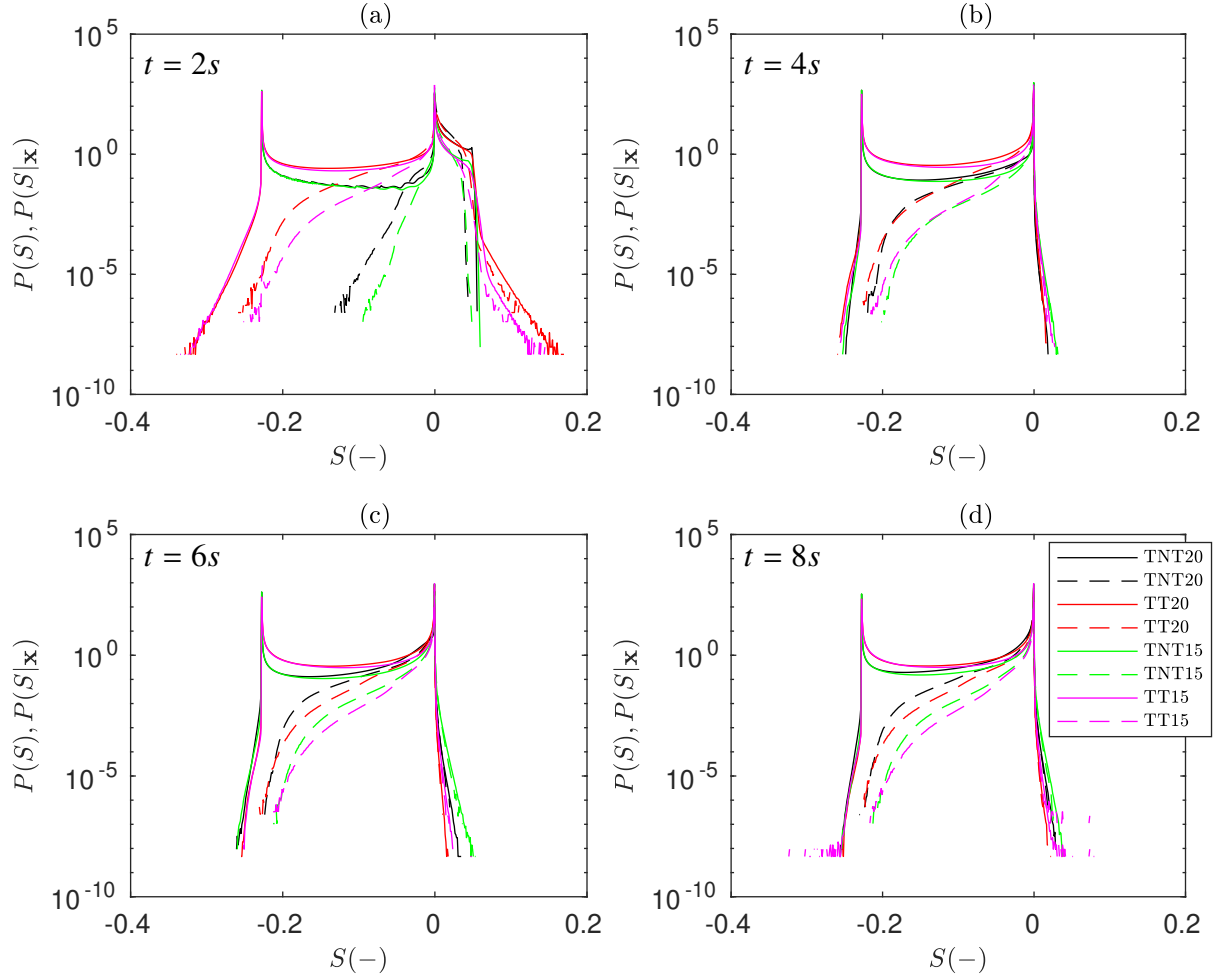


Figure 7.7: PDF of the supersaturation S conditionally sampled on the droplet locations (dotted lines) at (a) $t = 2s$, (b) $t = 4s$, (c) $t = 6s$ and (d) $t = 8s$ for simulations TNT20 (black), TT20 (red), TNT15 (magenta) and TT15 (green). Also shown are the PDFs of the supersaturation in the numerical domain (solid lines) at the respective times for the same simulations.

7.3.3 Droplet size distributions

In this section, we look at the evolution of the Droplet Size Distribution (DSD) for the different simulations. Figure 7.6 shows the time evolution of the probability density functions (pdfs) of the droplet radii in the numerical domain for the simulations TNT20 (figure 7.6a), TT20 (figure 7.6b), TNT15 (figure 7.6c) and TT15 (figure 7.6d). The left tail of the DSD represents the shrinking of droplets due to evaporation. For the same radius, the T-NT simulations have a much narrower DSD than the T-T simulations. One of the reasons for this could be the fact that the droplets in the T-T simulations experience more negative supersaturation than those in T-NT simulations (to be analysed later in the section). As is the case for the droplets, the scalar filaments are advected further in the environment in the case of the T-T simulations. When

the vapor fluctuations decay below the saturation value, the droplets in those locations start shrinking.

Due to the small magnitudes of positive supersaturation in the domain, droplets do not experience significant amount of excess water vapor diffusing onto their surface. The DSD peaked for a simulation without collision-coalescence (not shown) at $20.2\mu m$ with no broadening of the DSD to the right. Hence we conclude that the right tail of the DSD indicates droplet growth through collision-coalescence. Turbulence-enhanced collisions (Franklin, Vaillancourt, Yau, and Bartello 2005; Franklin, Vaillancourt, and Yau 2007; Ayala, Rosa, L.-P. Wang, and Grabowski 2008) in T-T simulations result in a broader right tail for the DSD and an extra pronounced peak in figures 7.6(b) and (d) compared to the T-NT simulations. TT20 has a much broader right tail compared to TT15. As was also seen in Perrin and Jonker (2015), a larger initial droplet radius is highly favorable for collisions with the resulting DSD becoming more broader. Larger settling droplets can collect more smaller droplets especially with the simplified collision-coalescence model considered here where the collection efficiency is set to be 100%.

Comparing the effect of initial droplet sizes, simulations TNT15 and TT15 have a narrower DSD (figures 7.6c and d) compared to TNT20 and TT20 (figures 7.6a and b), respectively. Smaller droplets have a smaller evaporation time scale³ (faster phase transition) which allows the flow and droplets to reach a thermodynamic equilibrium quickly (Perrin and Jonker 2015). This means that smaller droplets are more likely to reside in regions of less unsaturated air (less negative supersaturation).

