SUMMERTIME POST-COLD-FRONTAL MARINE STRATOCUMULUS TRANSITION PROCESSES OVER THE EASTERN NORTH ATLANTIC

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ABSTRACT OF THE DISSERTATION

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The Marine stratocumulus cloud system is a major component of the Earth’s energy budget. Mid-latitude stratocumulus are known to transition from a single, continuous cloud layer to a hybrid configuration that includes both stratocumulus and cumulus, and eventually to trade cumulus toward the tropics. Stratocumulus transitions are often observed in the wake of cold air outbreaks in the mid-latitude summertime marine boundary layer (MBL). Cloud morphology associated with two summertime cold fronts over the Eastern North Atlantic (ENA) is investigated using high resolution simulations from the Weather Research and Forecasting (WRF) model and observations from the Atmospheric Radiation Measurement
(ARM) ENA Climate Research Facility. Lagrangian trajectories are used to study the evolution of post-cold-frontal MBL clouds from solid stratocumulus to broken cumulus. Clouds within specified domains in the vicinity of transitions are classified according to their degree of decoupling, and cloud-base and cloud-top breakup processes are evaluated. The Lagrangian derivative of the surface latent heat flux is found to be strongly correlated with that of the cloud fraction at cloud base in the simulations. Cloud-top entrainment instability (CTEI) is shown to operate only in the decoupled MBL. A new indicator of inversion strength at cloud top that employs the vertical gradients of equivalent potential temperature and saturation equivalent potential temperature, which can be computed directly from soundings, is proposed as alternative to CTEI. Overall results suggest that the deepening-warming hypothesis suggested by Bretherton and Wyant explains many of the characteristics of the summertime post-frontal MBL evolution of cloud structure over the ENA, thereby widening the phase space over which the hypothesis may be applied. A subset of the deepening-warming hypothesis involving warming initially dominating over moistening is proposed. It is postulated that changes in climate-change induced modifications in cold frontal structure over the ENA may be accompanied by coincident changes in the location and timing of MBL cloud transitions in the post-cold-frontal environment.
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Chapter 1

Introduction

1.1 Motivation

Marine boundary layer (MBL) clouds exhibit a seemingly endless array of complex configurations and cover a large fraction of the Earth’s oceans. They are seminal components of the planetary radiation budget that act to cool the ocean surface by significantly impeding incoming shortwave radiation due to their high albedo, while minimally affecting longwave radiation losses to space, since their cloud-top temperatures are only slightly cooler than the ocean surface beneath them. They are also potentially susceptible to global climate change. Due to their climatological importance, it is essential to understand underlying processes during various stages in their life cycle, and accurately parameterize them in regional and climate models. An extensive and variable MBL cloud system is present over the Eastern North Atlantic (ENA) that undergoes a morphological transition with latitude. This region can be qualitatively explained as the following: moderate or strong subsidence associated with a subtropical anticyclone produces adiabatic compression that leads to a sharp difference between the potential temperature
of air in the lower troposphere and the potential temperature of the air immediately above the ocean surface with the former temperature being much greater than the latter. The very large heat capacity of the ocean leads to the formation of a stable layer adjacent the ocean surface that is capped by a temperature inversion. The primary factors that enhance this inversion and regulate the depth of the marine boundary layer include weak turbulence induced by wind shear near the ocean surface and cloud-top radiative cooling that produces negatively buoyant parcels, which provide the bulk of the turbulent kinetic energy required to maintain a mixed layer. Clouds over the northern reaches of the ENA tend to be layered and tend to be comprised of shallow turbulent moist stratus decks overlain by a strong temperature inversion and warm dry air, while those to the south tend to be more broken. Conceptual models of this cloud transition depict reductions in inversion strength and increasing sea-surface temperatures toward the Intertropical Convergence Zone accompanying the evolution to broken cloud structure. These large-scale changes in the upper and lower boundary conditions of the MBL are related to the latitudinal evolution of semi-permanent subtropical high-pressure systems that are part of the Hadley circulation. Given the importance of marine boundary layer clouds in the Earth’s radiation budget, changes in the location or function of the ENA cloud transition region in response to anthropogenic warming would likely impart significant changes in the regional and planetary radiation budgets (Bretherton et al., 2013).

Stratocumulus, shallow cumulus, and complex combinations of these cloud
types, often exhibiting mesoscale organization, are present in the transition MBL cloudiness over the ENA. Several studies have detailed the MBL cloud morphology, thermodynamic environment, and precipitation during the summertime (Albrecht et al. (1995), Miller and Albrecht (1995); Wood (2005); Dong et al. (2014a,b); Wood et al. (2015); and others), while additional studies have examined the basic life cycle of clouds through the transition process (Bretherton and Pincus (1995); de Roode and Duynkerke (1997); Bretherton et al. (1999); Lloyd et al. (2018)).

However, a much smaller body of literature has addressed the large scale environment in which MBL clouds reside, although scale interactions have long been recognized as a critical determinant of cloud configuration in the marine boundary layer in general. Conspicuously absent from the literature are studies detailing the life cycle of MBL clouds in the transition regions. For example, Lilly (1968) writes in reference to California stratocumulus: “In a sense the model only pushes the problem back one step and substitutes the question of origin of the cloud layer which must be present at the time subsidence commences. This original cloud layer might be a remnant of the frontal disturbances that frequently pass through the Gulf of Alaska in summer, or it may simply be produced from evaporative moistening of a previously clear mixed layer”. Steady advances have increased our knowledge of MBL clouds and it is important to fully understand the life cycle of MBL clouds in the ENA cloud transition region. This is particularly true given the known challenges in simulating MBL cloud systems in models of
all types. Understanding the cloud life cycle in the ENA transition region is an exercise in scale interactions.

Changes in cloud morphology over the ENA are often related to a process known as decoupling (Nicholls, 1984), whereby the MBL is composed of two layers separated by an intermittent, weak inversion: a moist sub-cloud layer immediately above the ocean surface and a cloud layer above capped by the marine inversion (Albrecht et al., 1995). The Atlantic Stratocumulus Experiment (ASTEX) was an important study that was aimed at investigating processes responsible for the transition between solid stratocumulus and trade cumulus cloud regimes over the ENA (Albrecht et al., 1995). It was carried out during June 1992, utilizing island, aircraft, ship, and satellite measurements. The results from ASTEX highlighted the important role of decoupling in the atmospheric boundary layer in stratocumulus cloud transitions, as well as deepening of the boundary layer, solar absorption in clouds, and drizzle, all of which impact the decoupling process. As the decoupling process takes its course, the solid deck of stratocumulus transitions into mesoscale, cellular structures that can be maintained by mesoscale convective systems that result from the accumulated moisture in the boundary layer.

A deepening-warming decoupling process first proposed by Bretherton and Wyant (1997) is thought to be a key initiator of the transition from a sheet of stratocumulus to more broken cloud structures. According to this hypothesis, the cloud-base buoyancy flux increases in proportion to latent heating, while the
MBL average buoyancy flux does not, leading to decoupling. At the onset of
decoupling and the transition in cloud structure, the lifting condensation levels
(LCLs) in updrafts and downdrafts gradually diverge and the cloud layer dries.

Past modeling studies have employed 1-D mixed-layer models (Schubert et al.
(1979); Wakefield and Schubert (1981); Nicholls (1984); Albrecht (1984); Brether-
ton and Wyant (1997)), and 2-D eddy-resolving models (Moeng and Arakawa
(1980); Krueger et al. (1995); Wyant et al. (1997)) to investigate marine stra-
tocumulus cloud transitions and the role of decoupling in the transition process.
Some of the earliest regional simulations included a two-layer, 1-D model of the
stratocumulus transition, which produced a regional gradient in the cloud struc-
ture (Wang et al., 1993), and a mesoscale model with 5-km horizontal resolution
that was used to test cloudiness parameterizations (Mocko and Cotton, 1995).
Regional simulations designed to test the impacts of drizzle and microphysics on
mesoscale organization showed that mesoscale structures were created in simu-
lations using 2-km horizontal resolution when many physical processes were re-
solved, especially those involving drizzle production, but not when the resolution
was increased to 18-km and parameterizations were required (Mechem and Kogan,
2003). A regional simulation using a mesoscale model with a resolution compati-
ble with current climate models (60-km), which used MBL turbulence and shallow
convection parameterizations, was able to successfully simulate the stratocumulus
to cumulus transition (Bretherton et al. (2013); McCaa and Bretherton (2004)).
A key finding of this study was that a shallow convection scheme was required
to faithfully reproduce the stratocumulus to cumulus transition. A later study demonstrated that mesoscale models with coarser resolution are sensitive to the parameterization of shallow convection and to the parameterization of penetrative mixing at the top of the cumuli, which acts to deepen the trade inversion (Bretherton et al., 2004). Sensitivities in the representation of cloud-top entrainment were also reported in another regional study (Wang et al., 1993).

Cascading cold frontal cloud bands are integral components of the ENA transition region and are observed in all seasons (Reed (1960); Giangrande et al. (2019)). Cold fronts in this region have higher average maximum and minimum integrated water vapor contents than North Pacific fronts in the summertime, a difference that can be attributed to higher sea-surface temperatures and, consequently, higher evaporation and moisture flux in the region (McMurdie and Katsaros, 1991). A recent study by Naud et al. (2018) documented the climatology of post-cold-frontal conditions over the ENA associated with 77 cold frontal passages, 15 of which occurred during the summertime. They reported that “post-cold frontal periods (including all seasons) were more dynamically active, drier, and more unstable” than periods that did not involve frontal passages. Naud et al. (2018) also found that post-cold-frontal MBL clouds are deeper, colder, and have higher cloud-tops, and possess higher liquid water paths than non-post-frontal clouds. Cloud depth was suggested in their study to be more dependent upon surface forcing than to inversion strength when winds were northerly. Another
finding in their study was that the air-sea temperature gradients in post-cold-frontal situations likely enhance cloud liquid water path and that the weaker inversions and deeper MBLs that are observed in these environments tend to be more decoupled.

These studies motivate us to investigate the applicability of the Bretherton and Wyant (1997) deepening-warming hypothesis in the context of MBL cloud transitions often observed in satellite images behind cold fronts in the ENA region. On a broader scale, the simulations presented herein represent an effort to determine the association between the deepening-warming hypothesis, the mesoscale clusters of cumulus-coupled stratocumulus that are observed over the ENA, and the air-mass modifications that follow marine cold frontal passages. We examine the life cycle of MBL clouds associated with two summertime cold fronts that moved through the ENA region. High-resolution, large domain simulations using the Weather Research and Forecasting (WRF) model are used to produce a Lagrangian time series of the MBL cloud evolution in two post-frontal cases over periods of several tens of hours. Remote and in situ data from the ENA site are used to evaluate the results of these simulations.

1.2 Scientific Objectives

The goal of this study is to improve understanding of the decoupling process and its impact on MBL cloud morphology in summertime post-cold-frontal air masses traversing the Eastern North Atlantic and beyond. Another goal is to
determine if the deepening-warming hypothesis can be used to explain MBL cloud transitions in post-cold frontal air masses. One particular focus is the feedback between decoupling and the surface latent heat flux, which is thought to be a driver of the transition process in the deepening-warming schema. In addition, the simulations presented herein do not employ a shallow convective parameterization and are thus intended to reduce uncertainties associated with lower resolution models that require such a parameterization. Convection arises in a grid cell in our simulations primarily as a consequence of the interactions between the sub-grid scale turbulence and surface flux parameterizations, which are driven by the external conditions supplied to the cell. The cloud fraction reported at each height in each grid cell ranges from zero to one. If the cloud fraction is one at a given height, we view the convection as being “explicitly resolved” at that height, but if it is less than one, the sub-grid scale structure of the convection is determined by the turbulence scheme and is not explicitly resolved.

Many convective clouds over the ENA and in the MBL in general have dimensions that are smaller than the 1350 m horizontal and ∼100 m vertical resolution used in our simulations and would require Large-Eddy Simulations with scales on the order of 100 m or less to fully resolve. The simulations presented herein straddle the mesoscale-LES model continuum, so MBL turbulence including the mixing process at cloud top must still be parameterized. Finally, the simulations are compatible with measurements of transition structure using cloud remote sensing technology deployed at ENA on scales of many days. This synergism
provides a means to evaluate the results of the transition simulations at a single location.

The organization and flow of important cornerstones within chapters in this dissertation is summarized in the table below:

| Step | Description |
|------|-------------|
| 1    | Two high resolution WRF simulations of regional summertime post-cold-front MBL clouds in July 2017 and 2018 were used to investigate post-cold frontal MBL cloud transitions. |
| 2    | Used Lagrangian particle dispersion model FLEXPART-WRF to follow evolution of individual MBL columns in each simulation through the transition process. |
| 3    | Quality of simulations were compared with coincident surface and remote sensor data collected at the ENA site, located on Graciosa island in the Azores archipelago. |
| 4    | Comparable MBL depths simulated by WRF in the two post-frontal cases to those measured at ENA, although 100-200 m deeper than the observed depths. Post-frontal cloudiness was also more broken and deeper in both simulations than observed structures. |
| 5    | Used Jones et. al (2011) decoupling diagnostic based upon the vertical moisture gradient, to separate cloud populations into more coupled vs. more decoupled clouds. |
| 6    | Examined cloud-base and cloud-top processes with respect to coupled and decoupled clouds over a domain at the onset of transition from solid deck of marine stratocumulus to broken cloud. |

Figure 1.1: A concise pipeline of the flow of the study as presented in this dissertation.
2.1 Marine Stratocumulus

Attempts to model the transition processes of turbulent marine cloud layers under a strong subsidence inversion, and understanding the impact of the interaction between large-scale atmospheric phenomena and thermal convection on these processes perhaps date back to Lilly (1968). This early study focused on cloud-top radiative heat loss as the main contributor to the maintenance of the sub-cloud mixed layer that spans between 500 m to 1 km or more from the ocean surface, rather than the surface shear-generated turbulence. Therefore, the study primarily considered cloud-top instability in the event of entrainment of dry air above cloud top into the cloud layer as the driver of the transition to broken cloud structure. The results of the Lilly (1968) study are applicable to non-precipitating cases consisting of thin liquid water clouds. Such conditions are typically encountered in coastal ocean upwelling regions, for example immediately adjacent to the California or Portuguese coastlines or in the summertime high latitude regions.

When air from the free troposphere penetrates into the cloud layer, its temperature is reduced due to evaporation of cloud water droplets into the dry air.
This mixed air will be negatively buoyant and sink further in the cloud layer if it reaches saturation at a colder temperature than the surrounding air. If this process occurs spontaneously, it represents an instability that will continue until the cloud vanishes. The condition for the stability of the cloud-top layer with respect to penetration of the dry air aloft in Lilly (1968) was chosen such that the overlying air would have equal or higher wet-bulb potential temperature, $\theta_w$, than that at the cloud top. By definition, the wet-bulb potential temperature is the temperature an air parcel would have if it were cooled until reaching saturation and adiabatically brought to a reference pressure. Thus, the temperature of the entrained parcel after reaching saturation through the evaporation of surrounding cloud water would not be lower than the latter, prohibiting negative buoyancy that would result in unstable sinking of the parcel as a convective downdraft. Thus, the entrained parcel would remain in the cloud and become part of it as a result of entrainment.

The results of the moist cloud model by Lilly (1968) showed that in steady state, the cloud layer is maintained by active convection, with the virtual heat flux moving upwards. This convective energy is supplied by the latent heat of evaporation from the sea surface which is later released as it is condensed in the cloud base. Whereas, the sub-cloud layer is driven by downward virtual heat flux, transporting sensible heat into the sea, since the sea surface is virtually colder than the surface air.

The Lilly (1968) 1-D model successfully predicted a positive vertical gradient
in $\theta_w$ at the inversion consistent with observations. One of the main findings of the study was that the general character of the steady-state solution was irrespective of the choice of an entrainment hypothesis within the prescribed bounds. It was conjectured that the existence of a low, radiatively effective cloud cover is key to maintaining such a strong inversion characteristic of the marine layer of coastal California and similar regions. Without this element, a $15 - 20$ degree inversion at a height of $500 - 1000$ meters seemed impossible to maintain by kinetic energy for any observed combination of subsidence, convection, shearing turbulence. Furthermore, Lilly (1968) speculated that this cloud layer might be a residue of the frontal disturbances that commonly pass through the Gulf of Alaska in summer, or simply generated by evaporative moistening of a previously clear mixed layer. In other words, the original genesis of the cloud layer described in the model was unknown.

Randall (1980b) further investigated the criterion for cloud-top instability with respect to entrainment of the cloud-top air that could lead to buoyant convection in the cloud layer, the so-called “Cloud-Top Entrainment Instability” (CTEI). The underlying motivation of this investigation was an attempt to uncover the processes that lead to the transition of a relatively steady-state stratocumulus deck into broken cloud elements. This CTEI study focused on the entrainment process itself, regardless of the cloud-top radiative cooling that is known to stimulate convection and turbulence in the cloud layer (Lilly (1968); Randall (1980a)). The CTEI criterion was linked to whether entrainment leads to the destruction or
generation of turbulence kinetic energy in a stratocumulus cloud. In a statically
stable layer, the buoyancy force tends to attenuate or almost completely prevent
the penetration of the dry air from aloft into the cloud layer. The work against
this force is supplied by Turbulence Kinetic Energy (TKE).

Randall (1980b) considered a uniform turbulent and saturated cloud layer
underlying a quiet and unsaturated layer. Virtual dry static energy, \( s_v \), was
employed in the study to account for the effect of vapor and liquid water in the
cloud parcels on their relative buoyancy, defined as

\[
s_v = c_p T_v + gz
\]  

(2.1)

where \( T_v \) is the virtual temperature, which is

\[
T_v = T(1 + \delta q - l).
\]  

(2.2)

In this expression, \( q \) and \( l \) are water vapor and liquid water mixing ratios,
respectively, \( c_p \) is the specific heat at constant pressure, and \( \delta = 0.608 \). As
conservative variables, the total water mixing ratio \( (q + l) \) and the moist static
energy \( h \equiv c_p T + gz + Lq \) were used in this study, where \( L \) is the latent heat of
vaporization.

Entrainment of cloud-top air into the cloud layer would promote convection,
or equivalently increase turbulent fluxes of \( s_v \), \( F_{s_v} \), at the highest level within the
cloud under the condition that

\[ \beta \Delta h - \epsilon L \Delta (q + l) < 0 \tag{2.3} \]

where \( \epsilon \equiv \frac{c_p T}{L} \), \( \beta \equiv \frac{1 + (1 + \delta) \gamma \epsilon}{1 + \gamma} \), \( \gamma \equiv \frac{L}{c_p} \left( \frac{\partial q^*}{\partial T} \right)_p \), \( q^* \) is the saturation mixing ratio, and \( \Delta \) is the difference between variables in levels just below and above the cloud top, \( B \) and \( B^+ \), respectively. In order to eliminate the effect cloud-top radiative cooling, the thickness of the layer between \( B \) and \( B^+ \) is assumed to be infinitely thin. Eq. 2.3 can be re-written in terms of a critical value for the difference in \( s_v \) between layers \( B \) and \( B^+ \),

\[ \beta \Delta h - \epsilon L \Delta (q + l) = \Delta s_v - (\Delta s_v)_{crit} \tag{2.4} \]

where

\[ (\Delta s_v)_{crit} = \left[ \frac{1 - (1 + \delta) \epsilon}{1 + \gamma} \right] L (q^*_B - q_{B^+}) \tag{2.5} \]

From Eq. 2.3 and Eq. 2.4, the criterion for the onset of this type of cloud-top instability, termed by Randall (1980b) as “Conditional Instability of the First Kind Upside Down”, or CIFKU, can be written as

\[ \Delta s_v < (\Delta s_v)_{crit} \tag{2.6} \]

According to Eq. 2.6, the requirement for the onset of this type of cloud-top
instability is fulfilled when $\Delta s_v$ is smaller than a critical value, $(\Delta s_v)_{\text{crit}}$, which has an inverse relationship with the relative humidity of the air atop the cloud layer. This imposes a more stringent requirement than that of Lilly (1968), which considers decrease in the wet bulb potential temperature with height at cloud-top as the criterion for cloud-top instability, which is equivalent to $\Delta h < 0$, while with CIFKU $\Delta h$ needs to be smaller than a negative value; $\Delta h < \epsilon L \Delta (q + l)/\beta < 0$.

The main difference between convective downdrafts of CIFKU and cumulus convective updrafts (or “Convective Downdraft of the First Kind” (CIFK)), apart from the opposing directions of buoyancy forces, is that CIFKU downdrafts are driven by cloud-top evaporative cooling, while cumulus updrafts are induced by condensation heating concentrated at the cloud base. Also, while downdraft cooling occurs only in the cloud layer, updraft heating finds its way to the conditionally unstable layer aloft the top of the PBL. For the case of cumulus updrafts, the dry and low-energy air entrained into the cloud, as well as the friction induced by momentum exchange act to diminish it by diluting its cloud mass. However, the entrainment into downdrafts plays a vital role for the generation of CIFKU.

Randall (1980b) concluded that the instability created by CIFKU which acts to decrease the fractional cloudiness within a cloud layer, is responsible for the partial disintegration (breakup) of the subtropical marine stratocumulus at their westward and equatorward boundaries. Fig. 2.1 illustrates how the marine stratocumulus regimes transition to tradewind cumulus and ITCZ regimes on their equatorward journey towards higher sea surface temperatures and weaker large
scale subsidence. In between these two regimes is the transition zone, at the poleward boundaries of which CIFKU commences, marking the breakup of the stratocumulus deck as it moves into the transition zone. On the other hand, the equatorward boundary of the transition zone marks the onset of CIFK. Another major distinction between these two regimes is that the marine stratocumulus cloud top is where the top of PBL is usually thought to be, whereas, this level is associated with the trade cumulus regime.

Figure 2.1: A schematic illustration of the role of CIFKU in determining the tropical and subtropical distributions of cloudiness, Fig.5 from Randall (1980a)

In a separate study, Deardorff (1980) found similar results to Randall (1980b) for the cloud-top instability criterion with respect to entrainment of dry air into the cloud top.

The vertical structure of the turbulence in the marine boundary layer and
its potential impacts was originally addressed by Turton and Nicholls (1987) and Nicholls and Turton (1986) in a series of studies. Nicholls and Turton (1986) noted that as the subsidence rate decreased and the marine boundary layer deepened, the supply of turbulent kinetic energy from the LW cooling at cloud top would eventually become insufficient to maintain a well-mixed layer. At this point, the marine boundary layer would separate into two distinct internal boundary layers, one driven by LW cooling at cloud top and the other driven by wind shear near the ocean surface. A weak inversion would form at the interface between these two layers. Once the separation was complete, vapor and moist static energy would accumulate in the layer adjacent to the ocean surface, prevented from moving higher by the weak inversion separating the two layers. Thus, the upper layer, or the “decoupled” layer, would become desiccated through dry air exchanges with the drier free troposphere above, potentially evaporating or thinning the stratocumulus beneath the inversion.

The consequences of decoupling included a second thermodynamic process because the moist lower layer would accumulate convective available potential energy (CAPE) if the decoupling persisted for a sufficient length of time. Moisture accumulation would also steadily decrease the LCL, initially located in the upper desiccated layer, until it breached the height of the weak thermal inversion separating the two layers. Once the LCL emerged into the moist lower layer, energetic thermals would saturate just beneath the inversion releasing latent heat that enabled the CAPE in the lower layer to be realized in the form of cumulus
convection. This newly formed convection would rise into the desiccated layer, moistening it through detrainment, and either immediately resupply the stratocumulus beneath the inversion with liquid water and aerosols, or slowly attenuate entrainment in the desiccated layer until subsequent convective elements were able to resupply the layer of stratocumulus. The models of Nicholls and Turton (1986) were partially validated during ASTEX, and the progression of decoupling leading to moisture accumulation, CAPE accumulation, the LCL entering layer near the ocean surface, and the onset of cumulus convection were observed by Miller and Albrecht (1995) and by Miller et al. (1998).

This intermittent decoupling, sometimes referred to as a “cumulus coupled” marine boundary layer, often exhibits a level of mesoscale organization (Miller and Albrecht (1995); and others). Mesoscale clusters of cumulus clouds, some reaching into the overlaying stratocumulus and resupplying it, are often observed in the marine boundary layer in the ENA region and beyond. These mesoscale clusters, sometimes referred to as “mushrooms” or “shrooms” are characterized by an extensive stratocumulus shield being fed by cumulus clouds from below. They produce extensive drizzle storms and occasionally evaporation-driven penetrating downdrafts in their wake. They resemble a miniature version of marine tropical deep convection. The association between “shrooms” and marine fronts observed during ASTEX was never quite clear. At least one such structure was clearly associated with a marine cold front as observed during ASTEX (M.A. Miller, personal communication), but others appeared to exist independent of the frontal
zone itself, but often in the post-cold-frontal air masses that passed when winds in the ENA were from the north.

Focus on cloud-top mixing as the primary driver of the marine stratocumulus to cumulus transition faded shortly after ASTEX as the role of cumulus convection in the transition process became more obvious. A series of 1-D modeling efforts led to the supposition that the transition process was driven from below by latent heat release associated with the cumulus convection. These 1-D simulations successfully simulated a transition from solid stratocumulus to cumulus and represented aspects of the intervening transition process in which cumulus and stratocumulus coexist in a “cumulus coupled” environment. The results of these 1-D models led to the introduction of the “deepening-warming” hypothesis, in which it is postulated that that the warming and moistening of the air mass adjacent to the ocean surface in conjunction with weakening subsidence leads to the observed latitudinal cloud transition. A hallmark of the hypothesis is the minimal role of cloud-top entrainment driven by LW cooling in the transition process.

The latitudinal deepening-warming has heretofore been viewed as a climatological process and the mesoscale clusters of cumulus rising into stratocumulus in a more or less local framework. There is no mathematical connection in the 1-D models between the mesoscale organization in the structures observed over the ENA and the deepening-warming hypothesis. Moreover, the association between the hypothesis, the clusters, and the frequently observed frontal structures over
the ENA and over the Earth’s mid-latitude ocean regions, is largely unknown. In essence, the tools to make such connections, high-resolution models capable of resolving these clusters and their relationship to the deepening-warming hypothesis and frontal structures, have been heretofore non-existent. Recent advances in computing power now enable such simulations and they are used in this dissertation as a first attempt to address the interplay between these major components of the cloud transition region over the ENA.

2.2 Marine Frontal Clouds

A prominent feature of cyclonic storms in the mid-latitudes is the resulting cloud systems that are characteristic of these regions. These cloud structures greatly alter vertical fluxes of latent heat, momentum, and moisture, and comprise a major part of the precipitation and cloud radiative forcing in the mid-latitudes, all of which have substantial climatic implications (Stewart et al., 1998). These cyclones form as a result of baroclinic instabilities present in these regions. During their life cycle, strong oceanic convective systems evolve into stratiform structures (e.g. Neiman and Shapiro (1993); Hoskins (1982); Neiman et al. (1993)).

Fronts are transition zones between air masses with contrasting thermal properties. Frontal zones are often characterized by significant weather, including sudden changes in cloud structures and precipitation, as well as drastic gradients of temperature, moisture, wind direction, and horizontal and vertical wind shear (Carlson, 1991). The significant role of fronts in cyclogenesis has been been well
established (Bjerknes (1919); Hoskins (1982); Bluestein (1986)). The clouds associated with mid-latitude cyclones are organized by the large-scale atmospheric dynamics, and cloud structures are different in each of the three (or more) air masses that are associated with the fronts. Fronts are generally synoptic-scale features, with mesoscale and cloud-scale motions taking place within them that act to modify moisture and temperature profiles, and consequently, are important features that require quantitative analysis (Stewart et al., 1998). Therefore, it is crucial to properly represent these heat and momentum transfers associated with the fronts and the corresponding air masses in climate models in order to adequately predict larger-scale features, and their impact on climate change.

However, a major source of uncertainty in climate model for predicting future climate can be traced to model representations of low-altitude clouds (Bony and Dufresne (2005); Medeiros et al. (2008); Williams and Webb (2009)) and marine stratocumulus clouds comprise a substantial portion of these cloud systems. Marine stratocumulus cloud systems are ubiquitous beneath anticyclones that occur under the subsiding branch of the Hadley circulation, as well as in post-cold-frontal regions of mid-latitude cyclones (Field and Wood (2007)). Trenberth and Fasullo (2010) discovered that most general circulation models suffer from negative cloud-cover bias that leads to higher rates of shortwave radiation absorption over the southern oceans. This bias is mostly associated with cold sectors of extratropical cyclone regions, and has been found to exist in the phase 5 of the Coupled Model Intercomparison Project (CMIP5) by Bodas-Salcedo et al. (2014),
the European Centre for Medium-Range Weather Forecasts (ECMWF) interim reanalysis (ERA-Interim) by Naud et al. (2014), as well as the NASA Modern-Era Retrospective Analysis for Research and Applications (MERRA).
Chapter 3

Overview of Data and Methodology

Two principal resources were utilized in this work: data collected using the suite of sensors deployed at the ENA site and the WRF model. These tools are described in the sections that follow.

3.1 Observation Data from ENA

Observations used in this study were collected at the Atmospheric Radiation Measurement (ARM) Eastern North Atlantic (ENA) Climate Research Facility located on Graciosa Island in the Azores archipelago (39°5′29.76″ N, 28°1′32.52″ W). This location and much of the instrumentation are described in Wood et al. (2015). Data from the surface meteorology station (SMET) are used to characterize the chronology of the surface temperature, relative humidity, pressure, and winds that are compared with output from the WRF model. The SMET sensors are mounted on a 10-m mast and include a Vaisala Model HMP45-D Temperature and Relative Humidity Probe, a Digital barometer, Vaisala Model PTB201A, and two R. M. Young Model 05106 Wind Monitors that consist of a propeller anemometer and a wind vane. The ENA site is also equipped with a
Doppler Lidar (DL) that detects aerosol backscatter and uses it to measure the Doppler velocity with an accuracy of 10 cm/s. The DL operates in the near-IR (1.5 μm) and transmits laser pulses with a range resolution of 30 m, a maximum measurement range of 9600 m, and a temporal resolution of about 1 second. When the DL pulse reaches the boundary of a cloud, its pulse is scattered such that it operates as a cloud-base height detector. Extremely thin clouds may allow the laser pulse to transmit through without being decimated thereby enabling additional cloud boundary detection above. Two minute averages of instantaneous vertical velocity measured by the DL that are centered on the half-hour output times of the WRF model are used in this study.

A K-a band, Zenith-pointing Radar (KAZR) operating at λ = 8.0 mm detects hydrometeors to a height of 18 km with an initial measurement height of 72 m. A profile of cloud location and hydrometeor Doppler vertical velocity is collected every 2-seconds in all but heavy precipitation when its beam is attenuated by liquid water absorption. When a cloud is drizzling and the droplet spectrum is bi-modal, the Doppler velocity becomes ambiguous unless spectral processing techniques are applied. These techniques may, at times, introduce considerable uncertainty in the estimation of the Doppler velocity of cloud droplets, so in-cloud KAZR measurements of the in-cloud vertical velocity are not used in this study. The KAZR data are used to compute the average, height-dependent cloud fraction over 30-min averaging interval.
3.2 WRF Configuration

Simulations were performed using WRF-ARW version 4.0 Skamarock et al. (2008) on NCAR’s Cheyenne supercomputer NCAR (2017). Two domains centered on Graciosa Island in the Azores were constructed using NOAA Earth System Research Laboratory’s WRF Domain Wizard, version 2.84 NOAA (2013) (Fig. 3.1). Analysis and three-hour forecast data from NCEP GDAS/FNL 0.25 Degree Global Tropospheric Analyses and Forecast Grids GDAS/FNL (2015) were used as input to WRF Preprocessing System (WPS). A horizontal resolution of 4050 m was chosen for the parent domain, which produces a downscaling ratio of approximately one-to-five. A parent-to-nest grid ratio of one-to-three equates to a horizontal resolution of the second domain of 1350 m. Both simulations were run for 72 hours (0000 UTC 17 July to 0000 UTC 20 July, 2017, and 0000 UTC 29 July to 0000 UTC 1 August, 2018) to capture the passage of the cold fronts, as well as the post-cold-frontal episodes downwind of the ACE-ENA site. The model outputs used in this study are from the second domain, which were written out every 30 minutes.

The dimension of the parent domain was chosen such that its center is approximately 1500 m from each edge following Lamraoui et al. (2018) to improve the timing of the passage of fronts and their strength. Hence the domains have sizes of $750 \times 750$ and $1050 \times 1050$ horizontal grid points, respectively. In addition, 82 vertical levels were designated such that the vertical grid spacing in the first 1 km is initially 15 m and becomes much larger beyond this point up to 50 mb.
Figure 3.1: Two domains centered on ACE-ENA site on Graciosa Island in the Azores, Portugal (39.1°N, 28°W), with horizontal resolutions 4,050 and 1,350 m, and 750×750, and 1050×1050 grid points, respectively. The domains were set using NOAA Earth System Research Laboratory’s WRF Domain Wizard, version 2.84.

Thus 41 levels are located in the lowest 3 km (~700 mb). To satisfy the Courant-Friedrichs-Lewy (CFL) criterion, time steps of 15 s and 5 s were used for the two domains, respectively, since the recommended time step is about 6 times the respective domain’s resolution (in km).

Detailed information regarding the technical aspects of running the simulations and additional settings, along with the namelist used for the 2018 simulation, are provided in Appendix A.
3.3 Parameterizations Used in WRF

The focus of the WRF simulations in this work was to better understand the life cycle of marine stratocumulus in the post-cold-frontal environment. To achieve the best possible representation of the observed conditions, various combinations of parameterizations and dynamic options were tested. Test simulations were conducted to the extent that the computational resources available at the time allowed. We found the combination of the following options that rendered the closest results to the satellite images and observation data from the site for the aforementioned periods. Table 3.1 shows a summary of the parameterization schemes used in this study, as well as their corresponding WRF options. More details on the complete set of options can be found in Appendix A. The following sections discuss the choice of parameterizations outlined in Table 3.1 in greater detail.

It must be noted that, since the duration of the simulations were not long enough (on the order of months or years), time-varying data such as monthly albedo values, sea-surface temperature (SST), and vegetation fraction were unnecessary and these fields remained constant and equal to their input values throughout the simulation period.

3.3.1 Cloud Microphysics Parameterization

An important factor determining the accuracy of atmospheric climate model simulations is representing clouds as correctly as possible. A critical aspect that
controls these representations is cloud microphysics and precipitation processes. However, accurate parameterization of these processes in climate models is still a work in progress, mainly because the cloud microphysical processes governing organization of hydrometeors are rather complex (Morrison and Milbrandt, 2015). There are two general approaches to representing cloud particles and their microphysical properties in climate models: the bulk method and the explicit bin-resolving method. Even though the latter approach leads to more accurate solutions to drop size distribution (DSD) than the former, their relatively high

Table 3.1: Parameterizations used in WRF simulations

| Parameterization                                      | WRF Option          |
|-------------------------------------------------------|---------------------|
| Cloud Microphysics                                   | mp.physics = 28     |
| Thompson aerosol-aware                               |                     |
| Planetary Boundary Layer (PBL)                       |                     |
| Mellor-Yamada Nakanishi and Niino Level 3 (MYNN3)    | bl_pbl.physics = 6  |
| TKE Advection                                       |                     |
| Stochastic eddy diffusivity mass flux (StEM)         | bl_mynn_edmf = 1    |
| Momentum transport in MYNN mass-flux scheme          | bl_mynn_edmf_mom = 1|
| TKE transport in MYNN mass-flux scheme               | bl_mynn_edmf_tke = 1|
| Cloud-scale mixing length in MYNN                    | bl_mynn_mixlength = 2|
| Longwave Radiation                                   | ra_lw.physics = 4   |
| Shortwave Radiation                                  | ra_sw.physics = 4   |
| Surface Layer                                        | sf_sfclay.physics = 5|
| Land Surface                                         | sf_surface.physics 2|
computational cost in climate models is a prohibitive factor. Therefore, the simpler bulk microphysical parameterizations that predict several DSD moments have been extensively implemented in mesoscale as well as some GCM models (Lim and Hong, 2010).

There are two main categories of bulk microphysics scheme: single-moment and multiple-moment. A single-moment scheme uses a distribution function, such as an exponential or gamma function, to represent hydrometeor size distributions for different categories of particle types, and then predicts the mixing ratios of these hydrometeors (Kessler (1969); Wisner et al. (1972); Lin et al. (1983); Cotton et al. (1986); Tao and Simpson (1993); Walko et al. (1995)). A double-moment scheme predicts mixing ratios of hydrometeors as well as the number concentrations of each hydrometeor category and the cloud condensation nuclei (CCN) (Ziegler (1985); Murakami (1990); Wang et al. (1993); Meyers et al. (1997); Reisner et al. (1998); Cohard and Pinty (2000b); Morrison and Pinto (2005); Thompson et al. (2008)). Despite higher computational costs of the double-moment scheme compared to the single-moment approach, it has significantly improved microphysical processes in mesoscale models (Lim and Hong, 2010), especially in the case of precipitating convective clouds simulations (Cohard and Pinty (2000a); Lee et al. (2004); Thompson et al. (2004); Milbrandt and Yau (2005); Phillips et al. (2007); Morrison et al. (2009)).