Figure 7.7 shows the pdfs of the supersaturation values conditionally sampled on the droplet locations (dashed lines) and the grid cells (solid lines) for the four simulations. The values are also averaged over 2s. Figure 7.7a clearly shows that the T-T simulations enjoy a much higher negative supersaturation in the first 2s. The enhanced initial entrainment and mixing due to the background turbulence in the cloud and environment layers in the T-T simulations results in more sub-saturated environmental air being mixed with the saturated cloudy air leading to more negative values for the supersaturation. This helps explain the narrow DSD for T-NT simulations compared to T-T simulations. The pdfs over the first 2s also suggest that the droplets

³single droplet evaporation scale is given by $\tau_{ev} = \frac{r^2}{2KS}$

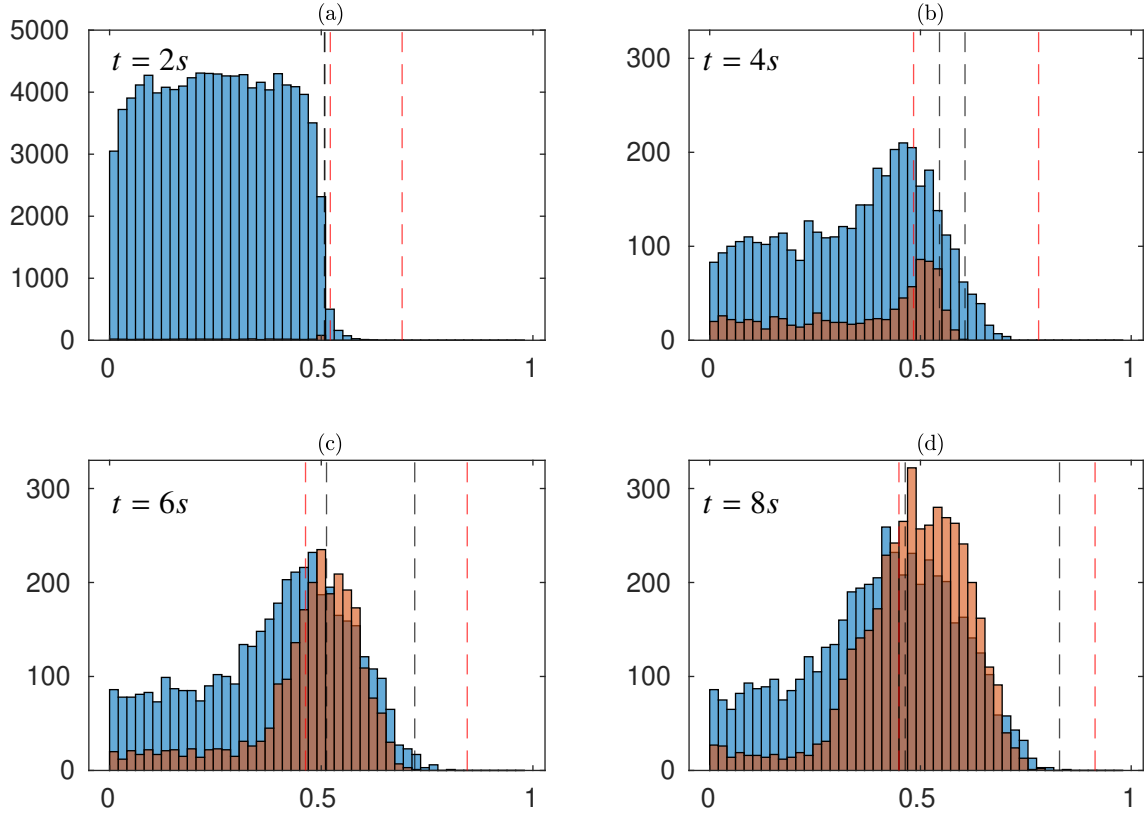


Figure 7.8: Number of collisions in the domain counted cumulatively every $2s$ and plotted as a function of the $\hat{x}$ coordinate for simulations TNT20 (orange) and TT20 (blue) at $t =$ (a) $2s$, (b) $4s$, (c) $6s$, and (d) $8s$. The black and red dashed lines show the inner and outer boundaries of the shell at the corresponding times for simulations TNT20 and TT20 respectively.

in the two T-T simulations experience a much broader magnitude of negative supersaturation due to the enhanced entrainment (red and pink dashed lines).

Comparing the grid values of supersaturation in the T-NT and T-T simulations for the same radius (black vs red and green vs magenta solid lines), it is clear that due to enhanced mixing in the T-T simulations, there are more grid cells with negative supersaturation, and accordingly, more droplets experiencing negative values of supersaturation. As mixing and entrainment proceeds, the droplets in the T-NT simulations (black and green dashed lines) start experiencing a broader range until the two left tails have the same range. At the end of the simulation, more droplets in the T-NT simulations experience a negative supersaturation.

Also, for all the plots in figure 7.7, the negative supersaturation experienced by the droplets for TT20 (dashed red) is always broader than TT15 (dashed magenta) which confirms that the smaller droplets are more likely to reside in regions of less unsaturated air.

Figure 7.8 shows the cumulative number of collisions between droplets in the domain (along

the $\hat{x}$ axis) over every $2s$. The histograms are plotted on the $\hat{x}$ coordinate for TNT20 (orange) and TT20 (blue) at (a) $t = 2s$, (b) $t = 4s$, (c) $t = 6s$ and (d) $t = 8s$. Also shown are the boundaries of the shell at these times x_b^- and x_b^+ (black dashed lines for TNT20 and red dashed lines for TT20). For TNT20, the number of collisions increases as the shell develops. A very high percentage of these collisions occur in the visible part of the shell and the part of the cloud core adjoining the shell. The highly turbulent nature of these regions are responsible for the increased number of collisions here. However, in stark contrast, collisions occur across the cloud layer in TT20. The initial TKE in the cloud layer leads to enhanced collisions in this region in the first $2s$. This could also explain the broader right tail of the DSD for the T-T simulations. As the TKE decays in the cloud layer, the number of collisions reduce in the cloud layer. However with the shell developing, the number of collisions simultaneously increases in the shell and adjoining cloud regions for later times. Detailed analyses to quantify the turbulence enhanced collision-coalescence in the shell region (increase in relative velocities and clustering processes) will be done in future studies.