In this study, test simulations were run with the following double-moment bulk microphysical parameterizations in WRF: Morrison double-moment scheme
(Morrison et al., 2009), WRF Double-Moment 6-class (WDM6) scheme (Lim and Hong, 2010), and Thompson aerosol-aware scheme Thompson and Eidhammer (2014). The Morrison scheme predicts the mixing ratios and number concentrations of cloud droplets, cloud rain, graupel, ice, and snow. This scheme is an improvement on the parameterization proposed by Morrison and Pinto (2005), since prognostic variables for the mixing ratio and number concentration of graupel are also added to the model. WDM6 scheme supplemented double-moment predictions of warm-phase mixing ratios and number concentrations of cloud and rainwater to WRF single-moment 6-class (WSM6) scheme (Hong et al. (2004); Hong and Lim (2006)), while adopting the same ice-phase microphysics of Hong et al. (2004). An important feature of this scheme is that it incorporates a prognostic variable for CCN that helps to activate cloud water and ice particles. The activation process in WDM6 is governed by the interaction between the number of activated CCN and supersaturation (Twomey (1959); Khairoutdinov and Kogan (2000)). Thus, this scheme handles the process of the growth of cloud water by first computing the cloud drop nucleation process before proceeding to the condensation phase. However, WDM6 ignores all other CCN sink-source terms except the CCN activation and cloud droplet evaporation, and the CCN activation process adopted follows a simplified form of the Kohler equation which requires accurate estimation of the environmental supersaturation value, hence the CCN activation process is not adequately represented (Lim and Hong, 2010).
The importance of cloud-aerosol interaction in cloud microphysics and radiative properties modeling is demonstrated by Ramanathan et al. (2001), Wang (2005), and Khain et al. (2008). It is crucial to accurately represent the role of CCNs (known as aerosol effect) in cloud microphysics parameterizations, as it not only directly dictates the rate of generation of cloud water and ice particles, but has many indirect effects, as well. Among the most prominent studies on indirect aerosol effect are the first and second indirect effects proposed by Twomey et al. (1974) and Albrecht (1989), respectively. The first aerosol effect refers to the increased cloud-top albedo due to generation of larger numbers of smaller droplets for a given cloud liquid water content as a result of higher aerosol concentration. The smaller sized cloud droplets, on the other hand, lead to reduced precipitation, causing the cloud to have a longer lifetime. This is known as the second indirect effect. However, it is a complex task to accurately quantify the aerosol effect on microphysical processes that, in turn, impact cloud radiation, precipitation, and dynamics, due to various interactions between aerosol and cloud ice particles, as well as many feedback processes involving other aspects of cloud dynamics (Levin and Cotton, 2008).

The improved Thompson aerosol-aware bulk microphysics scheme (Thompson and Eidhammer, 2014), that is based on the parameterization proposed by Thompson et al. (2008), incorporates the cloud and ice droplet nucleation processes by CCNs and ice nuclei (IN) aerosols, respectively, and explicitly predicts the number concentrations of cloud water droplets and the available CCN and
IN. The Thompson et al. (2008) scheme includes treatments of microphysical processes for cloud water, cloud ice, rain, snow, and a hybrid graupel–hail category. Implementations of this scheme in WRF demonstrated good performance in terms of forecasting precipitation when compared to precipitation measurements (Liu et al., 2011). Thompson aerosol-aware parameterization provides an aerosol climatology dataset of monthly-averaged mass mixing ratios of aerosol variables, emitted from both natural and anthropogenic sources, from a seven-year (2001-07) global model simulation (Colarco et al., 2010). These aerosol particles are modeled explicitly using multiple-sized bins for various aerosols species by the Goddard Chemistry Aerosol Radiation and Transport (GOCART) model (Ginoux et al., 2001). These aerosol variables include water-friendly species (organic carbon, black carbon, sea salts, sulfates), as well as dust aerosols that are known to be important cloud ice activators and are found in abundance in the atmosphere (DeMott et al. (2003); Richardson et al. (2007); Hoose et al. (2010); Murray et al. (2012)). Thompson aerosol-aware scheme was also designed to be well-suited for use in high-resolution simulations.

Thompson and Eidhammer (2014) conducted a series of experiments using high-resolution (4-km grid spacing) 72-hour WRF simulations of a winter storm event over the entire contiguous United States to evaluate the performance of this new aerosol-aware scheme and the effect of changing hygroscopic aerosol concentrations on the development processes of clouds and precipitation compared to the non-aerosol scheme of Thompson et al. (2008). The results showed increased
number concentration of cloud droplets with significant drop in their mean size, heightened cloud albedo consistent with the first aerosol indirect effect, as well as reduced warm-rain rates that were expected on the basis of the second aerosol indirect effect, following increased aerosol concentration.

Using this last microphysical parameterization in our simulations yielded the best results, specifically in terms of maintenance of non-precipitating low marine stratocumulus decks. We think this is mostly due to the more comprehensive treatment of the aerosol effects on cloud water and ice nucleation processes, cloud droplet size and concentration distribution, and precipitation processes. Therefore, the Thompson aerosol aware was the microphysical scheme that we ultimately opted to use in our simulations.

3.3.2 Planetary Boundary Layer (PBL) Parameterization

A crucial aspect of mesoscale models that significantly impacts forecast inaccuracy is the representation of lower tropospheric turbulent mixing that dictates the vertical thermodynamic and kinematic atmospheric profiles in this region. (Jankov et al. (2005); Stensrud (2009); Hacker (2010); Nielsen-Gammon et al. (2010); Hu et al. (2010)). The lower tropospheric air is in close contact with and directly affected by the earth’s surface through heat, moisture and momentum exchanges with the surface. Turbulent eddies in this region lead to a mixing process that accommodates these exchanges. Since the spatio-temporal scales of these eddies are smaller than the grid scales and temporal resolution in most mesoscale
models, they cannot be explicitly resolved. That is why mesoscale models need to employ parameterizations to represent the subgrid-scale lower tropospheric turbulent motions.

Fig. 3.2 depicts the temporal evolution of the PBL. The surface layer is the closest to the earth’s surface. It is in this region that the vertical shear is the strongest and molecular diffusion can be considered in the momentum equation (Holton, 1973). During the daytime, convection fueled by the heat fluxes from the surface lead to a convective mixed layer. The resulting convective plumes can generate cumulus cloud layers at the intersection with the entrainment zone which lies above the capping inversion. As daytime comes to a close and solar heating recedes, the surface starts to cool, and a stable nocturnal boundary layer forms in the lower PBL, with the remnants of the earlier convective layer residing atop this layer. In other words, the upper part of the PBL becomes decoupled from the surface.

PBL parameterization schemes estimate turbulence by decomposing equations of motion into mean and perturbation components, where the former represents the time-averaged variables that define the background atmospheric state, while the latter captures the turbulent fluctuations, or deviations, from the mean state. The problem that is encountered with respect to the perturbations is that there are always more unknown than known terms, and the order of the unknown terms surpasses all the other terms. Therefore, in order to be able to solve the set of equations, $n^{th}$-order turbulence closure is needed to provide the relationship
between unknown terms of moment $n+1$ and known terms of lower moments. One major area where various PBL schemes differ is the order of turbulence closure. The other significant distinction among them is whether they employ a local or non-local mixing approach. Local closure schemes only consider vertical levels adjacent to a given point to determine variables at that point, while this is not a necessary requirement in the case of non-local closure schemes.

Since the largest eddies in the PBL are responsible for the vertical mixing process throughout this region for the most part, and are mainly untouched by the local fluctuations in static stability, non-local schemes more accurately represent the mixing processes in the PBL (Stensrud, 2009). During daytime, heat from the surface is transported upward by these large eddies regardless of the localized stability maxima, and it is these eddies that can find their way to the top of the mixed layer, thereby entraining the air from the free atmosphere into the
mixed layer, and deepening the PBL (Stull, 1988). However, using higher orders of turbulence closure (Mellor and Yamada (1982), Nakanishi and Niino (2009)) at a higher computational cost can improve local schemes.

### 3.3.2.1 Mellor-Yamada (MY)

Mellor (1973) developed a Mean Reynolds Stress (MRS) turbulence closure model for the constant-flux surface layer. In this model, prognostic equations for the fluctuating components of Reynolds stress ($u_iu_j$) and heat conduction moments ($u_i\theta$) (Eqs. 3.1, 3.2, 3.3) is obtained by combining equations of motion for the mean and fluctuating components of velocity and potential temperature, denoted here by capital and small letters, respectively, and ensemble averages by overbars,

\[
\begin{align*}
\frac{\partial u_i u_j}{\partial t} + \frac{\partial}{\partial x_k} \left[ U_k u_i u_j + \bar{u}_k u_i u_j - \nu \frac{\partial}{\partial x_k} \bar{u}_i u_j \right] + \frac{\partial}{\partial x_j} \bar{p} u_i + \frac{\partial}{\partial x_i} \bar{p} u_j \\
+ f_k (\epsilon_{ijkl} u_l u_i + \epsilon_{ijkl} u_l u_j) = -\bar{u}_k u_i \frac{\partial U_j}{\partial x_k} - \bar{u}_k u_j \frac{\partial U_i}{\partial x_k} - \beta (g_j u_i \bar{\theta} + g_i u_j \bar{\theta}) \tag{3.1}
+ \bar{p} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - 2\nu \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k}
+ \frac{\partial u_j \bar{\theta}}{\partial t} + \frac{\partial}{\partial x_k} \left[ U_k \bar{u}_j + \bar{u}_k u_j - \alpha u_j \frac{\partial \bar{\theta}}{\partial x_k} - \nu \frac{\partial}{\partial x_k} \bar{u}_i u_j \right] + \frac{\partial}{\partial x_j} \bar{p} u_i + \frac{\partial}{\partial x_i} \bar{p} \bar{\theta} \\
+ \epsilon_{ijkl} f_k u_l \bar{\theta} = -\bar{u}_j u_k \frac{\partial \bar{\theta}}{\partial x_k} - \bar{\theta} u_k \frac{\partial U_j}{\partial x_k} - \beta g_j \bar{\theta}^2 + \bar{p} \frac{\partial \bar{\theta}}{\partial x_j} \tag{3.2}
\end{align*}
\]
\[
\frac{\partial \theta^2}{\partial t} + \frac{\partial}{\partial x_k} \left[ U_k \theta^2 + u_k \theta^2 - \alpha \frac{\partial \theta^2}{\partial x_k} \right] = -2 u_k \theta \frac{\partial \theta}{\partial x_k} - 2 \alpha \frac{\partial \theta^2}{\partial x_k \partial x_k} \quad (3.3)
\]

where \( p \) is the perturbation kinematic pressure, \( g_j = (0, 0, -g) \) the gravity vector, \( f_j = (0, f_v, f) \) the Coriolis parameter, \( \nu \) the kinematic viscosity, \( \alpha \) the kinematic heat conductivity, and \( \beta = -(\partial \rho / \partial T)_p / \rho \) the coefficient of thermal expansion.

Mellor (1973) followed Rotta’s energy redistribution hypothesis (Rotta, 1951) and Kolmogoroff’s hypothesis of local, small-scale isotropy (Kolmogorov, 1941) to approximate higher moment terms that appear in the set of prognostic equations. Rotta’s model simplifies the energy redistribution term that appears in the Reynolds stress equation by suggesting that it may be proportional to Reynolds stress and mean wind shear. Following the assumption that the constitutive coefficients are isotropic tensors

\[
p \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = - \frac{q}{3 l_1} \left( u_i u_j - \frac{\delta_{ij}}{3} q^2 \right) + C q^2 \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) \quad (3.4)
\]

The same logic is applied to the equivalent term in the heat conduction moments equation

\[
\frac{\partial \theta}{p \partial x_j} = - \frac{q}{3 l_2} u_j \theta \quad (3.5)
\]
where \( q \equiv (\overline{u_i^2})^{\frac{1}{2}} \), and the lengths \( l_1 \) and \( l_2 \), and the constant \( C \) are empirically determined. Mellor and Yamada (1974) also used Kolmogoroff’s model to estimate the dissipation terms, as follow

\[
2 \nu \frac{\partial u_i \partial u_j}{\partial x_k \partial x_k} = \frac{2}{3} \frac{q^3}{\Lambda_1} \delta_{ij} \quad (3.6)
\]

\[
2 \alpha \frac{\partial \theta \partial \theta}{\partial x_k \partial x_k} = \frac{2}{\Lambda_2} q \overline{\theta^2} \quad (3.7)
\]

However, since an isotropic first-order tensor is non-existent,

\[
(\alpha + \nu) \frac{\partial u_j \partial \theta}{\partial x_k \partial x_k} = 0 \quad (3.8)
\]

Other simplifications involve ignoring pressure diffusional terms \( \overline{p u_i} \) and \( \overline{p \theta} \) following Hanjalić and Launder (1972), and scaling 3rd-order moment turbulent velocity diffusion terms to 2nd-order gradients (Eqs. 3.9, 3.10, 3.11),

\[
\overline{u_k u_i u_j} = -q \lambda_1 \left( \frac{\partial u_i u_j}{\partial x_k} + \frac{\partial u_i u_k}{\partial x_j} + \frac{u_j u_k}{\partial x_i} \right) \quad (3.9)
\]

\[
\overline{u_k u_j \theta} = -q \lambda_2 \left( \frac{\partial u_i \theta}{\partial x_i} + \partial u_j \theta \right) \quad (3.10)
\]

\[
\overline{u_k \theta^2} = -q \lambda_3 \frac{\partial \theta^2}{\partial x_k} \quad (3.11)
\]

where \( \lambda_1 \), \( \lambda_2 \) and \( \lambda_3 \) are length parameters.

Mellor and Yamada (1974) offered a hierarchy of four PBL turbulence closure models based on the turbulent moment equations derived by Mellor (1973). The different levels of closure models are obtained by ordering terms as products of
the degree of anisotropy, $a$, with $a = 0$ denoting isotropy, and $q^3/\Lambda$. $a$ is assumed to be small, and have the same order as the non-dimensional measure of the departure from isotropy, $a_{ij}$

$$u_i u_j \equiv \left( \delta_{ij} + a_{ij} \right) q^2 \quad (3.12)$$

The Level 4 model retains all the terms in the Reynolds stress model equations presented by Mellor (1973) after implementing the aforementioned simplifications to Eqs. 3.1, 3.2, and 3.3, except for those including the Coriolis parameter, since their values are comparatively small in the boundary layer. The only further assumption was that all length scales are proportional to the boundary layer length scale, $l$, as such:

$$l_1, l_2 = A_1 l, A_2 l \quad (3.13)$$

$$\lambda_1, \Lambda_2 = B_1 l, B_2 l \quad (3.14)$$

where $A_1$, $A_2$, $B_1$, and $B_2$ were empirically determined, and $l$ is the boundary layer length scale. Following Blackadar (1962)

$$l = \frac{kz}{1 + kz/l_0} \quad (3.15)$$

where $k$ is the von Karman constant and $z$ is the height from the surface. As $z$ approaches to zero, $l \sim kz$, while as $z$ increases to infinity, i.e. exits the bounds
of the PBL, \( l \sim l_0 \). Mellor and Yamada (1974) adopted the following expression for \( l_0 \) that incorporates features of the turbulence field,

\[
l_0 = \alpha \frac{\int_0^\infty z q \, dz}{\int_0^\infty q \, dz}
\]  

(3.16)

where \( \alpha \) is a constant that is empirically determined, with a suggested value of 0.1 by Mellor and Yamada (1974). Finally, it was assumed that \( \lambda_3 = \lambda_2 = \lambda_1 \), and equal to 0.23\( l \) following Mellor and Herring (1973).

Under the assumption that diffusion and advection terms are \( O(a) \), more precisely \( O(a \frac{q^2}{\Lambda}) \), neglecting \( O(a^2) \) terms such as time-rate of change, advection and diffusion terms for the anisotropic components of turbulence moments yields the Level 3 model. This closure model retains prognostic equations only for TKE and \( \theta^2 \). Mellor and Yamada (1982) introduced a modification of Level 3 closure model, referred to as level 2.5, that serves as an intermediate step between Level 3 and Level 2 models. In this model, the material derivative and diffusion terms in the prognostic equation for \( \theta^2 \) are ignored, as opposed to neglecting advection and diffusion terms from the set of prognostic equations (Level 2) (Mellor and Yamada, 1974). This model still benefits from retaining the isotropic components of transient and diffusive turbulent processes as Level 3 model, while reducing its computational cost by eliminating one differential equation.

### 3.3.2.2 Mellor-Yamada Nakanishi and Niino Level 3 (MYNN3)

Nakanishi and Niino (2004) introduced improvements to Mellor and Yamada
(1974) (henceforth, MY) closure models Level 3 and 2.5, including optimizing constants in the closure schemes as well as the master length scale. These improvements to the MY Level 3 model helped remedying the underestimation of the convective boundary layer’s depth (Sun and Ogura, 1980), as well as the decaying magnitude of TKE in a stably stratified nocturnal PBL (Turton and Brown, 1987), based on comparisons with large-eddy simulation (LES) data. This new model performed better than the improved version of the MY 2.5 Level model, although the latter is computationally less expensive.

Despite superior performance of the Level 3 Nakanishi and Niino (2004) model compared to the MY Level 3 model, it suffered from computational instability during the simulation. This problem was later addressed by Nakanishi and Niino (2006) by ensuring that their model could be realized under the full breadth of conditions encountered in the PBL. They proposed a scheme that imposed a set of constraints on the turbulent terms such as the temperature and velocity variances and the length scale in the case of turbulence. This model is heretofore referred to as MYNN. In the model proposed by Nakanishi and Niino (2004), $S_M$ and $S_H$ are stability functions for momentum, and heat and moisture, respectively, and components of the eddy diffusivity coefficients of the turbulent flux terms in the Level 3 model. In other words, they added a stability correction to regulate the turbulence so as to prevent runaway turbulence under conditions of rapid PBL growth. These stability correction terms are written as the sum of their expressions in the 2.5 Level model and the difference between Level 3 and Level
2.5 models, denoted by the subscript 2.5 and a prime, respectively (Eqs. 3.18).

\[ S_M = S_{M2.5} + S_M' \]  \hspace{1cm} (3.17)

\[ S_H = S_{H2.5} + S_H' \]  \hspace{1cm} (3.18)

The denominators of the stability functions, \( D \) and \( D' \) are functions of the stability ratio \( G_H \), defined as

\[ G_H = \frac{L^2}{q^2} \frac{g}{\Theta_0} \left( \beta_\theta \frac{\partial \Theta_l}{\partial z} + \beta_q \frac{\partial Q_w}{\partial z} \right) \]  \hspace{1cm} (3.19)

where \( L \) is the master length scale, \( q^2/2 \) TKE per unit mass, \( \Theta_0 \) the reference potential temperature, \( \Theta_l \) the liquid water potential temperature, \( Q_w \) the total water content, and \( \beta_\theta \) and \( \beta_q \) are functions of water vapor fluctuations determined from the condensation process (Nakanishi and Niino, 2004).

In this scenario, \( D \) and \( D' \), may change signs with changes in \( G_H \) due to variations in stability in the flow, leading to a singularity problem. For unstable stratified conditions, constraints proposed by Helfand and Labraga (1988) prevent the singularity problem. In stable stratified boundary layers, \( D' \) can become non-positive. To avoid this, Nakanishi and Niino (2006) found the following restriction on \( L/q \),

\[ \frac{L}{q} \leq \left[ \frac{g}{\Theta_0} \left( \beta_\theta \frac{\partial \Theta_l}{\partial z} + \beta_q \frac{\partial Q_w}{\partial z} \right) \right]^{-1/2} \text{ for } G_H < 0 \]  \hspace{1cm} (3.20)
Since the vertical gradient of virtual potential temperature, $\partial \Theta_v / \partial z$ can be written as the sum of the terms in parentheses in Eq. 3.20, the condition on $L$ prescribed by Eq. 3.20 reduces to $L \leq q/N$, where $N$ is the Brunt-Väisälä frequency. This condition constrains the vertical distance that a parcel of air can move upward against the buoyancy force in a stable layer.

Perhaps, the main improvement of MYNN over MY is the specification of $L$. Unlike Mellor (1973) that disregarded effects of stability on $L$, MYNN proposed a new specification for $L$, such that it is constrained by the smallest of $L_S$, $L_T$, and $L_B$

$$\frac{1}{L} = \frac{1}{L_S} + \frac{1}{L_T} + \frac{1}{L_B}$$  \hspace{1cm} (3.21)

where $L_S$ is length scale in the surface layer that is proportional to $kz$, $L_T$ is similar to Eq. 3.16, except that $\alpha = 0.23$, which depends on the length of the turbulent field in the PBL, and $L_B$ is the buoyancy length scale and proportional to $q/N$. Nakanishi and Niino (2009) further improved MYNN model by re-evaluating the turbulence closure constants, as well as the proportionality constants in the stability functions, using LES data for convective PBLs.

3.3.2.3 University of Washington Moist Turbulence parameterization (UW)

Bretherton and Park (2009) introduced the University of Washington Moist Turbulence (UWMT) parameterization that is an improved and numerically stable
version of the second-order turbulence closure scheme proposed by Grenier and Bretherton (2001) (hereafter, GB01), designed for implementation in Community Atmosphere Model version 3 (CAM3). This model was proposed with the goal of providing a realizable treatment of marine stratocumulus. GB01 enhanced representation of stratocumulus-capped boundary layers (SCBLs) in comparison to a number of other turbulence closure parameterizations, such as Burk and Thompson (1989) and Gayno (1994). They all employed moist-conserved variables to handle changes in boundary layer stratification due to saturation. However, GB01 succeeded at producing sharp inversions, in contrast to the diffused inversions above SCBLs rendered by other models, using an explicit entrainment closure model for determining entrainment diffusivity at the boundary of convective layers.

The moist-conserved variables used in UW scheme are total specific humidity $q_t = q_v + q_l + q_i$, and liquid-ice static energy $s_t = c_p T + g z - L q_t - (L + L_f) q_i$, where $q_v$, $q_l$, and $q_i$ are the specific humidity of water vapor, liquid water, and ice, respectively, and $L$ and $L_f$ are the latent heats of vaporization and freezing. Moreover, since conditions are well-mixed within a turbulent layers, profiles of momentum and scalar variables remain rather unaltered by non-local scalar transport. Hence, diffusivities of these variables in this region was based on local TKE ($e$) estimation (Bretherton and Park, 2009). Turbulent fluxes of horizontal velocity ($u$ and $v$) and moist-conserved variables $s_i$ and $q_t$ are represented as
downgradient diffusion

$$w'\chi' = -K_{\chi} \frac{\partial \chi}{\partial z}$$  \hspace{1cm} (3.22)

with eddy diffusivity and viscosity defined as

$$K_h = l S_h e^{1/2}$$  \hspace{1cm} (3.23)

$$K_m = l S_m e^{1/2}$$  \hspace{1cm} (3.24)

where \( l \) is the turbulent master length scale characterizing TKE dissipation, \( S_h \) and \( S_m \) nondimensional stability functions following Galperin et al. (1988), and \( l S_h \) and \( l S_m \) are stability-corrected length scales attributed to the vertical mixing length scale. UW uses Blackadar (1962) formulation for \( l \) (Eq. 3.15), with \( l_0 = \eta h \) approximating \( l \) asymptotically in the turbulent layer except in the surface layer, where it is estimated by \( k z \). \( h \) is the thickness of the turbulent layer, and Bretherton and Park (2009) determined \( \eta \) from LES simulations as the following

$$\eta = 0.085 \{2 - \exp[min(Ri^{CL}, 0)]\}$$  \hspace{1cm} (3.25)

where \( Ri^{CL} \) is the bulk Richardson number for the convective turbulent layer. Based on this expression, \( \eta \) is much larger in turbulent layers that are strongly convective, where \( Ri^{CL} \) takes on negative values.
The main difference between UW parameterization scheme (Bretherton and Park, 2009), and MY and MYNN, is that in the UW scheme TKE is diagnostic rather than prognostic. UW neglects TKE storage, and models the production, transport and dissipation components of the horizontal mean TKE equation. The buoyancy and shear TKE production terms, \( B \) and \( P_s \), are prescribed as

\[
\begin{align*}
P_s &= -\overline{w'u'} \frac{\partial U}{\partial z} - \overline{w'u'} \frac{\partial V}{\partial z} = K_m S^2 \quad (3.26) \\
B &= \overline{w'b'} = -K_h N^2 \quad (3.27)
\end{align*}
\]

where \( S^2 = \left( \frac{\partial U}{\partial z} \right) + \left( \frac{\partial V}{\partial z} \right) \) is the vertical shear squared, \( b' \) buoyancy perturbation, and \( N^2 \) the buoyancy frequency, which is formulated in terms of vertical gradients of \( s_l \) and \( q_t \), with their coefficients depending on cloud fraction. TKE dissipation rate, \( D \), is parameterized by Bretherton and Park (2009) as

\[
D = \frac{e^{3/2}}{b_1 l} \quad (3.28)
\]

where \( b_1 = 5.8 \). The TKE turbulent transport term, \( T_e \), the convergence of the sum of vertical TKE flux and work done by pressure, is only considered in convective layers in UW, and is modeled in terms of turbulent-layer-mean TKE \( \langle e \rangle \) (Bretherton and Park, 2009):

\[
T_e = a_e(\langle e \rangle - e) e^{1/2}/l \quad (3.29)
\]
where $a_e$ is TKE relaxation rate. Bretherton and Park (2009) empirically determined $a_e = 1$ for a convective layer from LES data.

An important feature of the UW model is that when buoyancy fluxes become negative in the turbulent layer, it decouples and the conditionally unstable convective layer with moist saturated updrafts and unsaturated dry downdrafts that ensue are handled by cumulus parameterization. In a stably stratified turbulent layer, the UW model ignores turbulent TKE transport and storage, and the closure model simplifies to a first-order one. UW follows the Nicholls and Turton (1986) entrainment closure model at the top and bottom edges of convective layers. This entrainment closure depends on the evaporative cloud-top cooling, that acts to promote entrainment of the air above inversion into the cloud-top air, and sinking of this mixture into the layer.

### 3.3.2.4 Comparison between MYNN3 and UW PBL Parameterizations in WRF

Simulation accuracy in WRF, particularly as it related to cloud distribution and cover, proved particularly sensitive to the selection of the PBL parameterization. Multiple test simulations were run using the same input data as initial and boundary conditions, and physical domain specifications over Graciosa island for the same period of time with different PBL schemes, including UW (Bretherton and Park, 2009), which is adapted from CESM climate model for WRF, and the prognostic TKE PBL schemes Mellor-Yamada Nakanishi and Niino Level 2.5 and
These tests indicated that MYNN3 produced the closest qualitative representation of the clouds as compared to satellite observations and data collected at ACE-ENA and was the PBL scheme that was ultimately used. This PBL scheme is based on the Mellor-Yamada model (MY) Mellor and Yamada (1974, 1982), both of which are prognostic turbulent kinetic energy (TKE) schemes. To review, TKE quantifies the magnitude of turbulence in the PBL, which is comprised of contributions from vertical wind shear, buoyancy, turbulent transport, and dampening due to molecular viscosity. An alternative PBL scheme that uses MY as its base and predicts TKE values is the Mellor-Yamada-Janjic (MYJ) Janjić (1994). It is a 1.5-order closure scheme that is an improvement upon MY Level 2.5 turbulent closure model. A 1.5-order closure parameterization scheme incorporates diagnostic second-order moments for variables such as variances of potential temperature and mixing ratios, and first-order moments for other variables to predict second-order TKE (Cohen et al., 2015). As noted below, this alternative was dismissed on the basis of a past study.

Huang et al. (2013) used WRF in single column mode to conduct three case studies over subtropical oceanic regions to assess the performance of various PBL schemes. Included in their study were MYNN, MYJ, and YSU (Yonsei University PBL (Hong et al., 2006)) parameterizations, as well as the total energy-mass flux (TEMF) (Angevine et al., 2010), and the results were evaluated according to their ability to represent stratocumulus and shallow cumulus clouds when compared
to LES data from those regions. Their study concluded that in all three cases, MYNN better simulated vertical profiles of liquid water and potential temperature, and provided the least-biased thermodynamic structures than MYJ.

In our study, we also utilized the following optional settings in MYNN3: TKE advection, stochastic eddy diffusivity mass flux (StEM) Sušelj et al. (2013), momentum and TKE transport in mass flux scheme, a modified cloud-scale mixing length Ito et al. (2015), and cloud-top radiational cooling contributing to TKE production.

Figure 3.3: Downward longwave flux at surface (Wm$^{-2}$) on 2330 UTC 17 July 2017 using MYNN3 (left) and UW (right) PBL schemes.

Fig. 3.3 shows downward longwave flux at surface (Wm$^{-2}$) on 2330 UTC 17 July 2017 with MYNN3 (left) and UW (right) PBL schemes. This figure shows a considerable difference between the two PBL parameterizations in terms of cloud production. The image on the left from Fig. 3.5, shown later, exhibits
the MODIS Aqua true-color image from NASA Worldview on mid-day July 17, 2017. Unfortunately, the plots from the 2017 simulation using UW scheme are temporally discordant from the satellite view; they are applicable several hours later. Data storage restrictions on the Cheyenne system prevented us from saving all data from the UW simulations, but our observation while monitoring clouds during each simulation was the lack of cloud production from all PBL schemes that were tested with the exception of MYNN3 (and MYNN2.5). These two PBL schemes were able to maintain clouds throughout the simulation, including mid-day July 2017.

In the case of MYNN3 (and MYNN2.5), the clouds comprising the frontal band strengthen as the front passes over Graciosa island, and later break up and form patches of growing cumulus cloudiness that are supported by moisture fluxes from below. However, we observed that these clouds gradually perish over time in simulations that employed UW PBL parameterization, with no new clouds being generated by the model, which is evident in the ensemble of plots in Fig. 3.4 showing the evolution of cloud structures over a 24-hour period. Similar mesoscale cloud structures can be seen to the south east of the domain, in the left images of both Fig. 3.5 (satellite image) and the simulation plot using MYNN3 in Fig. 3.3. These structures are altogether absent in the UW plot in Fig. 3.3.

As discussed in the preceding subsections, the MYNN stability-adjusted specification of the turbulent master length scale, $l$, incorporates a buoyancy length scale, $L_B$, while UW follows the approach taken by Mellor and Yamada (1974) to
define $l$. The master length scale greatly impacts the behavior of stability functions ($S_M$ and $S_H$ for MYNN3, and $S_m$ and $S_h$ for UW), especially in turbulent convective boundary layers. Moreover, MYNN3 retains a prognostic second-order closure model for TKE, while UW adopts a diagnostic equation for TKE. We surmise that these two major differences between MYNN3 and UW PBL parameterizations are critical levers that play major roles in determining whether realistic cloud cover is produced in the WRF simulations over ENA. However, we acknowledge that other factors might have been responsible for the under-performance of UW scheme in terms of representing clouds in this domain, including interactions between UW and other physical parameterizations. There may be useful information about cloud dynamics and physics that could be gained by further analyzing the differences in the performance of MYNN3 and UW schemes, which could be the subject of further in-depth analyses.
3.3.3 Radiation Parameterization

It is crucial to correctly estimate the atmospheric radiative forcing in climate models in order to ensure their prediction accuracy. Among the various radiation transfer models available in WRF, the Rapid Radiative Transfer Model for GCMs (RRTMG) (Iacono et al., 2008), which is a modified version of RRTM (Mlawer et al., 1997) that can be readily applied to GCMs, was used in the longwave and shortwave radiation calculations in the model simulations in this study. RRTM and RRTMG are based on the line-by-line radiative transfer model (LBLRTM), which is an efficient and accurate model that applies to the full spectral range (Clough et al. (1992); Clough and Iacono (1995)). LBLRTM accounts for all significant molecular absorbers, and includes the continua of carbon dioxide, oxygen, nitrogen, ozone, and Rayleigh scattering extinction.

RRTM was developed for both the longwave (LW) and shortwave (SW) regions, and designed with the goal of increasing the accuracy of radiative fluxes and cooling rates (Mlawer et al., 1997). In order to accurately account for radiative transfer due to scattering in the atmosphere, a radiative transfer model needs to have ample information about the absorption coefficient distribution of species in the atmosphere. RRTM adopts correlated-\(k\) method to calculate radiative fluxes and cooling rates for an inhomogeneous atmosphere, which is significantly less computationally expensive compared to line-by-line models, and completely adaptable to accelerated multiple-scattering calculations. The correlated-\(k\) method heavily relies on detailed information on absorption coefficients for the
primary and minor molecular species. RRTM adopts these absorption coefficients from LBLRTM. It accounts for molecular absorbers such as water vapor, carbon dioxide, methane, nitrous oxide, ozone, oxygen, nitorgen, CFC-11, CFC-12, CFC-22, and CCL\textsubscript{4} in the longwave, and water vapor, carbon dioxide, ozone, methane and oxygen in the shortwave. Moreover, it considers extinction from aerosols, clouds and Rayleigh scattering.

RRTMG is structured mostly on the same physics and absorption coefficients as RRTM, with the addition of several modifications to enhance the computational efficiency of RRTM, and represents subgrid-scale cloud variability, in order to be compatible with GCMs. RRTMG shows reasonable accuracy relative to LBLRTM and RRTM, in the longwave and shortwave regions, respectively for clear sky conditions; a flux accuracy of 1.5\textit{Wm}\textsuperscript{−2} and 3\textit{Wm}\textsuperscript{−2} in the entire atmosphere, and heating rates accuracy of 0.2\textit{Kd}\textsuperscript{−1} and 0.1\textit{Kd}\textsuperscript{−1} in the troposphere, and 0.4\textit{Kd}\textsuperscript{−1} and 0.35\textit{Kd}\textsuperscript{−1} in the stratosphere, for the RRTMG\textsubscript{LW}, and RRTMG\textsubscript{SW}, respectively (Iacono et al., 2008). In order to alleviate the complexity of representing random subgrid-scale cloud variability, including cloud overlap, when multiple scattering exits, the Monte Carlo Independent Column Approximation (McICA) (Barker et al. (2002); Pincus et al. (2003)), which is a statistical technique, has been adopted by RRTMG\textsubscript{LW} and RRTMG\textsubscript{SW}.

The advantage of using RRTMG as the radiation transfer scheme in our simulations, aside from its accuracy, was that we took advantage of the option provided by WRF to input climatological water and ice-friendly aerosols data (aer\_opt =
3), which is compatible with Thompson microphysics. This option is particularly useful because the quality of representing radiative processes associated with water vapor, ozone, and long-lived greenhouse gases, directly impacts the accuracy of cloud simulations in the model.

### 3.3.4 Land Surface and Surface Layer Parameterizations

The surface sensible and latent heat fluxes are important drivers of the PBL. The PBL schemes directly impact the structure of clouds, especially in the case of cloud-topped boundary layers, and are very sensitive to surface fluxes. In order to capture mesoscale circulations driven by variations in surface parameters, such as temperature, albedo, soil moisture, and vegetation, subgrid-scale fluxes need to be taken into account.

Fortunately, in the case of this study, the complexities of land surface variability and hydrology processes are substantially mitigated, due to the fact that the majority of the simulation domain is located over the ocean. The large heat capacity of the ocean prevents drastic diurnal temperature gradients as those characteristic of land surfaces. Also, the surface properties of the ocean is considerably more stable than those on land; multiple factors affecting land surface features, such as snow cover, soil texture, vegetation, orography, seasonal surface emissivity, and urban land-use, are absent in the case of the ocean.

The land surfaces on the islands within the simulation domains in this study were parameterized using the unified Noah land surface model (Tewari et al.,
This scheme has four soil layers (10, 30, 60, and 100 cm thick), and solves for prognostic land states, such as surface skin temperature, total and liquid soil moisture, and soil temperature at each layer, canopy water content, and physical snow depth. The initial conditions for these prognostic equations are provided by the preprocessed input data generated by WRF Preprocessing System (WPS).

The coupling between the surface skin layer and the first atmospheric model level is parameterized by a surface layer scheme. This scheme provides exchange coefficients for sensible and latent heat and moisture to the land surface scheme, and the friction stress and water/surface fluxes of heat and moisture directly to the PBL scheme. These fluxes are particularly sensitive to the treatment of the thermal and moisture roughness lengths, that are estimated by the surface layer scheme. Since MYNN3 was used as the PBL scheme, the MYNN surface layer was required for simulations in this study.

3.3.5 Cumulus Parameterization

Processes associated with cumulus clouds substantially impact the large-scale temperature and moisture fields. Cumulus-induced subsidence leads to large-scale warming and drying of the air below, while cumulus detrainment results in large-scale cooling and moistening (Arakawa and Schubert, 1974). In the atmosphere, shallow and deep convective clouds usually coexist with each other. Shallow convection operates on lower altitudes than those where precipitation processes are activated, resulting in non-precipitating, low-level cumulus clouds.
These convective updrafts strongly modify the depth of the boundary layer, temperature, moisture, wind, and cloud structures by taking the surface mixed-layer air to the lower free troposphere (Bretherton et al. (2004); Kain (2004); Wang et al. (2004a); Wang et al. (2004b)).