7.4 Concluding remarks

The effect of initial droplet size distributions on the strength of the subsiding shell at the edges of shallow cumulus clouds is investigated. Direct numerical simulations are performed to study the temporal mixing at the cloud-environment interface. Two sets of simulations are performed: turbulence-turbulence setups with background turbulence in the cloud and environment, and a temporal plume setup with a quiescent environment. A positively buoyant cloud layer is considered in both setups to mimic an actively growing cloud. A monodisperse distribution of droplets of size $R = 15\mu m$ and $20\mu m$ are seeded in the cloud layer initially. Evaporation of droplets due to entrainment leads to cooling and the formation of a subsiding shell which grows with time.

Turbulence in the environment leads to droplets detrained into unsaturated filaments staying in the environment for a longer time. Droplets are advected further in a turbulent environment while in a quiescent flow, settling droplets are free to follow a vertically downward trajectory.

The initial shell formation and growth is significantly faster for simulations with turbulence in the environment. As a result, these simulations also have a thicker shell at the end of the simulations compared to T-NT simulations. After an initial slow growth rate, the growth rate of the shell in the T-NT simulation increases linearly.

A stronger shell, in terms of the negative buoyancy, is established in TT15. In TT15, a larger number of smaller droplets ($R = 15\mu m$ compared to TT20 with $R = 20\mu m$) evaporate, leading to a higher buoyancy contribution to TKE production. The weakest shell is produced in TT20 at the end of the simulation. A dynamical positive feedback is established where the droplet evaporation increases the mean TKE. The increased TKE in the system drives further entrainment of unsaturated air leading to more evaporation.

The droplet size distribution is narrow for T-NT simulations compared to T-T simulations. Droplets in the T-T simulations experience a broader range of negative supersaturation. Also, smaller droplets are more likely to reside in less unsaturated areas due to their smaller evaporation time scale. Hence simulations with initial droplet radius $R = 15\mu m$ have a narrower DSD compared to those with $R = 20\mu m$.

Droplet growth through water vapor diffusion is not significant due to the small magnitudes of positive supersaturation in the cloudy domain. Growth by collision-coalescence is maximum for TT20 as a larger initial droplet radius can collect more smaller droplets. A broader right tail and an extra peak is observed in the DSD for the TT20 simulation compared to TT15. A narrow DSD as in TT15 is not conducive for collision-coalescence as is evident in the narrow right tail compared to TT20. The T-T simulations have a high number of collisions in the cloud region in the first 2s as a result of the background TKE. For both T-T and T-NT simulations, as the shell forms and thickens, the collisions peak in the near shell region which includes the visible part of the shell and the adjacent cloud core region.

The setups in chapters 4 and 5 included a volumetric forcing in the cloud layer to prevent the formation of a highly transient mixing layer. However, nudging the cloud layer using droplets would be highly expensive and the analysis in this chapter is performed on a highly transient shell region. Also, the study is highly idealized and the applicability of the results to actual clouds comes with a few caveats. The domain size is quite small and this means that the range

of spatial and temporal scales considered in this study is limited. Additionally, temperature lapse rate or pressure variations with height is not considered. A monodisperse distribution of droplets is considered initially. A polydisperse distribution would be more realistic and is the next logical future step in this study. Additionally a collection efficiency of 100 % and the lack of separate treatment for droplet-droplet interactions also adds to the idealization.

Chapter 8

Conclusions

In this thesis, the interaction between mixing and entrainment at the cloud edge, and the dynamics of particles/droplets is investigated. Detailed conclusions and discussions have been presented in each chapter; some of the key findings and contributions of the thesis are summarized here.

8.1 Summary

8.1.1 Case-setups and Methodology

Direct numerical simulations (DNS) capture small-scale features of the flow as they resolve scales down to the Kolmogorov scale. In this thesis, the DNS code SPARKLE was extended with a hybrid Eulerian-Lagrangian method: the flow velocities and thermodynamic scalars are represented on an Eulerian grid and the particles/droplets are treated using a Lagrangian frame of reference. A new canonical setup was developed whereby a developing, positively buoyant temporal plume is used as a paradigm for a small portion of the edge of a cloud. The cloud-edge mixing is represented as close to real-life clouds as possible, and this includes an actively growing cloud, the negatively buoyant subsiding shell and an environment. Three variants of the setup are used: in combination with a volumetric forcing term, the setup is used to characterise the dynamic growth of the shell in chapter 4. A new bulk condensation scheme was implemented in SPARKLE to represent the cloud thermodynamics for this analysis. By introducing tracer particles, the dynamics of particles crossing the different interfaces at the

lateral edge of a cloud was studied in chapter 5. A Lagrangian particle tracking routine, which includes particle interpolation, integration and communication (originally developed by Perrin and Jonker 2015) routines, was implemented and validated in SPARKLE for this study. In chapter 7, more realistic conditions were created with droplets introduced in the cloud layer and background turbulence in the environment layer. The correlation between initial cloud droplet sizes and entrainment-mixing was studied. For this analysis, a complete microphysics routine with droplets growing (shrinking) through condensation (evaporation) and growing through collision-coalescence, was implemented.

A different, but novel setup was implemented in chapter 6. Gravity plays an important role at the lateral edge of the cloud since heavier droplets at the cloud boundaries can settle out into the environment and evaporate. Also, larger settling droplets can grow by colliding and coalescing with smaller droplets. The aim of this chapter was to study the effect of gravity on the important phenomenon of preferential concentration in inertial particles in a simpler setting with homogeneous, isotropic turbulence. Drawing inspiration from grid-generated decaying turbulence in wind tunnels, a temporal setup was developed which simulated the flow at the exit of a grid and follows it in time. This is analogous to following a fluid blob as it exits the active grid and moves downstream along the wind-tunnel. Isotropic, homogeneous turbulence was generated and the effect of gravity on particle clustering and geometric collisions was studied. The setup also allows comparisons with data from wind-tunnel experiments.

8.1.2 The subsiding shell

Numerous LES and cloud-resolving model studies on the generation and impact of the subsiding shell on entrainment and detrainment rates can be found in literature. In this thesis, a systematic DNS study of the dynamics of the subsiding shell at the lateral edge of an actively growing cloud was performed. Scales down to the Kolmogorov scales were resolved and an improved understanding of the small-scale features of the flow in the shell was obtained. Bridging the turbulence community and the atmospheric science community, integral relations originally developed for axisymmetric free shear flows was used to characterise entrainment at the cloud edge in the presence of a subsiding shell.

Entrainment across the shell was investigated using DNS and Lagrangian particles for the first time. Four flow zones were identified at the cloud edge: the cloud core, visible shell, invisible shell and the environment. The interfaces between these zones were identified and the impact of choosing the correct interface for entrainment studies was highlighted. These interfaces were named the cloud core boundary, visible shell boundary and Turbulent-Non Turbulent Interface (TNTI). The TNTI, which we identify between the subsiding shell and the environment, is often neglected in LES cloud studies. This is a key finding and detecting this interface by applying thresholds on the enstrophy is a novel method. We also confirmed the mechanism of preferential entrainment originally identified by Dawe and Austin (2011) in LES studies.

8.1.3 Particle clustering and gravity

Inertial particles tend to preferentially concentrate or cluster in regions of low vorticity and high strain rate in turbulent flows. Particle clustering can lead to increased collision rates which is crucial in clouds. The role of gravity on clustering has not been extensively studied so far. In chapter 6, a comprehensive study of the role of gravity in a polydisperse distribution of droplets in isotropic homogeneous decaying turbulence was performed. The radial distribution function was used to quantify clustering and analysis revealed that gravity suppresses clustering in sedimenting droplets due to reduced droplet-turbulence interaction times. A comprehensive analysis of the RDF calculated from DNS showed very good agreement with analytic predictions for both non-sedimenting and sedimenting droplets. The kinematic collision kernel for the polydisperse distribution was calculated. Gravity reduces the collision kernel for collisions between same-size droplets and causes a significant increase in the kernel magnitude for unequal sized droplets.

8.1.4 Entrainment and droplet growth

In chapter 7, the effect of aerosol perturbations on cloud properties was studied using DNS by varying the initial droplet size distributions in the cloud layer. An increase in aerosol concentration in clouds leads to a higher droplet number concentration and a reduced mean

droplet radius. Different aerosol concentrations were simulated by varying the initial size distribution of droplets, and the resulting effect of entrainment on the droplet size distributions and shell strength was investigated. A background turbulence was imposed in the cloud and environment layers to make the setup more realistic.

Simulations revealed a dynamical positive feedback where enhanced evaporation due to an increased concentration of smaller droplets (as a result of increased aerosols) enhanced the evaporation at the cloud edge. This increased the turbulent kinetic energy which drives further entrainment causing further evaporation of droplets. The resulting droplet size distribution was found to be broader for initial size distributions with a smaller droplet radius (higher aerosol concentration). A broader droplet size distribution was conducive for the growth of droplets through collision-coalescence up to drizzle size, and could help explain the discrepancies between the time taken for warm rain initiation in observations and numerical models. Comparisons with simulations with a quiescent environment showed that there was enhanced entrainment due to the additional TKE at the interface mixing layer. This resulted in a broader droplet size distribution and a stronger positive feedback compared to a quiescent environment.

8.2 Concluding remarks

The complex interactions between small-scale turbulence, thermodynamics and microphysics at the cloud edge have been demonstrated in this thesis. From generating a subsiding shell, to broadening of droplet size distributions, the role of lateral entrainment cannot be overstated in shallow, warm clouds. An attempt has been made to correlate the process of lateral entrainment across cloud-environment interfaces and the behaviour of particles and droplets (including sizing and spatial distributions).

The generation of the subsiding shell has been recognized in literature since the early 90's. A very clear picture of the mixing at the lateral cloud edge has emerged from chapters 4,5 and 7 in this thesis. Droplets evaporating at the cloud edge results in evaporative cooling and the formation of a horizontal buoyancy gradient across the cloud edge. All evidence points towards a buoyancy driven shell, with an increased contribution of the buoyancy production of kinetic

energy leading to an increase in the total turbulence kinetic energy available at the cloud edge. This further drives the entrainment of unsaturated air leading to more droplets evaporating and establishing a dynamical positive feedback which drives the shell growth. Characteristic scales are defined for the in-shell buoyancy, vertical velocity and thickness using integral properties of the flow. With a bulk condensation scheme, the growth of the shell thickness is shown to be linear and the minimum magnitude of the mean buoyancy inside the shell settles to a constant (in time) value. As the shell thickens, it accelerates ballistically, however the mean velocity is expected to be dynamically unimportant and slaved to the buoyancy. A detailed analysis of the self-similarity of the shell reveal that the flow does not behave like a classical self-similar flow, and that the TKE budget and velocity moments scale with the buoyancy and not the mean velocity.

Two regimes were identified in the flow inside the shell: the 'drag phase' and the 'buoyancy phase'. Theoretical analyses reveal that the flow inside the shell is determined by a balance between the integral buoyancy B and the horizontal transport of vertical momentum $\overline{u'w'}|_{x_b^-}$ at the inner boundary of the shell. When the latter term dominates, the drag phase occurs with the in-shell mean buoyancy being negative, but the shell being dragged up by the cloud core. The onset of the buoyancy phase occurs when B overcomes the vertical momentum flux $\overline{u'w'}|_{x_b^-}$ and the shell starts subsiding.

We demarcated two zones within the shell: a visible shell and an invisible shell, with the invisible shell bounded by the TNTI. The TNTI is explicitly detected for the first time at the cloud edge in this thesis. Also, detecting the TNTI in a more realistic setup in LES is highly significant. Using a threshold for the enstrophy to detect the TNTI can have applications in the identification of coherent structures in LES studies, such as updrafts, downdrafts/shells or environmental subsidence in the boundary and cloudy layers of shallow convection. Particles crossing the TNTI exhibit a sharp jump in enstrophy and buoyancy values. The interface commonly considered in entrainment studies, the visible shell boundary, where the cloud liquid water drops to zero, is shown to be a cross-over station where particles do not undergo a significant change in properties. Even though the visible shell boundary is dynamically unimportant, it is still a relevant interface over which entrainment rates can be calculated, i.e.

the different interfaces attain importance based on the application. The TNTI gains importance as an interface while studying the mass-flux transport. We confirm a previously held result that the upward mass flux in the cloud core is compensated by the downward mass flux in the subsiding shell. By using conditionally averaging mass flux in the different zones, we were able to highlight that it is actually the invisible shell that is responsible for the majority of the downwards mass flux with almost no net exchange across the TNTI and the environment in the mid-cloud layer. However, this does not mean that the air is not transported from the cloud to the environment. We postulate that eventually the cloud and the invisible shell will dissipate with the humid air in the cloud moistening the environment. This is a radically different mechanism compared to direct mixing between the cloud and the environment and more studies are needed to confirm this. It would be interesting to see the zone-wise contribution to droplet evaporation and growth to understand if droplets react differently to the different interfacial layers in the shell.