The role of a cumulus parameterization scheme in climate models is to estimate the rate of convective precipitation, latent heat release, as well as the convective vertical redistribution of heat, moisture, and momentum, in the subgrid scale (Kain and Fritsch, 1990). However, because the resolution of the parent domain in our simulations was fine enough to explicitly resolve deep convection ($< 10\text{km}$), no cumulus parameterization scheme was required in our case.

### 3.4 Identifying Fronts

Despite the importance of marine fronts in creating intense weather systems in the lower troposphere and being an integral component of synoptic scale structure in the atmosphere, no comprehensive climatology of marine fronts exists in the literature. Moreover, no generally-accepted definition of marine fronts is found in the literature; definitions vary according to the application. This may be a consequence of the fact that, conventionally, detailed marine frontal analysis has been conducted manually based on case studies often derived from short-term experiments, which was a time-consuming task. There exists only a handful of such studies that are based on the manual surface analyses (Schumann and Van Rooy (1951); Reed and Kunkel (1960); Morgan et al. (1975); Flocas (1984);
Utsumi et al. (2014)). Perhaps most importantly, acquiring process-level data that can be used to diagnose and characterize frontal behavior over the oceans is extremely difficult. Vertical profiles of atmospheric thermodynamic structure, which are based on radiosondes, are piecemeal, and retrievals of thermodynamic structure from satellites do not have sufficient resolution to resolve the frontal structure in detail. Remote sensors that are used effectively on land to collect detailed surveys of frontal structures are not deployed widely over the oceans, and when they are, conventional instruments such as radar often function at a degraded manner due to operational limitations.

Increased computational capability and the emergence of global reanalysis datasets in recent decades have led to the development of automated schemes for constructing frontal climatologies ((Hewson (1998); Santurette and Joly (2002); Hewson and Titley (2010))), which has paved the way for more studies since the 1990s (e.g. Sanders and Hoffman (2002); Berry et al. (2011a); Berry et al. (2011b); Simmonds et al. (2012); Catto et al. (2013); Schemm et al. (2015); Thomas and Schultz (2019a); Thomas and Schultz (2019b)). Yet, these schemes only offer subjective approaches for defining fronts with varying degrees of strengths and weaknesses in producing a reasonable frontal climatology (Jenkner et al. (2010); Berry et al. (2011b); Schemm et al. (2015); Thomas and Schultz (2019a)). Thomas and Schultz (2019a) offered the following five components for defining and diagnosing fronts: a) a thermodynamic quantity or quantities, such as (equivalent) potential temperature, and wind, for identifying fronts; b) a function(s) acting on
a quantity (e.g. frontogenesis and gradient functions), to create the field used to
detecting fronts; c) a level(s) to operate the function(s) on the quantity, including
surface layer, 850 hPa, or 1 km above sea level; d) a threshold field value(s)
beyond which a frontal structure is recognized; e) identifying the category (e.g.
warm or cold) and the spatial scales of the frontal zone.

In this study, fronts in the vicinity of the Azores and at the ENA site were
detected in two phases. We initially identified potential frontal passages in the
area of interest using MODIS/AQUA satellite images from NASA WORLDVIEW
for the summers of 2017 and 2018. The two shown in Fig. 3.5 were chosen as
potential cold front examples for our study because of their distinct frontal cloud
structures advancing south around a low pressure system. The first of these cases,
July 17, 2017, occurred during the Aerosol and Cloud Experiment-Eastern North
Atlantic (ACE-ENA), which adds to usefulness of these simulations for future
studies because the Gulfstream-1 aircraft sampled the post-frontal cloudiness.

Next, surface meteorological data from the ENA were analyzed to detect the
temporal gradients in five dynamical variables at the surface that would indicate
a cold front passage. Fig. 3.6 shows the time series of surface wind speed and
wind direction, pressure, relative humidity and temperature over the ENA site.
The same variables from the WRF simulations at the same location are plotted
in conjunction with the ENA observations in order to compare the performance
of the model.
Figure 3.5: MODIS Aqua true-color images obtained at NASA Worldview centered on Azores showing the cold front advancing from the north-west on (left) mid-day July 17, 2017, and (right) mid-day July 29, 2018, respectively. (https://worldview.earthdata.nasa.gov)

Passage of cold fronts in the 2017 and 2018 cases were accompanied by a small drop in surface air temperature, which are somewhat masked by island thermal effects that are responsible for the diurnal temperature changes in the observations and the simulations. Evidence of the passage of these weak cold fronts is found in the decrease in the daytime and nighttime maximum and minimum temperatures during the first two days in the 2017 case and in the nighttime temperatures in the 2018 case. In addition, decreased relative humidity, a surface pressure minimum, and veering of the surface winds from southerly to northerly/north-westerly are observed as the fronts pass over the ENA.

Post-cold-frontal conditions are assumed to conclude when the surface temperature, pressure and winds return to their pre-frontal state. In the summer 2017 case, the leading edge of the front passed Graciosa at approximately 0200 UTC 18 July 2017, and the post-frontal region persisted until approximately 1800 UTC
19 July 2017 when an abrupt change in the wind direction signaled the onset of a new synoptic regime. Around this transition period the wind speed decreased from $6\, ms^{-1}$ to $2\, ms^{-1}$, and winds gradually shifted from north-westerly to south-easterly. Also, surface pressure reached a minimum of about 1017.5 hPa from a pre-frontal maximum of 1025.0 hPa. A corresponding decrease in surface air temperature and relative humidity can be seen around this point. However, simulated values of these two variables show a cold daytime bias that can be linked to the island effect phenomenon. The drop in measured surface relative humidity values was from 100% to a little less than 70%, while simulated relative humidity only decreased by about 20%. Surface temperature values from measurements decreased from about $26^\circ C$ to $20^\circ C$, whereas the simulated values dropped from $25^\circ C$ to a little less than $20^\circ C$.

Larger perturbations in the surface variables were observed and simulated in the 2018 case. The front reached the Azores at approximately 1800 UTC 29 July 2018 and the post-frontal environment existed until early on 31 July 2018. Winds veered as the front passed the ENA site, as expected, and a more northerly flow was observed in the post-frontal environment than was observed in the 2017 case. In association with the frontal passage in the 2018 case, wind speed changed from 9 to about $1\, ms^{-1}$. Relative humidity from observed values dropped from about 90% to a little above 50%, while those from simulation decreased from 100% to 80%. Also, surface temperature decreased from $25^\circ C$ to $20^\circ C$, and $23^\circ C$ to $16^\circ C$ for those obtained from measurements and WRF model, respectively.
Figure 3.6: Time-series of surface wind direction and wind speed, surface air pressure, relative humidity and temperature over the three-day WRF simulations during July 2017 and 2018, obtained from surface meteorology data from ACEENA (dot-dash blue line) and WRF (solid red line) located over Graciosa Island, Azores.
Potential temperature and horizontal wind fields at 850 hPa during the passage of fronts over the Azores, which lie in the geometric center of the plots, for the two simulations are shown in Fig. 3.7. In both cases, sharp gradients in both variables are evident in the first two plots in the leftmost column. Similar to the time-series analysis of the five surface variables used to detect fronts discussed above, it can be seen in Fig. 3.7 that the frontal passage of July 2018 seems to be more vigorous than that of July 2017, judging from the larger spatial gradient in horizontal wind direction and the potential temperature, as well as southward advancement of the front in 2018. This analysis further bolsters those obtained from surface variables.

Overall, the WRF simulations for the two cases reasonably reproduce the surface observations of the frontal and post-frontal environments at the ENA site, as demonstrated in Fig. 3.6. Island effects, which have been reported in past studies from islands in this region (Miller and Albrecht, 1995), are evident in the observations and in the simulations. The daytime cold bias in the temperature simulations, which also leads to increases in the surface relative humidity, is likely attributable to sampling biases because a portion of the model’s grid cell lies over the ocean. Given that WRF model simulations did a reasonable job of reproducing surface changes associated with the passage of these weak cold fronts, we are relatively confident that the simulated frontal and post-frontal environments over the entirety of the ENA domain bear some resemblance to reality.
3.5 Simulated and Observed MBL Structure at ENA

Next we examine aspects of the observed and simulated vertical structure of the MBL. Figs. 3.8-3.9 show time series of the vertical structure of hydrometeor location, vertical velocities (W (m/s)) in the column (WRF) and in the sub-cloud layer (ENA observations), vertical structure of horizontal velocity, and lifting condensation level (LCL) over the specified 72-hour periods in summer 2017 and 2018, from ENA observations and WRF simulations of conditions at Graciosa Island. The observed hydrometeor locations in the observations, shown in the
first and third panels in Figs. 3.8-3.9, are from the KAZR and represent the fractional coverage of all hydrometeors, cloud droplets and falling precipitation. In contrast, the WRF cloud fraction includes only cloud droplets, so the black dots at cloud base flag the presence of precipitation that exceeds a rain water mixing ratio of 0.01 g/kg anywhere beneath the cloud base.

Figure 3.8: Time series of vertical structure of cloud fraction, vertical and horizontal velocities and lifting condensation level (LCL) from observation and WRF data at Graciosa Island for 2017 simulation, respectively. Note that DL can measure vertical velocity (W) only below the cloud base.
Even though the simulated cloud structures are not exactly the same as those from observation data for each year, they follow a similar trend in most places along the time series. Average marine boundary layer heights (judging by the cloud-top height values) during the designated 3-day periods are deeper in WRF simulations than those observed by approximately 120 m and 190 m in summer 2017 and 2018, respectively. Sub-cloud vertical wind velocities are considerably weaker in model simulations, however simulated horizontal wind velocities are
consistent with the observed values in both cases. Lastly, LCLs simulated by WRF are lower than ENA observations by 200 m and 300 m on average for 2017 and 2018 cases, respectively, although their general trends are the same. This difference is due to island effects; simulated variables at grid scale over the island used to calculate LCLs are biased towards conditions over the ocean, and thus are smaller than those obtained from measurements over the island because the land warms faster than the ocean surface.

In general, the simulated MBL and cloud structures produce marine boundary layer clouds and MBL structures that appear relatively similar to those observed at ENA, though some important differences are evident. Updrafts in the simulations represent grid-scale vertical velocities in the subcloud layer, while the observations are two-minute averages of one-second profiles from the DL of the vertical velocity with 30-m vertical resolution. Averaging of the DL data are necessary because the observations are not comparable on a one-one basis. Applying a time-space conversion, average wind speeds in the MBL for the two simulations have an upper bound of \(\sim 8-9\) m/s, so the velocity mean at each level corresponds to nearly 1000-1100 m horizontal distance, which is roughly compatible with the grid scale velocity in the simulations. This analysis suggests that vertical velocities at grid-scale are considerably weaker in model simulations than those suggested by time-space conversion of the DL data, and do not demonstrate the repeating patterns of strong updrafts/downdrafts evident in the latter, however simulated horizontal wind velocities are consistent with the observed values in
both cases.

The MBL cloudiness on July 18, 2017 at ENA is thicker and less broken than the WRF-simulated structure. Similarly, MBL clouds are observed to be less broken in the July 30, 2018 case and, in addition, possess considerably more vigorous subcloud vertical velocities than those in the simulations. These observations echo a trend found in comparison with satellite images in these cases: that WRF simulations produce less MBL cloud than observed in post-cold-frontal conditions. In both cold frontal cases, simulated low-cloudiness appears more broken than the observed structures by the time the column has reached ENA. This may be due to the deeper MBL in the simulations than observed. Nonetheless, there is enough similarity to justify a further investigation of the upstream cloud transitions in the simulations.
Chapter 4
Cloud Life Cycle Overview

In both 2017 and 2018 simulations, the cold fronts were accompanied by a solid deck of stratocumulus in their wake. As the fronts journeyed south, this stratocumulus disintegrated into fragments and gradually became transition cloudiness, which was characterized by the presence of both cumulus and stratocumulus in various combinations. To study the transition process of the boundary layer and cloud structures in the simulations, we used FLEXPART-WRF version 3.3.2 Brioude et al. (2013) to calculate forward Lagrangian trajectories initialized in the solid stratocumulus decks in 3D. FLEXPART-WRF is a free Lagrangian particle dispersion model (LPDM) that uses mesoscale meteorological output from WRF to simulate trajectories of infinitesimally small air parcels (particles) in three-dimensional space (latitude, longitude, and altitude). Hegarty et al. (2013) studied three LPDMs, including FLEXPART, Hybrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) and Stochastic Time-Inverted Lagrangian Transport (STILT), using North American Regional Reanalysis (NARR) and a number of different WRF configurations as meteorological inputs and found all three to be competent models to compute plume trajectories. The model’s reliability has been further demonstrated in Brioude et al. (2011) and Brioude et al. (2012b),
where FLEXPART-WRF is used to conduct successful simulations of pollutant transport for two case studies. Further details on FLEXPART-WRF configuration used in this study are provided in Appendix B.

Figure 4.1: Forward lagrangian trajectories performed with FLEXPART-WRF on the 2017 and 2018 simulations (top and bottom rows, respectively). The starting point is the northernmost point, and the red star shows the location of the tracked parcel at respective time shown above each plot.

The output of FLEXPART-WRF consists of latitude, longitude, and altitude information of the centers of mass of different clusters of air tracer particles released from a specified point during their evolution, as well as the location information of the center of mass of all clusters. The trajectories of the mass center
of all clusters following passive air tracer particles released from a $0.02 \times 0.02$ degree domain located in the stratocumulus deck are shown in Fig. 4.1 for the 2017 and 2018 simulations. The red star indicates the location of the parcel at each of the three times indicated above the respective plots and the black line depicts the trajectory that the parcel followed to reach this point. In both cases, a prominent band of simulated cloud demarcated the leading edge of the cold front and the solid cloud layer located north of the frontal zone evolved into broken mesoscale cloud elements over a period of a few hours. Fig. 4.2 depicts conditions along the entirety of the Lagrangian trajectory, start-to-finish, and serves as an over-arching view of the conditions experienced by the parcel. Detailed mesoscale views illustrating conditions over vertical cross-sections of less than 100 km in length centered at the location of the red stars and aligned with the direction of the parcel trajectory at those points are shown in Figs. 4.3-4.4.

The process of marine stratocumulus breakup is depicted in full 32-hour time-series of the Lagrangian cloud fraction, vertical velocity (W), vertical structure of the horizontal wind, cloud-base and cloud-top heights ($z_b$ and $z_t$, respectively), LCL, two-meter air temperature (T2), and the upward latent flux at the surface (LH) along the trajectories in Fig. 4.2 for 2017 and 2018 simulations. In both cases, the solid stratocumulus decks were accompanied by weak updrafts and nearly constant LCL. Initially, the stratocumulus deck undergoes erosion at its base with time as LH and T2 rise along the trajectory. Along with these changes, the LCL increases and downdrafts appear when the deck begins to disintegrate.
Figure 4.2: Time series of cloud fraction, vertical and horizontal velocities, cloud-base and cloud-top heights ($z_b$ and $z_t$, respectively), lifting condensation level (LCL), temperature at 2 m ($T_2$) and latent heat flux from surface (LH) along trajectories shown in Fig. 4.1 for 2017 and 2018 simulations, respectively.
Figure 4.3: Vertical cross-sections of vertical velocity (W), horizontal wind speed, vertical structures of cloud fraction, cloud-base and cloud-top heights ($z_b$ and $z_t$, respectively), LCL, two-meter temperature ($T_2$), and LH, centered on the red star at each respective time shown in Fig. 4.1 and aligned with the Lagrangian trajectory of the parcels at that point for 2017 simulation. Cloud fraction is overlain the first two variables (the top two panels). Vertical axes of the first three panels in each column show the height from surface (m), and the left and right axes of the lowest panels correspond to $T_2$ (K) and LH ($Wm^2$), respectively.

As the conditions become more unstable further along the trajectory as indicated by frequent fluctuations in LCL, LH and T2, the breakup process accelerates both from below and above the cloud until the stratocumulus deck breaks into individual cloud elements. The broken cloud structure on July 18, 2017 after 7:30 and on July 29, 2018 after approximately 14:00 are similar, although the clouds
linger for a slightly longer period in the 2018 simulation. One notable difference between the two cases is the larger LH values in 2017, which may be related to the simulated differences in post-breakup cloud structure.

Mesoscale height-distance cross-sections covering distances of $\sim 100$ km for the 2017 (Fig. 4.3) and 2018 (Fig. 4.4) cases provide a more detailed perspective of the spatial distribution of the cloud structure immediately upstream and downstream of the tracked parcel (red star) along its path. These cross-sections center on the parcel location and align with the direction of the trajectory thereby representing
instantaneous moments in time at three stages of the evolution of the tracked particles in the cloud layer.

Initially the stratocumulus cloud deck existed under rather quiescent conditions characterized by relatively weak vertical velocities and relatively weak wind shear for both simulations in the northernmost latitudes (leftmost column). These quiescent periods were sporadically interrupted by temporary fractures in the solid cloud deck, although, overall, stratified structures prevailed. Moving from a location upstream of the parcel to a location downstream (Figs. 4.3-4.4), the LCL, LH and T2 slowly rose. While it is more subtle in the 2018 simulation, the breakup of the cloud deck appeared to begin mainly from the cloud base (left panels) because it rises and cloud-base cloud fraction decreases without similar changes at cloud top.

As the column moved further south-east, the solid cloud deck decomposed into cloudy fragments accompanied by notable disturbances in all variables (4.3-4.4, center column). Steadily increasing SSTs, erratic fluctuations in cloud fraction, vertical structures of wind, LCL, LH, and T2 corresponded to the destruction of the clouds both at the base and top. Columns upstream and downstream of the parcel’s location were intermittently cloudy and clear in both simulations, and mesoscale circulations were indicated by oscillations in the variables. As the column became more diluted from above and below, downdrafts became dominant, and the column became periodically decoupled from the ocean surface moisture source. Multilevel cloud layers coexisted with convective clusters in this phase of
Almost half a day after the onset of the breakup of the stratocumulus deck, the column transitioned into widely scattered, large mesoscale cloud clusters (4.3-4.4, rightmost column). These clusters contained relatively strong deep cumulus updrafts rising to nearly 1.5 km, and laterally detrained stratocumulus. These elements extend at least 300 m deeper than the broken clouds earlier along the trajectory (center column). A primary source of transporting moisture from the PBL to the upper troposphere, particularly in the Tropics and mid-latitudes in the summer, are these cumulus convective clouds (Xu and Randall, 1996). The anvil clouds produced by the lateral detrainment of cumulus clouds also comprise...
the major component of stratiform precipitation associated with mesoscale convective systems (Houze Jr, 1977).

Figure 4.6: Column average cloud water mixing ratio (g/kg) and vertical velocity of mesoscale cumulus structures 1, 2, and 3, on 1000 UTC 18 July 2017, demarcated on the left plot in Fig. 4.5.
Figure 4.7: Column average cloud water mixing ratio (g/kg) and vertical velocity of mesoscale cumulus structures 1, 2, and 3, on 0700 UTC 30 July 2018, demarcated on the right plot in Fig. 4.5.

Three such structures have been chosen and represented in Fig. 4.5 by red stars for each simulation. Column averages of cloud water mixing ratio (g/kg)
and vertical velocity (cm/s) are shown in Figs. 4.6-4.7. In all cases, strong updrafts are concentrated in the central regions of the cloud structure, which also exhibit the largest cloud depths. A much larger area within these structures is occupied by thinner stratus that surrounds the central updrafts and is accompanied by weak downdrafts.
Chapter 5

Decoupling Diagnostics

Simulated post-frontal clouds experienced breakup prior to their arrival at ENA in both cases, which lead to the supposition that the simulated transition occurred too far upstream. It is of interest, therefore, to analyze the physical processes operating before and after the transition in the simulations in hopes of gaining insight into model behavior and, perhaps, the transition process itself. Past studies have documented that decoupling is an important contributor to the breakup of a solid deck of stratocumulus. Bretherton and Wyant (1997) (hereafter, BW97) attributed decoupling in subtropical cloud-topped boundary layers to negative buoyancy fluxes below cloud base that acted to suppress convection in the sub-cloud region. They suggested that, as the cloud moved over warmer SSTs, increased surface latent heat fluxes (or equivalently, surface moisture fluxes) accompanied by lower surface relative humidity due to cloud-top mixing were the instigators of decoupling. As the Bowen ratio decreased, the increase in the surface latent heat/moisture flux caused increased buoyancy and liquid water fluxes within the cloud proportional to the surface fluxes, and subsequently led to a cloud-base minimum in the buoyancy flux. The difference between cloud-base and in-cloud buoyancy fluxes created a stable region below the cloud, marking
the onset of decoupling. As the surface latent heat flux became greater than the
net in-cloud radiative cooling, the stratocumulus layer became less well-mixed
and drier, and the gap between the lifting condensation level and cloud-base
widened, a phenomenon that was referred to as “deepening warming”. To study
sub-cloud and cloud-top processes that contributed to the breakup of the ma-
rine stratocumulus deck in the simulations and the effect of decoupling on these
processes, rectangular regions that straddled the transition from solid cloud to
broken cloudy patches for the 2017 and 2018 simulations shown in Fig. 5.1 were
selected for further analysis.

Classifying the clouds in these regions as residing in a coupled or decoupled
environment required an objective criteria. It must be noted, however, that we
adhere to the notion that decoupling is a continuum and there is no rigid threshold for clouds to instantaneously change from a coupled state to a decoupled one. What we seek is a measure that can separate the clouds that are either still coupled to the sub-cloud layer or in nascent stages of decoupling from those that are further into the decoupling process, as efficiently as possible. We label them as “coupled” and “uncoupled” clouds, respectively, for want of better terms that can convey our definitions of these two groups explained in the previous statement. There are various decoupling diagnostic measures proposed in the literature. The decoupling metrics explored in this study are discussed in the following sections.

5.1 Minimal Decoupling Criteria

BW97 proposed a “minimal decoupling criterion” for the mixed-layer model of a cloud-topped boundary layer (CTBL) driven radiatively atop areas with fixed SSTs, while ignoring drizzle. This criterion for negative sub-cloud buoyancy fluxes is given by

\[
\Delta F_R \leq A\eta(\delta z_c/z_i) \approx 0.45
\]

where \(\Delta F_R\) is the net radiative flux divergence across the stratocumulus cloud-topped boundary layer. In their model, BW97 assumed that \(\Delta F_R\) is the sole diabatic forcing in the CTBL and that its value is fixed. This flux divergence is given by \(F^+ + F_R - F_R(0)\), where \(F^+\) is the net radiative flux atop the cloud, and \(F_R(0)\), the net upward radiative flux at surface. In Eq. 5.1, \(F_L(0)\) is latent heat flux from
surface, $A$, a non-dimensional entrainment efficiency, $\delta z_c$, the cloud thickness, and $z_i$, the inversion height. Lastly, $\eta \approx 0.9$ is a thermodynamic coefficient that is weakly dependent on pressure and temperature.

This criterion was defined for typical values in subtropical stratocumulus and pertains to the moment when the sub-cloud buoyancy flux at the cloud base becomes negative. As acknowledged in BW97, this is the “broadest possible criterion for decoupling in that any negative buoyancy fluxes below cloud base indicate decoupling.” According to Eq. 5.1, decoupling initiates when the ratio of radiative flux divergence in the CTBL to the surface latent heat flux ($\Delta F_R/F_L(0)$) becomes smaller than a threshold value. This threshold is directly proportional to $\delta z_c/z_i$, that reflects the fraction of the boundary layer occupied by the cloud layer, and the parameter representing the efficiency of entrainment, $A$. The threshold value of 0.45 in Eq. 5.1 is obtained for the typical case in which the cloud layer fills approximately 25% of the depth of the boundary layer, and $A = 2$.

Adopting this diagnostic proved particularly challenging in this study, due to the fact that radiative fluxes at cloud top are not provided by WRF, therefore the net cloud-top radiative flux, $F^+_R$, and consequently, the radiative flux divergence across the cloud layer cannot be readily computed from the WRF simulations. The only approach for estimating the radiative flux divergence at cloud top would be to use the cloud-top radiative fluxes with those at TOA (that are available from WRF outputs) as a surrogate for this variable. To do this, it needs to be assumed that the longwave (LW) emission and shortwave (SW) albedo at TOA are very
close to their magnitudes at cloud-top, and that there are no high-altitude clouds above those in the vicinity of the boundary layer that are the subjects of this study in the domain of interest. A closer inspection revealed that the approximated flux ratio would not respond strongly to the transition from coupled to decoupled clouds, which may have partly been due to the implementation of these coarse approximations.

5.2 Jones Decoupling Criteria

Jones et al. (2011) proposed three separate decoupling diagnostics that were investigated in this study. The first decoupling diagnostic proposed by Jones et al. (2011) takes the vertical structure of the boundary layer into account in the context of changes in two moist-conserved variables, $\theta_\ell$ and $q_T$, between the surface and inversion, where $\theta_\ell$ is the liquid potential temperature and $q_T$, the total water mixing ratio. These definitions are

$$\begin{align*}
\theta_\ell & \approx \theta - \frac{L}{c_p} q_\ell \\
q_T & = q_\ell + q_v
\end{align*}$$

where $\theta$ is the potential temperature, $L$ the latent heat of vaporization, $c_p$ the dry air specific heat at constant pressure, and $q_\ell$ and $q_v$ are liquid water and water vapor mixing ratios, respectively. When the MBL is well-mixed, $\theta_\ell$ and $q_T$ are approximately constant beneath the capping inversion. Conversely, vertical
gradients in $\theta_T$ and $q_T$ are observed when the MBL is decoupled. This decoupling diagnostic quantifies the vertical gradients of moisture and temperature, and is given by

$$\Delta q = q_{bot} - q_{top}$$

$$\Delta \theta_T = \theta_{T, top} - \theta_{T, bot}$$

where variables with subscripts “bot” and “top” are calculated as the mean over the lower and upper 25% of the boundary layer below the inversion. Note that the subscript $T$ has been omitted in Eq. 5.4 and hereafter in this section. Jones et al. (2011) found profiles where $\Delta q > 0.5 \text{ gkg}^{-1}$ and $\Delta \theta_T > 0.5 K$ to be decoupled, based on data collected during the VOCALS Regional Experiment (VOCALS-REx) in October-November 2008 in the MBL over the Southeast Pacific.

These metrics have two advantages in comparison to the one discussed earlier in this section; they capture the definition of decoupling in MBL clouds, hence the decoupling mechanism, in their formulation, and both can be easily and directly calculated from the output of WRF simulations. Therefore, they appeared promising metrics to adopt for the purposes of this study.
The second decoupling diagnostic suggested by Jones et al. (2011) is a subcloud decoupling measure prescribed by the difference between LCL and cloud-base height, $z_b$, which is expressed as

$$\Delta z_b = z_b - z_{LCL}$$  \hspace{1cm} (5.6)

A smaller $\Delta z_b$ indicates a well-mixed boundary layer where cloud base is in close proximity to the LCL. As the boundary layer becomes more decoupled, the gap between the cloud base and LCL widens, and $\Delta z_b$ increases. The decoupling threshold recommended by Jones et al. (2011) is $\Delta z_b > 150$.

The final decoupling diagnostic proposed by Jones et al. (2011) is referred to as the “mixed layer cloud thickness” and is the difference between the inversion height ($z_i$) and LCL, or

$$\Delta z_M = z_i - z_{LCL}$$  \hspace{1cm} (5.7)

When the MBL is well-mixed, $\Delta z_M$ is equivalent to the cloud thickness. Latent heat released due to condensation within moist updrafts generates a buoyancy flux within the cloud layer. Thus, a thicker cloud layer can have larger values of vertically integrated buoyancy flux along its depth, and consequently, more in-cloud turbulence. A more turbulent cloud layer generates more entrainment, which in turn facilitates mixing of dry and warm air above the inversion with the in-cloud air mass and helps the cloud layer become decoupled from the sub-cloud
layer. Therefore, larger values of $\Delta z_M$ should correspond to more decoupled cloud layers.

The procedure used in Jones et al. (2011) was adopted to determine which of the diagnostics was best suited for use with the WRF simulations, so we tested the second and third decoupling criteria against $\Delta q$, which represented the first diagnostic. In order to calculate $\Delta q$, the capping inversion height $z_i$ is required. Because the capping inversion in the simulations is not sharp in most cases, two methods have been adopted to identify and cross-check $z_i$. The first method is from Jones et al. (2011), where $z_i$ is determined as the vertical level with the minimum temperature and relative humidity of at least 45%. The second approach identifies the inversion height as the level where $\frac{d}{dz} \theta_l$ and $\frac{d}{dz} q_T$ are maximum, while the relative humidity is greater than or equal to 45%. The results were almost the same in both cases for both 2017 and 2018 simulations, and wherever they did not coincide, the $z_i$ from the first approach was chosen.

Figs. 5.2-5.3 show scatterplots of $\Delta z_b$ and $\Delta z_M$ with respect to $\Delta q$, respectively, from the rectangular domains for the 2017 and 2018 simulations shown in Fig. 5.1. Note that the color schemes in all scatterplots in this study reflect the density of points, with dark red and dark blue signifying the areas with the maximum and minimum point densities for each given plot, respectively. The correlation between $\Delta z_b$ and $\Delta q$ in both 2017 and 2018 simulations is almost negligible, as seen in Fig. 5.2, while $\Delta z_M$ exhibits a positive correlation with $\Delta q$ in both cases (Fig. 5.3). However, no clear decoupling threshold in terms of $\Delta z_m$
could be determined in the data from the designated domains that would also coincide with a corresponding decoupling threshold value in $\Delta q$, which would be suitable for both simulations. The fact that the model is prescribed with discrete vertical levels for the entire atmosphere could partly explain the inefficiency of $\Delta z_b$ and $\Delta z_m$ as successful decoupling diagnostics for the model data. Cloud-base and inversion heights in the model can only be estimated in terms of fixed vertical levels and this rather crude estimation could negatively impact the ability of second and third decoupling diagnostics to successfully characterize the decoupling range. Hence, the first decoupling diagnostic suggested by Jones et al. (2011) is employed in this study.

Fig. 5.4 shows the composite profiles of $q_T$ (dark blue line), $\theta_e$ (black line), and cloud fraction (green line) with different ranges of $\Delta q$ as the decoupling measure. The dashed black and red lines are $z_i$ and LCL, respectively. To improve the
Figure 5.3: Scatterplots of $\Delta z_M$ and $\Delta q$ on 1800 UTC 17 July 2017 (left) and 1130 UTC 29 July 2018 (right), respectively.

Visualization, 10 times cloud fraction is plotted. In order to create the composites, first the profiles were interpolated over the same number of vertical levels below the LCL, between LCL and $z_i$, and between $z_i$ and 1500 m, to ensure that LCL and $z_i$ were aligned across all profiles. The variables were then averaged across all profiles, and the vertical axis was scaled so that $z_i$ and LCL reflected mean $z_i$ and LCL values. Clouds with $\Delta q > 2.0$ and $\Delta q > 2.1$ for 2017 and 2018 simulations, respectively, exhibit a higher degree of decoupling, since $q_T$ and $\theta_\ell$ values change with height from surface to the inversion height. Those with $\Delta q < 1.6$ and $\Delta q < 1.7$, on the other hand, indicate well-mixed boundary layer conditions, judging by how $q_T$ and $\theta_\ell$ remain relatively constant in the region below the capping inversion.

We note that decoupling is a gradual process whereby the conditions in the
Figure 5.4: Composite profiles for a) $\Delta q < 1.6 \text{ (g/kg)}$ and $\Delta q > 2.0 \text{ (g/kg)}$ on 1800 UTC 17 July 2017 (leftmost two plots), and b) $\Delta q < 1.7 \text{ (g/kg)}$ and $\Delta q > 2.1 \text{ (g/kg)}$ 1130 UTC 29 July 2018 (rightmost two plots). $q_T$ is indicated by the navy blue line, and $\theta_e$ by the black line. The green line shows 10 times the cloud fraction for better visualization. The inversion height $z_i$ and LCL are also shown in dashed black and red lines, respectively.
boundary layer become less well-mixed (i.e. the cloud element becomes less coupled, until the cloud-base and in-cloud regions form separate stable entities). Therefore, we suspect that there is no exact threshold value for distinguishing between the decoupled and coupled clouds, and we adhere to this assumption in our attempts to classify clouds in the simulations according to their coupling state. Hence, the plots designated as “coupled” and “decoupled” clouds in the following sections are not necessarily those that reside in absolutely well-mixed conditions, or are completely decoupled from the sub-cloud region, respectively, but rather encompass examples that fall somewhere in the decoupling range, leaning towards being more coupled or decoupled than otherwise, respectively.

With this explanation, for both simulations, we designated cloud layers with $\Delta q < 1.6$ as coupled and those with $\Delta q > 2.1$ as decoupled, and neglect those that fall somewhere in between these values. While these threshold values have an element of subjectivity, they are consistent with the decoupling continuum that exists during the decoupling process in both simulations.

5.3 Buoyant Production of TKE (QB) and Vertical Velocity (W)

Prior to exploring the decoupling diagnostics discussed above, the decoupling measure that was adopted for use in this study was the sub-cloud buoyant TKE production (QB) values, following BW97. This variable seemed like a reasonable first choice based on past observations that the extent of turbulent mixing due to
buoyancy below cloud base would be a good indicator of the degree of decoupling of the cloud layer with respect to the sub-cloud region. The buoyant turbulent mixing below the cloud base significantly dictates the supply of TKE and moisture to the cloud layer. Perhaps a more precise variable representing the maintenance of clouds by sub-cloud moisture would be the vertical moisture flux, however, unlike QB and W, it was not a WRF output variable. Figs. 5.5 and 5.6 show the same cross-sections as in Figs. 4.3 and 4.4 for 2017 and 2018 simulations, respectively, but for the vertical profiles of W and QB (vertical velocity panels are included again for easier comparisons between regions with different values of QB and W).

The solid layer of stratocumulus in the top-most panels of Figs. 5.5 and 5.6 coincide with sub-cloud regions exhibiting positive QB and weak vertical velocities. These sub-cloud regions also exhibit small negative values of QB in the majority of the cloud layer, except in a shallow layer immediately below the cloud top. These in-cloud negative QB values in the stratocumulus-topped boundary layer prior to the breakup process indicate statically stable conditions within the cloud layer, and that the circulation is mainly driven by the sub-cloud layer, while only a small depth below the cloud top is sustained by cloud-top radiative processes. This is surprisingly at odds with the general understanding of how overcast stratocumulus clouds are maintained, which is mainly by cloud-top processes (BW97). As the breakup process initiates, QB values below the cloud base are reduced to the point that the positively buoyant layer periodically detaches completely from
Figure 5.5: Vertical cross-sections of vertical velocity \( W \), horizontal wind speed, and buoyant production of TKE \( QB \), centered on the red star at each respective time shown in Fig. 4.1 and aligned with the Lagrangian trajectory of the parcels at that point for 2017 simulation. Cloud fraction is overlain the variables and the vertical axes are the height from surface (m).

the cloud layer, and hence no longer continually supplies it with moisture and TKE (the second and third panels in Figs. 5.5 and 5.6). The regions where the cloud layer is diluted are marked with receding positive QB in the cloud layer, as
well as downdrafts extending all throughout the cloud and sub-cloud layer, while the mesoscale patches of cloudiness are still attached to a sub-cloud positive layer of QB and rather strong updrafts in the entirety of the boundary layer.

These observations supported our initial use of QB (and W) as a decoupling criteria. We note that arriving at a threshold value for sub-cloud QB values and
the depth below the cloud base across which it should be considered is subjective
and was based solely upon the observed values from the simulations used in this
study. In Figs. 4.3 and 4.4, we identified decoupled clouds as those that are atop
regions of more disturbed LCL and surface latent heat fluxes, and where positive
QB became completely detached from the cloud-base as seen in Figs. 5.5 and 5.6.
Therefore, we defined a decoupling indicator as the average value of QB over a
few layers below the original stratocumulus deck being smaller than a threshold
value close to zero: $QB_{subcloud} < 10^{-4} \text{ m}^2\text{s}^{-2}$. This indicator identified simulated
cloud elements that are most probably decoupled. Clouds that did not meet
this condition were assumed to be somewhere in the decoupling continuum; they
were either completely coupled or are in the process of becoming decoupled. To
reduce the ambiguity in defining coupled clouds across this continuum, we applied
a second condition. Coupled clouds had to satisfy the condition $QB_{subcloud} >
10^{-3} \text{ m}^2\text{s}^{-2}$. The threshold values of $QB_{subcloud}$ for both conditions were chosen
based on the ranges of QB in Figs. 5.5 and 5.6.

However, after further studying the efficiency of both QB and W in determin-
ing the coupling state of clouds and considering the correlations between these
two variables and $\Delta q$ as discussed in Jones et al. (2011), it became clear that
neither of these two variables are reliable decoupling metrics. Figs. 5.7-5.8 show
scatterplots of average sub-cloud vertical velocity ($W_b \text{ (cm/s)}$) and buoyant TKE
production ($QB \text{ (m}^2\text{s}^{-2})$) across 100 m below cloud base, respectively, and $\Delta q$
(g/kg) for clouds within the rectangular domains shown in Fig. 5.1 for 2017 and
Vertical velocity at cloud base seemed to be a slightly preferable decoupling metric relative to $\text{QB}$ because it exhibited a slightly linear relationship with $\Delta q$ values smaller than 1.5 g/kg, especially in 2018, but no robust correlation was found between these two variables. Based on the results in Fig. 5.7, points with $W_b$ greater than approximately 5 cm/s roughly correspond with $\Delta q$ values less than 2 g/kg. In the same interval, there are a considerable number of points with smaller $W_b$ values (mainly negative). Therefore, with $W_b$ as the decoupling criteria, many examples that would otherwise fall under the category of “coupled” clouds were classified as “decoupled”.