We highlight the important role gravity plays in droplet growth. The effect of gravity on the clustering of droplets over a large range of Stokes numbers and settling velocities considered in chapter 6 show that the reduced interaction times between droplets and turbulent eddies causes a reduction in clustering. The collision kernel is also reduced for geometric collisions between unequal sized droplets. However, the inclusion of collision-coalescence and hydrodynamic interactions between droplets would provide a better picture. The Taylor Reynolds numbers of the current simulations are several orders of magnitude below those of actual clouds and hence extrapolating these results to real-life clouds would require a better understanding of the Reynolds number dependence of clustering of sedimenting droplets. At the cloud edge, larger settling droplets can experience a broader range of negative supersaturation leading to a broader droplet size distribution. This broad DSD has implications on droplet growth due to collision-coalescence since larger droplets formed due to coalescence can further collect smaller droplets as they settle.

We highlight the role of entrainment in the broadening of droplet size distributions and the associated increase in collision-coalescence. A clear enhancement in the number of collisions in the visible shell and the adjacent cloud core region is shown. This can result in bigger

droplets and a subsequent broadening of the size distributions. Conversely, the differences in entrainment in clean and polluted clouds can be studied by varying the initial aerosol number concentrations which is achieved by varying the initial size distributions in the cloud layer. An increased number of smaller droplets are observed to be evaporating in polluted clouds resulting in a stronger shell at the cloud edge. However, the associated size distribution is much narrower compared to clean clouds. This could have implications on the cloud albedo and precipitation as shown in LES studies. An increase in cloud albedo due to an increased number of smaller droplets (higher particle concentration) and the suppression of precipitation due to a narrow size distribution and the delaying of the onset of collision-coalescence is expected. However, simulating the DNS till droplets reach drizzle size would require a much bigger domain as well as increased computational cost. This is currently outside the capabilities of DNS but such simulations are extremely useful to visualize and quantify small-scale interactions between turbulence and microphysics.

8.2.1 Contributions to COMPLETE

One of the main objectives of the COMPLETE project was to improve the understanding of the dynamics of turbulent entrainment of dry environmental air to the cloud, and the microphysical and dynamical effects of turbulent mixing following the entrainment. Another objective was to quantify the dynamics of aerosols and particles in clouds with particular focus on the differences in the dynamics of inertial and non-inertial particles in shear- and buoyancy-driven flows. The results presented in this thesis certainly achieves these objectives and the DNS data, along with data from field measurements by means of expendable smart mini balloons, will be used to setup an open access cloud Lagrangian data base. We also envisage the DNS data to be used to help develop better collision kernels for coalescence growth and to develop new methods to characterize particle size distributions in clouds/aerosols. There is also scope for the data to be used to quantify predictive relationships of important processes in the aerosol life cycle.

8.3 Future work

Multiple avenues of research have been opened up with this thesis. A few interesting possibilities are mentioned in the following subsections.

8.3.1 *Dynamic evolution of the shell with droplet evaporation*

As mentioned in chapter 4, the transient nature of the growth of the shell at the expense of the cloud layer necessitated the implementation of the volumetric forcing in the cloud layer. Studying the dynamical evolution of the shell (possibly till the establishment of a self-similar regime) by replacing the bulk scheme in chapter 4 and introducing droplets as in chapter 7, would require a similar form of nudging. In order to maintain the positive buoyancy in the cloud layer, the droplet concentrations in the 'nudging zone' would have to be constantly monitored and maintained by introducing more droplets. We envisage such a simulation to be highly expensive but still possible within the realms of hybrid Eulerian-Lagrangian DNS. However, a polydisperse distribution with sizes over a large range, and making significant computational gains by implementing a more efficient, possibly implicit, time-integration scheme (which would allow larger particle time steps) is necessary for this to happen.

8.3.2 *Extension to stratocumulus clouds*

DNS has been suggested to be a complementary tool to LES for stratocumulus cloud research (Mellado et al. 2018). The DNS setup in this thesis can be used to study key processes such as interactions between turbulence, evaporation, radiation and microphysics in the cloud-top entrainment zone. An interesting question that has been identified to be suitable for DNS investigations in Mellado et al. (2018) is quantifying whether entrainment can be considered a purely interfacial process or driven by large turbulent eddies. Another question pertains to the effect of evaporative cooling, droplet sedimentation, and shear broadening on the mean entrainment velocity at the cloud top. Additionally, DNS can be used to study the effect of the different interfacial layers in the cloud-top entrainment zone on the evolution of the droplet size distribution in stratocumulus clouds.

8.3.3 *Collection efficiency*

There is considerable scope for studying the evolution of the droplet size distribution in the current setup. One aspect would be to consider the aerodynamic interactions between droplets. For the collision-coalescence process, local aerodynamics or hydrodynamic interactions are important even for a dilute volume fraction. A three-way coupling can occur with the turbulent flow affecting the motion of the droplets through interfacial viscous drag, particle motion being affected by the presence of other particles in the system, and the background fluid turbulence defining the far-field conditions and the local environment for the hydrodynamic interactions. These interactions can be studied by using a hybrid DNS approach which consists of solving for the undisturbed flow through DNS and representing the local particle-induced small-scale disturbance flows analytically (Ayala, Grabowski, and L.-P. Wang 2007).

8.3.4 *Moist fountain model for cumulus clouds*

Cumulus clouds have a similar structure to turbulent fountains. A fountain is a turbulent flow driven up by momentum flux from a source and arrested by an opposing buoyancy force. Clouds and fountains can be studied using the plume theory. Parallel research is ongoing in our research group where entrainment at the lateral edges and at the top of a moist fountain (as a paradigm for a shallow cumulus cloud) is studied using the bulk condensation scheme implemented in SPARKLE as part of this thesis. Traditional fountains assume a homogeneous interior with the entrained air being mixed instantaneously. This is not the case in cumulus clouds with both homogeneous and inhomogeneous mixing observed. Also, a quasi-steady state is considered in fountain entrainment while real clouds are time-dependent and could be actively growing, decelerating or dissolving. This can be addressed by controlling the source region to generate a time-dependent fountain. Traditional fountain studies are performed in a uniform environment. However clouds develop in a stratified environment and to address this, a stratification and a temperature lapse rate is also planned to be implemented in the environment. There is also scope for introducing droplets from the base of the fountain and allowing them to grow with background supersaturation that varies with height.

8.3.5 *Comparisons with experiments*

The case-setup in chapter 6 is developed to replicate the test section in wind-tunnel experiments very closely. Few comparison studies between experiments and numerical simulations have managed similar flow conditions. An important problem that is often the focus of both numerical and experimental studies, and hence apt for comparison, is the two-way coupling between turbulence and the dispersed particles. Here, in addition to turbulence affecting particle motion through viscous drag, the particles in dispersions with high mass-loading modify the fluid turbulence energy as well. We plan to study two-way coupling by performing DNS simulations at a higher mass-loading in a similar setup and comparing with data from wind-tunnel experiments.

8.3.6 *A versatile SPARKLE*

The implementation of the Lagrangian particle tracking routine and cloud microphysics routine in SPARKLE has been done in such a way that the implemented routines can be easily reused for solving problems from different fields such as ash transport in plumes, aerosol activation, moist fountains etc. The effectiveness of SPARKLE can be further enhanced by implementing a higher order implicit time scheme which would allow larger time steps for solving droplet equations of motion. Currently, the cloud droplet routine in SPARKLE is limited by the really small particle time steps necessitated by the droplet evaporation. Different treatments are currently made to switch between implicit and explicit schemes for cloud droplets as mentioned in chapter 7. We plan to implement a higher order implicit scheme such as the Adams-Moulton scheme which does not suffer from the numerical instability faced by the Adams-Bashworth schemes for relatively large time steps. This would significantly reduce the computational cost.

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Appendices

A Sensitivity to forcing parameters

The case-setup presented in chapter 4 is unique due to the introduction of the volumetric nudging inside the cloud layer. This was done primarily to prevent the shell layer from exhausting the cloud layer which then leads to a very transient flow. However, forcing the cloud layer can have several effects on the flow, primarily with respect to how fast the shell grows or thickens. We perform an analysis to study the sensitivity of the results to the forcing in the cloud layer. This is done by varying the length of the cloud layer (and hence the length over which the forcing is applied), and by changing the time scale of forcing. Two extra simulations B01 and B02 are performed; in B01, τ_c the time scale of nudging is relaxed, and in B02, L_c the width of the cloud layer is changed. The new simulations are similar in all other parameters to simulation A03.

A.1 Effect of time scale τ_c

In simulation B01, L_c is fixed and τ_c is relaxed to twice the value used in A03, i.e. $\tau_c = \frac{2 L_c}{w_c}$. This results in a softening of the sharp step change in the velocity and the thermodynamic properties, resulting in a shear layer which is much reduced in intensity compared to that in simulation A03 as shown in figure A1 (a) and (b). An analysis of the length scale l^* for B01 clearly shows that the length scale is still increasing linearly with time as shown in figure A1(c). Additionally, figures A1(c) and (d) show that the relations $l_s = 2.2l^*$ and $\overline{w}_{\min} = 0.25 b^*(t - t_B)$ observed in section 4.4 holds for B01 as well. This allows us to conclude that the growth of the shell thickness remains unaffected by the intensity of the shear layer at the cloud boundary.

A.2 Effect of cloud thickness L_c

In simulation B02, τ_c is fixed and the thickness of the cloud layer is doubled, i.e. $L_c = 2m$. This increases the distance between the left boundary and the shell as shown in figure A1(c). In A03, since the shell forms around $2m$ from the left boundary, turbulent eddies of scales greater than $2m$ will be inhibited by the left boundary. By increasing the width of the cloud layer, eddies of larger scales are also allowed to develop. However, the presence of these larger eddies

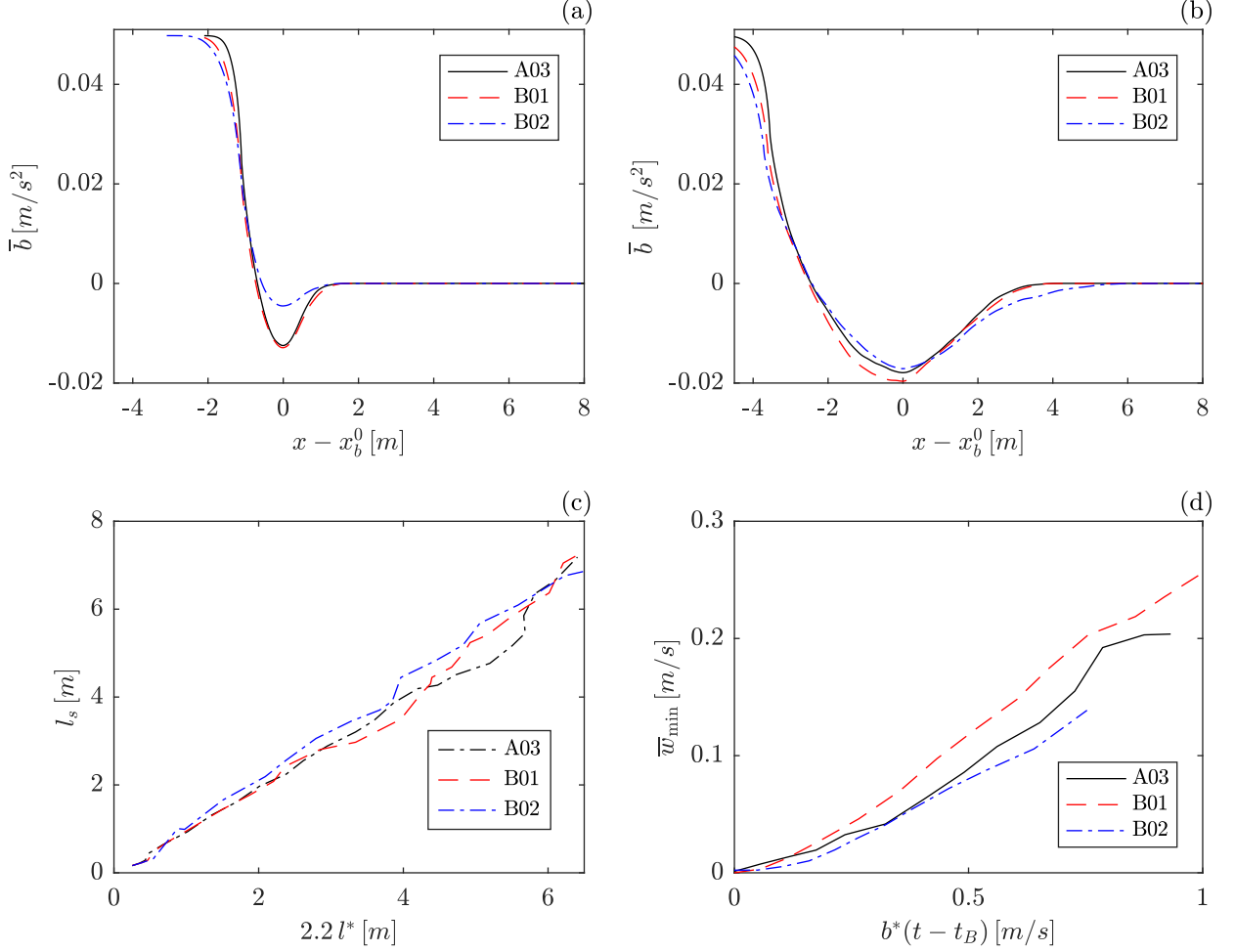


Figure A.1: Mean buoyancy profiles for simulations (a) A03 ($L_c = 1m$), (b) B01 ($\tau = \frac{2L_c}{w_c}$), and (c) B02, ($L_c = 2m$)