The same conclusion can be reached about QB as a decoupling metric based on Fig. 5.8. Contrary to what was expected, QB showed no discernible correlation with $\Delta q$ across all ranges. Therefore, it can be concluded that QB would not be an adequate decoupling metric to be used in this study. We assume that a
Figure 5.8: Scatterplots of buoyant TKE production (QB (m^2 s^{-2})) across 100 m below cloud base, and Δq (g/kg), for 2017 and 2018 simulations, respectively.

A contributing factor to the lack of success using this approach may be due to the subjectivity of the thresholds chosen to calculate the sub-cloud QB metric in the first place or because our observations were based on a handful of cross-section plots from select locations.
Chapter 6

Cloud-base Decoupling Processes

It is apparent from the plots in the leftmost column of Figs. 4.3-4.4 that the disintegration of solid layer of begins at cloud base, with no corresponding behavior at cloud top in the same location. Hence, the cloud-base processes that contribute to the thinning and ultimately breaking up of the stratocumulus decks located at the wake of the fronts in both simulations are studied first. In this chapter, we consider the role of latent heat flux from the surface (LH) and LCL in the decoupling process at cloud-base by looking at their correlations with the cloud-base cloud fraction, as well as the their Lagrangian derivatives. Next, the contributions of surface wind speed and relative humidity on variations in LH are investigated.

6.1 Correlations between latent heat flux from surface (LH) and cloud-base cloud fraction

Locations where the stratocumulus deck is starting to transition into broken cloud structures coincide with increases in LH shown in the leftmost panels of Figs. 4.3-4.4. Following BW97, we first compute the correlation between LH and cloud
fraction in the lowest 100 m of cloud layers (this cloud fraction is hereafter designated as $CLD_B$). The cloudy elements within the study regions shown in Fig. 5.1 are divided into coupled and decoupled categories based on the decoupling criteria described in the previous section. The top row of Fig. 6.1 shows the corresponding plots for the 2017 and 2018 simulations, respectively.

Figure 6.1: Correlations between a) average cloud fraction across the lower 100 m of MSC ($CLD_B$) and latent heat flux from the surface (LH) (upper panels), b) $\frac{D}{Dt}(CLD_B)$ and $\frac{D}{Dt}(LH)$ (lower panels), for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two panels) and 1130 UTC 29 July 2018 (rightmost two panels), respectively.

In both cases, $CLD_B$ for decoupled clouds does not show a strong correlation with LH; 0.305 and -0.216 for 2017 and 2018, respectively. The coupled $CLD_B$ exhibits a negative and relatively better correlation with LH as compared to the decoupled cloud elements for each simulation. The correlation coefficient
between coupled $CLD_B$ and LH in 2017 is -0.391, versus -0.54 in 2018. There also does not appear to be a threshold in LH value for the onset of decoupling (as suggested by BW97), at least in these WRF simulations, since in both cases, coupled and decoupled elements correspond to the same range of LH, with the majority of points roughly from 90 to 140 Wm$^{-2}$, and 120 to 170 Wm$^{-2}$, for 2017 and 2018 cases, respectively. It is also observed that values of LH and the correlation coefficient with coupled clouds are larger in 2018 than in 2017. It can be inferred that as long as the stratocumulus deck is coupled, changes in LH have a tendency to inversely affect cloud fraction in the lower levels of the cloud deck. Conversely, when the clouds become decoupled from the sub-cloud region and $CLD_B$ significantly decreases, changes in LH have little impact on $CLD_B$. This latter observation may be due to the buffering effect of decoupling, which enables moisture accumulation near the surface (Albrecht et al. (1995); Miller and Albrecht (1995); and others).

Fig. 4.2 as well as plots in the leftmost columns of Figs. 4.3 and 4.4 suggest that local fluctuations in LH, rather than a threshold value, coincide with areas where cloud-base thinning and decoupling commence and the solid cloud deck becomes broken. To investigate the effect of variations in LH directly below the cloud layer on changes in $CLD_B$ following the cloudy air parcels in the vicinity of the cloud base, we computed correlations between the average of Lagrangian derivatives (material or total derivatives) of cloud fraction across 100 m above cloud base and the Lagrangian derivative of LH directly below the cloud base.
The Lagrangian derivatives of $CLD_B$ and LH following the cloud base are laid out in Eqs. 6.1-6.2, respectively:

\[
\frac{D}{Dt} CLD_B = \frac{\partial}{\partial t} CLD_B + u \frac{\partial}{\partial x} CLD_B + v \frac{\partial}{\partial y} CLD_B + w \frac{\partial}{\partial z} CLD_B \tag{6.1}
\]

\[
\frac{D}{Dt} LH = \frac{\partial}{\partial t} LH + \bar{u} \frac{\partial}{\partial x} LH + \bar{v} \frac{\partial}{\partial y} LH \tag{6.2}
\]

The first term on the right-hand side of both equations above represents the local time derivative, and the rest of the terms characterize advection of each variable by the wind. The overbars in the right-hand side of Eq. 6.1 indicate that first cloud-base cloud fraction at each model vertical level that fell within the lowest 100 m of the cloud layer was used to estimate the local time derivative, as well as the advection terms for each of the zonal, meridional, and vertical components with the corresponding velocities at those levels ($u$, $v$, and $w$, respectively). $\frac{D}{Dt} CLD_B$ for each cloud element was then calculated as the average of the Lagrangian derivatives of cloud fraction at each level (equivalent to the sum of the time derivative and advection terms at the corresponding vertical level). Since we were interested in estimating the Lagrangian derivative of LH directly below the cloud, average horizontal velocities across the vertical levels within the lowest 100 m from the cloud base ($\bar{u}$ and $\bar{v}$) were used in the advection terms in Eq. 6.2. Finally, there is no advection of LH by the wind in the vertical direction, since LH is a 3-D variable with no vertical component.

The Lagrangian derivatives in Eqs. 6.1-6.2 using WRF data were then estimated by adopting the finite difference method. Eq. 6.3 and Eq. 6.4 show the
finite difference representation of the Lagrangian derivative terms on the right-hand side of Eqs. 6.1-6.2, respectively

\[
\frac{CLD_B^{n+1}_{i,j,k} - CLD_B^n_{i,j,k}}{\Delta t} + u^n_{i,j,k} \frac{CLD_B^n_{i+1,j,k} - CLD_B^n_{i-1,j,k}}{2\Delta x} + v^n_{i,j,k} \frac{CLD_B^n_{i,j+1,k} - CLD_B^n_{i,j-1,k}}{2\Delta y}
\]

\[
\frac{CLD_B^n_{i,j+1,k} - CLD_B^n_{i,j-1,k}}{2\Delta y} + w^n_{i,j,k} \frac{CLD_B^n_{i,j,k+1} - CLD_B^n_{i,j,k-1}}{2\Delta z}
\]

(6.3)

\[
\frac{LH^{n+1}_{i,j} - LH^n_{i,j}}{\Delta t} + \bar{u}_{i,j} \frac{LH^n_{i+1,j} - LH^n_{i-1,j}}{2\Delta x} + \bar{v}_{i,j} \frac{LH^n_{i,j+1} - LH^n_{i,j-1}}{2\Delta y}
\]

(6.4)

where \( n \) refers to the current time step, \( i, j, k \) are the zonal, meridional and vertical spatial directions, and \( u, v, w \) are the zonal, meridional and vertical velocities, respectively. \( \Delta x, \Delta y \) are equal to the longitudinal and latitudinal length of each grid point and \( \Delta z \) is the vertical distance between the layer \( k \) and the one above it, while \( \Delta t \) is the simulation time step. Also, \( \bar{u}_{i,j} \) and \( \bar{v}_{i,j} \) in Eq. 6.4 are the average zonal and meridional velocities across the lowest 100 m from the cloud base at grid point \((i, j)\), respectively.

A point of clarification is that the Lagrangian derivative of LH is a means to examine how LH values would hypothetically change in locations as seen directly below the cloud following the cloudy parcel, and advected by winds proportional to the average values in the lower level of the cloud base. Therefore, the Lagrangian derivatives of LH here are not values of LH that would be advected by
the wind in the vicinity of the ocean surface. These LH values represent the integrated effects of all of the processes that contribute to the LH, such as the surface winds and the gradients of temperature and moisture between the atmosphere and ocean near the ocean surface.

Results of this analysis are shown in the second row of Fig. 6.1. The correlation coefficients for coupled cases are now much improved, -0.515 and -0.651 for 2017 and 2018, respectively, compared to the correlations between $CLD_B$ and LH for coupled clouds in each simulation. On the other hand, in the case of decoupled clouds, there is negligible correlation between total derivatives of $CLD_B$ and LH in 2017 (0.008) and it is weaker than the corresponding correlation for coupled clouds in 2018 (-0.376), although it is slightly better than the correlation between decoupled $CLD_B$ and LH in 2018. Therefore, erosion and breakup in the lower levels of the cloud deck ($CLD_B$) in these simulations is loosely linked to instantaneous fluctuations in the surface LH following the cloud base in coupled regions rather than the absolute values of latent heat flux from the ocean surface below the cloud. The coefficients of determination for the Lagrangian derivatives of LH and $CLD_B$ (square of the correlation coefficient) are 0.265 and 0.424 for the 2017 and 2018 cases, respectively, which means that approximately one-quarter and slightly less than half of the variance in the Lagrangian derivative of $CLD_B$ is explained by the Lagrangian derivative of LH. Hence, there are other processes that contribute to the changes in $CLD_B$. 
6.2 Correlations between lifting condensation level (LCL) and cloud-base cloud fraction

Latent heat flux modulates the LCL and past studies have also reported strong connections between the height of the LCL and the occurrence of coupled regions within a transition cloud field (Miller and Albrecht, 1995). Fig. 6.2 shows correlations between the LCL and $CLD_B$ (top panels) in the 2017 and 2018 cases. Moderate and strong correlations between the LCL and the $CLD_B$ in coupled clouds are found in both cases (-0.339 and -0.724, for 2017 and 2018, respectively). While the correlation for decoupled clouds in 2018 is poor (-0.194), a positive and moderate correlation is exhibited for decoupled clouds in 2017 (0.345).

The Lagrangian derivative of the LCL below the cloud base and $CLD_B$ is calculated similar to $\frac{D}{Dt} LH$ (Eqs. 6.2-6.4) and shown in the bottom panels of Fig. 6.2. The correlation coefficients for the Lagrangian derivatives compared to their counterpart in the top panel for coupled clouds is slightly improved in 2017 (-0.4 vs. -0.339), whereas it is smaller in 2018 (-0.629 vs. -0.724). The correlation coefficients for the decoupled clouds follow the same pattern as those for latent heat flux shown in Fig. 6.1; negligible and relatively weak correlations for the Lagrangian derivatives (0.107 and -0.268) in 2017 and 2018, respectively. In fact, the plots are virtually identical to those in Fig. 12, which reflects the strong relationship between LH and LCL. Similar to the case for latent heat flux, Lagrangian derivatives of the LCL demonstrate a moderate and strong correlation with the Lagrangian derivative of $CLD_B$ for coupled clouds, for 2017 and 2018.
simulations, respectively. However, in terms of absolute values, the local LCL is more important in determining $CLD_B$ than steady changes in the LCL observed following the parcel trajectory for coupled clouds only in 2018. While this relationship in 2018 is strong, this signal lacks the year-to-year consistency exhibited in the Lagrangian correlations between LH and $CLD_B$.

![Figure 6.2: Correlations between a) average cloud fraction across the lower 100 m of MSC ($CLD_B$) and LCL (upper panels), b) $\frac{D}{Dt}(CLD_B)$ and $\frac{D}{Dt}(LCL)$ (lower panels), for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two panels) and 1130 UTC 29 July 2018 (rightmost two panels), respectively.](image)

The results shown in Fig. 6.1 suggest that the changes in the surface LH following the cloud base may be partly responsible for the initiation of the decoupling process. There are at least two mechanisms that could lead to this link. One potential mechanism echoes the deepening-warming hypothesis; the LH release at cloud base becomes large enough that it fuels much larger updrafts within the
cloud, which in turn increase mixing at cloud top and initiate downdrafts that penetrate the cloud base and dry the air below, locally decoupling the cloud from the surface. Another possibility is that warming dominates moistening, deepening the boundary layer and consequently raising the LCL. A higher LCL leads to local moisture accumulation, which eventually lowers the LCL and enables cumulus to from at the top of the decoupled layer and rise to the base of the inversion. This process requires no inherent contribution from cloud-top instabilities. In decoupled regions, the cloud is no longer substantially supplied with buoyant TKE and moisture from below and, as such, exhibits limited response to changes in the surface LH and moisture flux. While it is possible that both of the LH-related breakup scenarios suggested above operate depending upon conditions, cloud-top processes are also explored to better understand stratocumulus breakup and changes in the decoupled cloud structures beyond the breakup point.

6.3 Correlations between horizontal wind speed and relative humidity, and surface latent heat flux

An increase in LH followed by the initiation of decoupling at cloud base should correspond with reduction in surface relative humidity (RH) due to cloud-top mixing, as described by the deepening-warming hypothesis proposed by BW97. Fig. 6.3 below shows the correlations between latent heat flux (LH) and relative humidity (RH) (upper rows) and the Lagrangian derivatives of LH and RH (lower rows) for 2017 and 2018 simulations. RH exhibits an inverse correlation with LH,
and increases in LH are strongly correlated with decreases in RH in almost all cases. Correlation coefficients between coupled and decoupled clouds in 2017 are noticeably different compared to those in 2018 (-0.812 and -0.505 for coupled and decoupled clouds, and -0.727 and -0.845 for those for 2017 and 2018, respectively). However, that is not the case for the Lagrangian derivatives of LH and RH following the cloud base, i.e. for each simulation, coupled and decoupled clouds have similar correlation coefficients and almost the same distribution (-0.712 and -0.710 for coupled and decoupled clouds in 2017, and -0.838 and -0.880 for those in 2018, respectively). Therefore, Lagrangian changes in RH and LH are more consistent in each simulation regardless of the coupling state of the cloud above.

Figure 6.3: Correlations between a) latent heat flux from surface (LH) and surface relative humidity (RH) (upper panels), b) $\frac{D}{Dt}(LH)$ and $\frac{D}{Dt}(RH)$ (lower panels), for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two panels) and 1130 UTC 29 July 2018 (rightmost two panels), respectively.

Finally, the same analyses were repeated, this time for surface wind speed, in
order to investigate their role in inducing variations in the LH along the trajectory of the clouds compared to that of surface RH. The contrast in correlation coefficients between coupled and decoupled clouds was also found in correlations between the surface latent heat flux and horizontal wind velocity at 10 m ($UV_{10}$), shown in Fig. 6.4 below. There is even a more stark disparity between coupled and decoupled clouds in the case of $UV_{10}$ than RH, as well as between the two simulations, with weak negative correlation coefficients between $UV_{10}$ and LH in 2017 in contrast to positive and moderately strong ones in 2018 (-0.259 and -0.092, and 0.660 and 0.207 for coupled and decoupled clouds in 2017 and 2018, respectively). However, similar to the Lagrangian derivatives of RH and LH, Lagrangian derivative of $UV_{10}$ below the cloud is strongly correlated with that of LH for both simulations, with positive correlation coefficients 0.735 and 0.831, and 0.815 and 0.883 for coupled and decoupled clouds in 2017 and 2018, respectively.

Concentrating on the Lagrangian correlations between RH and LH and $UV_{10}$ and LH because of their consistency and integrative nature, we conclude that both variables are contributors to the observed behavior in the Lagrangian changes in LH. Further, we note that their respective relationships with LH are consistent with the expected behavior of these surface variables in the context of BW97. We should also add that even though cloud-top mixing may perhaps play a role in reducing RH near the ocean surface under less well-mixed MBL conditions, we cannot definitely link these changes exclusively with cloud-top processes. The difference between correlation coefficients for coupled and decoupled clouds in the
Figure 6.4: Correlations between a) latent heat flux from surface (LH) and horizontal wind speed at 10 m ($U_{10}$) (upper panels), b) $\frac{\partial}{\partial t}(LH)$ and $\frac{\partial}{\partial t}(U_{10})$ (lower panels), for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two panels) and 1130 UTC 29 July 2018 (rightmost two panels), respectively.

case of Lagrangian derivatives is only minor for both 2017 and 2018 simulations, and there is an inconsistency in terms of comparing the magnitude of correlation coefficients between coupled and decoupled clouds in 2017 versus 2018. Although, coupled clouds encompass slightly larger values of RH, the trends and ranges of values of RH and LH is almost similar in all cases. Therefore, the impact of stronger cloud-top mixing on changes in surface RH due to updrafts from the cloud base in decoupled cases cannot be separated from other factors. The other dominant factor may be changes in SST; as the SST increases, for example, the RH will decrease in response, regardless of cloud-top processes, which in turn affects LH. Increased LH may also help further reduce RH, creating a feedback loop between the two variables.
Chapter 7

Cloud-top Processes

The cloud-top processes described herein are thought to help destabilize and potentially break up stratocumulus. They are compared in terms of their strength in diluting clouds in the upper 200 m of the simulated cloud deck. Each process is again examined in the context of coupled and decoupled clouds.

7.1 CLOUD-TOP BUOYANCY INSTABILITY

Among the most established cloud-top processes in the literature responsible for stratocumulus breakup are Randall’s “Conditional Instability of the First Kind Upside-Down (CIFKU)” (Randall, 1980b) and Deardorff’s “Cloud Top Entrainment Instability (CTEI)” (Deardorff, 1980). The instability criteria for stratocumulus-topped boundary layer inversions in both of these studies state that the differences in values of virtual dry static energy or equivalent potential temperature, respectively, between the layer immediately atop the cloud above the inversion and the in-cloud layer below inversion must be smaller than a threshold
value

\[
\begin{align*}
\text{CIFKU: } & \Delta s_v < (\Delta s_v)_{\text{crit}} \\
\text{CTEI: } & \Delta \theta_e < (\Delta \theta_e)_{\text{crit}}
\end{align*}
\]

(7.1)

where

\[
\begin{align*}
(\Delta s_v)_{\text{crit}} & \propto (q_{s}^{B+} - q^B) \\
(\Delta \theta_e)_{\text{crit}} & \propto (q_{w}^{B+} - q_w^B)
\end{align*}
\]

(7.2)

In this expression \(q_s\) is the saturation mixing ratio, \(q\) is the mixing ratio, \(q_w\) is the total water specific humidity, and \(B+\) and \(B\) refer to above-cloud and cloud-top layers, respectively.