do not have an effect on the length scale of the shell l^* as shown in figure A1(c). This also highlights the fact that entrainment is dominated by the small scale mixing and could also be an explanation for the agreement between the entrainment coefficients in this DNS study and the LES study in Romps (2010) (which also includes much larger scales of turbulent motion). The relations for l^* and $\bar{w}_{min}$ hold for this case setup as well.

B Derivation of equation 4.12

From equation 2.7 the mean liquid water potential temperature can be defined as,

$$\bar{\theta}_l = \bar{\theta} - \frac{\bar{\theta}}{T} \frac{L}{c_p} \bar{q}_l. \quad (1)$$

We define $A = \frac{\bar{\theta}}{T} \frac{L}{c_p}$ which can be considered to be relatively constant in comparison to q_l .

Differentiating equation 1 with time gives

$$\frac{\partial \bar{\theta}}{\partial t} = \frac{\partial \bar{\theta}_l}{\partial t} + A \frac{\partial \bar{q}_l}{\partial t}. \quad (2)$$

Similar to $\bar{\theta}_l$, the mean buoyancy $\bar{b}$ is

$$\bar{b} = g \left[\frac{\bar{\theta} - \theta_0}{\theta_0} + 0.608(\bar{q}_t - q_{t,0}) - 1.608\bar{q}_l \right].$$

Differentiating $\bar{b}$ with time gives

$$\begin{aligned} \frac{\partial \bar{b}}{\partial t} &= g \left[\frac{1}{\theta_0} \frac{\partial \bar{\theta}_l}{\partial t} + \frac{A}{\theta_0} \frac{\partial \bar{q}_l}{\partial t} + 0.608 \frac{\partial \bar{q}_t}{\partial t} - 1.608 \frac{\partial \bar{q}_l}{\partial t} \right], \\ &= g \left[\frac{1}{\theta_0} \frac{\partial \bar{\theta}_l}{\partial t} + 0.608 \frac{\partial \bar{q}_t}{\partial t} + \left(\frac{A}{\theta_0} - 1.608 \right) \frac{\partial \bar{q}_l}{\partial t} \right]. \end{aligned}$$

To calculate q_l using the bulk condensation scheme, the conditions in equation 2.11 is used.

For $\bar{q}_l = \bar{q}_t - \bar{q}_s$,

$$\begin{aligned} \frac{\partial \bar{b}}{\partial t} &= g \left[\frac{1}{\theta_0} \frac{\partial \bar{\theta}_l}{\partial t} + 0.608 \frac{\partial \bar{q}_t}{\partial t} + \left(\frac{A}{\theta_0} - 1.608 \right) \left(\frac{\partial \bar{q}_t}{\partial t} - \frac{\partial \bar{q}_s}{\partial t} \right) \right] \\ &= g \left[\frac{1}{\theta_0} \frac{\partial \bar{\theta}_l}{\partial t} + \left(\frac{A}{\theta_0} - 1 \right) \frac{\partial \bar{q}_t}{\partial t} + \left(\frac{A}{\theta_0} - 1.608 \right) \left(-\frac{\partial \bar{q}_s}{\partial t} \right) \right] \\ &= g \left[\frac{1}{\theta_0} \left(-\frac{\partial \overline{u'\theta_l'}}{\partial x} + \langle S_1 \rangle \right) + \left(\frac{A}{\theta_0} - 1 \right) \left(-\frac{\partial \overline{u'q_t'}}{\partial x} + \langle S_2 \rangle \right) + \left(\frac{A}{\theta_0} - 1.608 \right) \left(-\frac{\partial q_s}{\partial t} \right) \right] \\ &= -\frac{\partial \overline{u'b'}}{\partial x} - g \left(\frac{A}{\theta_0} - 1.608 \right) \left(\frac{\partial \overline{u'q_s'}}{\partial x} + \frac{\partial q_s}{\partial t} \right) + g \left[\frac{\langle S_1 \rangle}{\theta_0} + \left(\frac{A}{\theta_0} - 1 \right) \langle S_2 \rangle \right] \end{aligned}$$

For $\bar{q}_l = 0$,

$$\begin{aligned}
\frac{\partial \bar{b}}{\partial t} &= g \left[\frac{1}{\theta_0} \frac{\partial \bar{\theta}_l}{\partial t} + 0.608 \frac{\partial \bar{q}_t}{\partial t} \right], \\
&= g \left[\frac{1}{\theta_0} \left(-\frac{\partial \overline{u' \theta'_l}}{\partial x} + \langle S_1 \rangle \right) + 0.608 \left(-\frac{\partial \overline{u' q'_t}}{\partial x} + \langle S_2 \rangle \right) \right], \\
&= -\frac{\partial \overline{u' b'}}{\partial x} + g [\langle S_1 \rangle + \langle S_2 \rangle].
\end{aligned}$$

where $\langle \cdot \rangle$ denotes Reynolds averaging and

$$\begin{aligned}
S_1 &= \frac{\theta_{l,c} - \theta_l}{\tau} H(L_c - x), \\
S_2 &= \frac{q_{t,c} - q_t}{\tau} H(L_c - x).
\end{aligned}$$

In the final step, the term $\overline{u' b'}$ is introduced, the derivation for which is given below in subsection

B.1. On integrating within the limits of the shell, S_1 and S_2 goes to zero.

B.1 Calculation of $\overline{u'b'}$

$$\begin{aligned}
b &= g \left[\frac{\theta - \theta_0}{\theta_0} + 0.608(q_t - q_{t,0}) - 1.608q_l \right] \\
\bar{b} &= g \left[\frac{\bar{\theta} - \theta_0}{\theta_0} + 0.608(\bar{q}_t - q_{t,0}) - 1.608\bar{q}_l \right] \\
b' &= b - \bar{b} \\
&= g \left[\frac{\theta'}{\theta_0} + 0.608q'_t - 1.608q'_l \right] \\
b' &= g \left[\frac{\theta'_l}{\theta_0} + \frac{A}{\theta_0}q'_l + 0.608q'_t - 1.608q'_l \right] \\
b' &= g \left[\frac{\theta'_l}{\theta_0} + 0.608q'_t + \left(\frac{A}{\theta_0} - 1.608 \right) q'_l \right] \\
\overline{u'b'} &= g \left[\frac{\overline{u'\theta'_l}}{\theta_0} + 0.608\overline{u'q'_t} + \left(\frac{A}{\theta_0} - 1.608 \right) \overline{u'q'_l} \right] \\
&\quad \text{(i) } \bar{q}_l = \bar{q}_t - \bar{q}_s, \\
\overline{u'b'} &= g \left[\frac{\overline{u'\theta'_l}}{\theta_0} + 0.608\overline{u'q'_t} + \left(\frac{A}{\theta_0} - 1.608 \right) (\overline{u'q'_t} - \overline{u'q'_s}) \right] \\
\overline{u'b'} &= g \left[\frac{\overline{u'\theta'_l}}{\theta_0} + \left(\frac{A}{\theta_0} - 1 \right) \overline{u'q'_t} + \left(\frac{A}{\theta_0} - 1.608 \right) (-\overline{u'q'_s}) \right] \\
\frac{\partial \overline{u'b'}}{\partial x} &= g \left[\frac{1}{\theta_0} \frac{\partial \overline{u'\theta'_l}}{\partial x} + \left(\frac{A}{\theta_0} - 1 \right) \frac{\partial \overline{u'q'_t}}{\partial x} + \left(\frac{A}{\theta_0} - 1.608 \right) \left(-\frac{\partial \overline{u'q'_s}}{\partial x} \right) \right] \\
&\quad \text{(i) } \bar{q}_l = 0, \\
\overline{u'b'} &= g \left[\frac{\overline{u'\theta'_l}}{\theta_0} + 0.608\overline{u'q'_t} \right]
\end{aligned}$$

B.2 Derivation of $\frac{\partial q_s}{\partial t} + \vec{u} \cdot \nabla q_s$

In the bulk condensation scheme, q_s is calculated as a function of both θ_l and q_t ,

$$q_s = q_s(\theta_l, q_t).$$

Therefore,

$$\begin{aligned}
\frac{\partial q_s}{\partial t} + \vec{u} \cdot \nabla q_s &= \frac{\partial q_s}{\partial \theta_l} \frac{\partial \theta_l}{\partial t} + \frac{\partial q_s}{\partial q_t} \frac{\partial q_t}{\partial t} + \vec{u} \cdot \nabla \theta_l \frac{\partial q_s}{\partial \theta_l} + \vec{u} \cdot \nabla q_t \frac{\partial q_s}{\partial q_t} \\
&= \frac{\partial q_s}{\partial \theta_l} \left(\frac{\partial \theta_l}{\partial t} + \vec{u} \cdot \nabla \theta_l \right) + \frac{\partial q_s}{\partial q_t} \left(\frac{\partial q_t}{\partial t} + \vec{u} \cdot \nabla q_t \right) \\
&= \frac{\partial q_s}{\partial \theta_l} S_1 + \frac{\partial q_s}{\partial q_t} S_2 \\
\frac{\partial \bar{q}_s}{\partial t} + \overline{u' q'_s} &= \left\langle \frac{\partial q_s}{\partial \theta_l} S_1 \right\rangle + \left\langle \frac{\partial q_s}{\partial q_t} S_2 \right\rangle
\end{aligned}$$

C TNTI detection: Sensitivity to threshold values

A very popular method used to detect a TNTI is by applying a threshold on enstrophy which allows one to separate the turbulent region from the approximately irrotational, non-turbulent region (da Silva et al. 2014). This value can be selected from a range since statistics have been shown to be insensitive to the exact threshold value (Bisset, Hunt, and M. Rogers 2002). We perform an analysis to verify if the location of the TNTI is indeed insensitive to the choice of threshold values in our case setup.

We check a range of magnitudes for ω_{th}^2 from 10^{-3} to $10^{-6} s^{-2}$. In figure C.1, the interfaces obtained by applying the different thresholds are plotted. The overlapping interfaces obtained from this range of threshold values point to the fact that these ranges lie in the viscous superlayer observed in interfacial layers and any threshold magnitude within this range can be used as a robust technique to detect the TNTI. Hence, we settle on a value of $\omega_{th}^2 = 10^{-6} s^{-2}$ for this study.

Furthermore, the TNTI can be seen to coincide exactly with the outer boundary of the shell as determined from the isoline of the buoyancy field $b = 0$. The inner interface corresponding to the isoline $b = 0$ coincides with the CCB.

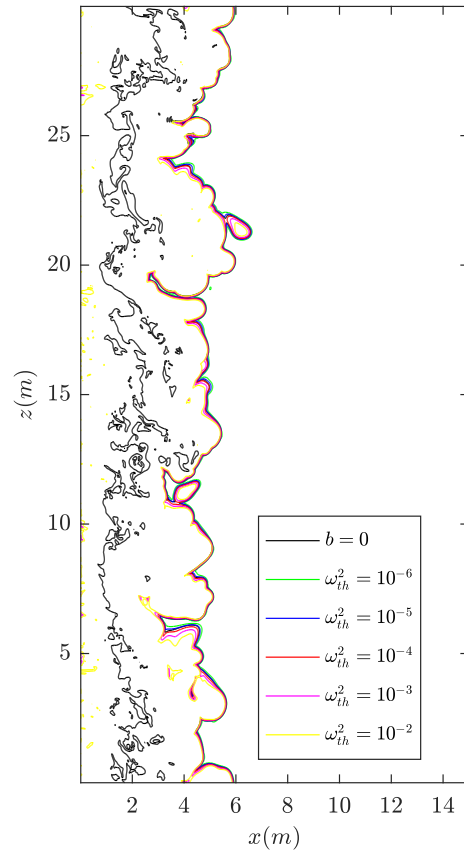


Figure C.1: Isolines of $b = 0$ (black) at the time of seeding (t_0). Superimposed are the different interfaces obtained by applying different threshold values to the enstrophy field ω_{th}^2 .