The physics behind both criteria are quite similar; after the dry and warm air atop the inversion mixes with moist in-cloud air due to the turbulence in the cloud layer and leads to the evaporation of cloud water, a new cloud parcel is generated that may become denser, or equivalently, its virtual potential temperatures can be less than the surrounding air. Consequently, it becomes negatively buoyant and sink ustably through the cloud. Consequently, the unhindered entrainment of dry air into the cloud top can further dilute the cloud mass. An equivalent buoyancy reversal criteria to both of the above expressions is the following Xiao et al. (2011)

\[
\kappa = \frac{c_p \Delta \theta_e}{L \Delta q_t}
\]

(7.3)
where $\Delta$ is the difference of the respective variables across the cloud-topped inversion, $q_t$, $c_p$, and $L$ are the total water mixing ratio, specific heat of air at constant pressure and latent heat of water evaporation, respectively. There are different threshold values for $\kappa$ proposed in different studies; the instability criteria found by Randall (1980b) and Deardorff (1980) is $\kappa > 0.23$, MacVean and Mason (1990) suggest that cloud-top buoyancy reversal is only observed for $\kappa > 0.7$, while a number of studies, e.g. Kuo and Schubert (1988) and Moeng (1986) have found no relationship between $\kappa$ and stratocumulus breakup at cloud-top.

Each of these cloud-top buoyancy instability criteria requires a reference for calculating values corresponding to level $B+$, which is immediately above the cloud top beyond the inversion. The inversion height is determined using the two methods explained in Section 4. Thus, $B$ is the last cloudy level below the inversion and $B+$ is the interpolated value of the desired variable 10 m above $B$.

Fig. 7.1 shows correlations between $\kappa$ from Eq. 7.3, hereafter referred to as “buoyancy reversal criteria”, and the average cloud fraction across 200 m in the cloud layer below the cloud top, $CLDU$, for 2017 and 2018, respectively. $CLDU$ for the decoupled clouds have moderate correlation coefficients with respect to the buoyancy reversal criteria compared to their coupled counterparts, both in 2017 and 2018 simulations. The correlation coefficients for the decoupled clouds are higher in 2017 (-0.516) than in 2018 (-0.332), while coupled clouds show weak correlations coefficients in both years, 0.007 and 0.146 in 2017 and 2018, respectively. It is worth noting that, in both simulations, coupled clouds correspond to
Figure 7.1: Correlations between buoyancy reversal criteria ($\kappa$) and average cloud fraction across the upper 200 m of MSC ($CLD_U$) for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two plots) and 1130 UTC 29 July 2018 (rightmost two plots), respectively.

higher values of buoyancy reversal criteria, spanning from 0.4 to 0.8, than the decoupled clouds that range from 0.2 to 0.7 in 2017 and 0.3 to 0.6 in 2018. In these simulations, we conclude that $CLD_U$ is moderately correlated with the buoyancy
reversal criteria only for decoupled clouds, whereas coupled clouds exhibit little or no correlation. An interesting observation from the results in Fig. 7.1 is that, even though coupled clouds have higher values of buoyancy reversal criteria than decoupled clouds, which is expected to enhance cloud-top entrainment instability and thinning, their $CLD_U$ values either varies independent of the buoyancy reversal criteria values (2017) or even show a slight positive albeit weak correlation with this variable. It can be inferred that, as long as the cloud layer is still coupled to the sub-cloud layer, cloud-top entrainment due to buoyancy instabilities have little effect in diluting the cloud from above. As the decoupling process progresses, however, these instabilities become more effective at eroding the cloud layer from above, and as the instabilities strengthen, the clouds become even further diluted at cloud top.

A shortcoming of the CTEI criterion is that in climate models and non-LES regional models, accurately calculating the cloud-top jumps in $\theta_e$ and $q_t$ requires assumptions and is not straightforward. The mixing processes that affect CTEI generally occur at scales on the order of a few meters, which are unresolved in our simulations and even in some LES models (e.g. Mellado (2017)). Hence, the cloud-top mixing processes associated with CTEI in our simulations arise from the MYNN turbulence parameterization, which is responsible for mixing free tropospheric air into stratocumulus. Our analysis of CTEI therefore represents the relationship between the parameterized cloud-top mixing and the simulated stratocumulus transition. Simulations from WRF in our study have an average
vertical resolution of 80 m at marine stratocumulus cloud top. Therefore, $\Delta \theta_e$ and $\Delta q_t$ need to be interpolated at cloud-top, which results in a rather rough estimation of $\kappa$ that may affect the correlation coefficients with respect to $CLD_U$. It is unclear whether this shortcoming significantly impacts our result, but other studies have found discouraging correlations (Stevens (2010), Mellado (2010), Mellado et al. (2009)).

### 7.2 Estimated Inversion Strength

Klein and Hartmann (1993) introduced LTS as a measure of lower-tropospheric instability, defined as the difference between potential temperature at 700 hPa and the surface, in an attempt to uncover the environmental variables that regulate low-level stratiform cloud amount. They found a reasonable correlation between LTS and regional mean cloud amount. LTS has been widely adopted by some models in boundary layer cloud parameterizations (e.g. Rasch and Kristjánsson (1998); Köhler et al. (2011)). However, Wood and Bretherton (2006) pointed out that since LTS was designed and studied for subtropical regions, it might not be appropriate to use as a parameterization for low clouds in the mid-latitudes. They proposed “estimated inversion strength” (EIS) as a new measure of the inversion strength for use in parameterizations of the low cloud cover fraction (CF), especially in subtropics and mid-latitudes. The EIS improves upon LTS by accounting for the moist-adiabatic potential temperature gradient at 850 hPa. Naud
et al. (2016) reinforced the conclusion of Wood and Bretherton (2006) by demonstrating improved correlations between post-cold-frontal CF and EIS relative to correlations with LTS over mid-latitude oceans in both hemispheres. The EIS is an approximation of potential temperature, $\theta$, at 850 hPa level which roughly corresponds to the typical inversion height for mid-latitude stratocumulus-topped boundary layers. Following Eqs 4 and 5 from Wood and Bretherton (2006), EIS is calculated as,

$$EIS = LTS - \Gamma_8^{s50}(z_{700} - LCL) \quad (7.4)$$

where $LTS = \theta_{700} - \theta_0$, $z_{700}$ is the height of the 700 hPa isobar, $\Gamma_m^{s50}$ is the moist-adiabatic potential temperature gradient at $T = (T_0 + T_{700})/2$ and, pressure $P = 850$ hPa, as a measure of the moist adiabatic lapse rate at 850 hPa, which is given by

$$\Gamma_m(T, P) = \frac{g}{c_p} \left[ 1 - \frac{1 + L_v q_s(T, P)/(R_a T)}{1 + L_v^2 q_s(T, P)/(C_p R_v T^2)} \right] \quad (7.5)$$

In this expression, $q_s$ is the saturation mixing ratio, $R_a$ and $R_v$ are the gas constants for dry and water vapor, respectively, and $L_v$ is the latent heat of vaporization.

Correlations between EIS and cloud-top fraction ($CLD_U$) as a measure of effectiveness of the contribution of EIS changes to MSC breakup are shown in Fig. 7.2. Correlation coefficients for both coupled and decoupled clouds are very
Figure 7.2: Correlations between EIS and average cloud fraction across the upper 200 m of MSC ($CLD_U$) for coupled and decoupled clouds, on 1800 UTC 17 July 2017 (leftmost two plots) and 1130 UTC 29 July 2018 (rightmost two plots), respectively.

Poor for both simulations (-0.005 and 0.129 in 2017 and -0.03 and 0.039 in 2018, respectively). Despite decoupled clouds being slightly better correlated with EIS than the coupled ones, the poor correlation coefficients indicate that when it is considered as the sole criterion, it fails to account for stratocumulus breakup at
cloud-top in the majority of cases. This may be due to the loss of their moisture and TKE supply from below, which enabled them to become more susceptible to cloud-top instabilities. One problem with the use of EIS as an indicator of breakup is that increases in LCL, decoupling, and the stratocumulus breakup happen nearly simultaneously. Based on Eq. 7.4, as the LCL increases, EIS coincidentally increases and this link seems contrary to the supposed role of inversion strength on cloud-top breakup, since as the cloud-top jump in moisture and equivalent potential temperature is reduced, the inversion becomes weaker. A weakened inversion should result in increased entrainment of dry and warm air above the inversion into the cloud, and its ultimate destruction.

### 7.3 A New Measure of Inversion Strength Designed for use in Large Scale Models

Because the existing measures of inversion strength studied earlier either fall short of explaining the breakup in the WRF simulations (EIS) or require interpolations to compute (the buoyancy reversal criteria, $\kappa$), we investigated an alternative measure which can be more easily calculated using data from climate and regional models with coarser vertical resolution than LES models.

Equivalent potential temperature ($\theta_e$) is another moist-conserved variable that incorporates the heating effect of latent heat release on potential temperature. As an entrained parcel ascends adiabatically across the inversion, a decrease in $\theta_e$ indicates a reduction in the latent heating due to reduced moisture content.
Therefore, vertical gradients in $\theta_e$ indicate moisture changes during adiabatic ascent and descent across the inversion. On the other hand, vertical gradients in the saturated equivalent potential temperature ($\theta_{es}$) indicate temperature changes during adiabatic ascents and descents across the inversion. Typically, $\theta_{es}$ above inversion is higher than below it because the air is warmer, while the opposite is true for $\theta_e$, since conditions above inversion are drier. The difference between $\theta_{es}$ and $\theta_e$ at the layers atop and below the inversion indicates how much drier and warmer the air above the inversion is relative to that just below the inversion. Warmer and drier conditions indicated by a greater difference between $\theta_{es}$ and $\theta_e$ atop the inversion lead to reduced instability of the inversion layer to downward motions from above. Therefore, the inversion is strengthened, i.e. there is a greater resistance to entrainment of air above inversion into the layer below. The reverse is true for smaller values of this difference; the inversion becomes more susceptible to downward entrainment of air above that acts to dilute the cloud layer below. Therefore, the profile of these two variables provides a sense of the strength of the inversion in terms of the contrast between both the moisture and temperature of the two air masses.

Fig. 7.3 shows the vertical profiles of equivalent potential temperature ($\theta_e$), saturated equivalent potential temperature ($\theta_{es}$), 100 times cloud fraction for ease of viewing, LCL and the capping inversion height ($z_i$) for a point in the stratocumulus deck (I) and a semi-broken cloud element (II), chosen from the domain shown in Fig. 5.1 in the 2018 simulation. In the case of point I, $\theta_e$ and
Figure 7.3: Vertical profiles of equivalent potential temperature, $\theta_e$ (solid black line), saturated equivalent potential temperature, $\theta_{es}$ (solid navy blue line), 100 times cloud fraction (solid green green line), LCL (dashed red line) and capping inversion height $z_i$ (dashed black line) for points I and II chosen from the domain in the 2018 simulation shown in Fig. 5.1, where I is a point from the solid stratocumulus deck, and II is in the broken cloud field downstream of the stratocumulus deck.

$\theta_{es}$ sharply diverge beyond the inversion height, while having the same value in the in-cloud region. The cloud element at point II is in the broken cloud field downstream of the stratocumulus deck, and is being diluted from above as well as from below, judging by the cloud-fraction values. Unlike point I, $\theta_e$ and $\theta_{es}$ start diverging slowly in the cloud region for point II. This suggests that the inversion has become weak enough, allowing the dry air to penetrate through the cloud, thereby destroying it from above.
Since the model is prescribed with discrete vertical levels, the layer above inversion may be at a different altitude depending on the inversion height. Therefore, in order to offset the bias of the different distances between inversion and the layer above it, the vertical gradient of $\theta_{es} - \theta_e$ at the inversion is used as a measure of the inversion strength. This variable is hereafter labelled “INV”

$$INV = \frac{d}{dz}(\theta_{es} - \theta_e)$$ (7.6)

INV is calculated for each example represented in Fig. 7.3, and as expected, it is greater in the case of a stronger inversion; 0.125 and 0.025 for the points I and II, corresponding to strong and weak inversions, respectively. Fig. 7.4 shows correlations between coupled and decoupled $CLD_U$ and $INV$, for 2017 and 2018 simulations, respectively. As expected, weakening of inversion strength is linked to reduction in cloud-top fraction, and that this variable correlates better with decoupled $CLD_U$. The correlation coefficient for decoupled clouds in 2017 is slightly improved compared to that for buoyancy reversal criteria (0.542 versus -0.516), while in 2018, it is slightly smaller than the latter (0.305 versus -0.332). However, there is a poor correlation between this variable and the coupled clouds (-0.175 and -0.049 in 2017 and 2018, respectively). One interpretation of this finding is that as long as the clouds are coupled, they are supplied with latent heat from the sub-cloud layer and can maintain their cloud-top stability, therefore not allowing for any or much entrainment from above the inversion. This notion is consistent with the greater number of clouds with $CLD_U$ exceeding 0.5 as compared to the
Figure 7.4: Correlations between the vertical gradient of the difference between \( \theta_e \) and \( \theta_s \) at cloud-top (\( INV = \frac{d}{dz}(\theta_es - \theta_e) \)) and average cloud fraction across the upper 200 m of MSC (\( CLD_U \)) for coupled and decoupled cases, on 1800 UTC 17 July 2017 (leftmost two plots) and 1130 UTC 29 July 2018 (rightmost two plots), respectively.

decoupled ones. However, a positive trend can be seen between those with \( CLD_U \) smaller than 0.5 and \( INV \), which can be related to how strongly coupled they are to the surface. In other words, those clouds are likely in the beginning of the decoupling process, and are more susceptible to changes in inversion strength at
cloud-top.

In conclusion, \( INV \) performs similar to the buoyancy reversal criteria (\( \kappa \)) in terms of quantifying the impact of inversion instabilities on the breakup of decoupled clouds, while being easier to calculate than the latter in non-LES models. And because it has proved more successful than EIS, it can be viewed as an alternative metric for explaining the relationship between cloud-top instabilities and cloud-top erosion. Also, it can be interpreted that cloud-top instability and inversion strength measures may perhaps be byproducts of the breakup processes at cloud base. The main evidence is that they only seem to be correlated with breakup at cloud top when the cloud has been further decoupled after cloud-base processes such as local fluctuations in LH beneath the cloud have eroded it from below.
Chapter 8
Discussion and Conclusions

Summertime cold frontal passages and associated post frontal cloudiness are an important component of the climate over the ENA. The post-cold frontal environment often exhibits a transition from a continuous MBL cloudiness in the northern ENA to broken cloudiness in the southern ENA. To investigate these post-cold frontal MBL cloud transitions, we used two high resolution simulations of regional summertime post-cold-front marine boundary layer clouds in July 2017 and 2018 to investigate the processes that lead to these cloudiness transitions. The resolution of our simulations negated the need for a shallow convection parameterization, so MBL clouds were generated by a combination of the surface flux and MYNN3 turbulence parameterizations. To track the evolution of cloud elements, we used a Lagrangian particle dispersion model (FLEXPART-WRF) to follow the evolution of individual MBL columns in each simulation through the transition process.

The WRF simulations produced a range of cloud configurations associated with the transition region that resemble cloud structures in satellite images from the simulation periods. To evaluate the quality of the simulations, we compared them with coincident surface and remote sensor data collected at the ENA site.
Surface variables agreed reasonably well with the simulations, though island effects on the surface temperature from WRF simulations led to daytime cold bias at the wake of the cold fronts at the location of the ENA site and influenced surface temperature comparisons. MBL depths simulated by WRF in the two post-frontal cases were comparable to those that are measured at ENA, though 100-200 m deeper than the observed depths. Comparisons between the sub-cloud and cloud structure measured using the ENA Doppler Lidar and KAZR cloud radar showed similar overall structures, but the post-frontal cloudiness was more broken and deeper in both the 2017 and 2018 simulations than the observed structure. The ENA-measured sub-cloud vertical velocities were noticeably larger than those in the simulations in the post-cold-frontal environment.

Decoupling of the cloud layer from the surface supply of moisture is known to be an important process in this region, especially as it relates to cloud transitions. We tested three diagnostic decoupling parameters suggested by Jones et al. (2011), as well as sub-cloud buoyant production of TKE following Bretherton and Wyant (1997), to classify the simulated cloud cover across the decoupling continuum and found that the diagnostic based upon the vertical moisture gradient yielded the best results. The Lagrangian cloud profiles as the MBL cloud layer evolved suggested changes at cloud base and cloud top as the clouds became more broken, so we examined processes at cloud base and cloud top separately in the context of more coupled and more decoupled cloud populations over a domain at the onset of the transition from solid deck of marine stratocumulus to broken cloud
structures, for each of the 2017 and 2018 simulations.

A finding of particular importance was that cloud-base erosion in the simulations was mainly the result of local fluctuations in LH, which preceded any changes at cloud top as the clouds became more broken. Correlations between the absolute value of LH and changes in the cloud fraction at cloud base were substantially lower than those between the Lagrangian derivatives of LH and cloud fraction at cloud base for more coupled clouds. Similar correlations to those involving LH were found when analyzing the LCL in the context of cloud-base changes, which is expected given that the surface LH and surface LCL are related. The relationship between the Lagrangian derivatives of 10-m wind velocity and the surface RH and LH following the cloud base were strong and positive for both coupled and decoupled clouds, uniformly exceeding 0.7, the implication being that changes in the surface wind and humidity conditions were likely influencing the cloud-base erosion process through their effect on LH as long as the cloud element was still coupled to the sub-cloud region. Changes in the surface relative humidity and LH were virtually simultaneous making it difficult to determine if the LH affected the humidity as a consequence of cloud-top mixing following deepening-warming or if surface warming led to a lower RH, which subsequently leads to an increase in the LH. In the latter case, a potential feedback loop would exist.

We examined the relationship between CTEI and EIS in the context of decoupling on cloud-top cloud fraction and found that CTEI was moderately correlated with changes in cloud-top cloud fraction only for more decoupled clouds, while EIS
exhibited weak correlations for both coupled and decoupled clouds. In addition, we tested a new cloud-top dilution diagnostic based upon estimating the inversion strength using the vertical gradients of the difference between the equivalent and saturation equivalent potential temperature in the vicinity of the capping inversion height and found that it preformed similar to CTEI as an indicator of cloud breakup at cloud top, while being readily computed from soundings. In summary, the degree of decoupling was found to significantly influence the extent to which both cloud-base and cloud-top processes affect the erosion of cloud elements at cloud base and cloud top, respectively. Our findings suggest that cloud-top processes are able to substantially alter the cloud structure only after significant decoupling has occurred.

Our results suggest that the deepening-warming process proposed by Bretherton and Wyant (1997) may be operating in the post-cold-frontal environment in ENA, which may broaden its applicability in the marine atmosphere. A variation of the deepening-warming hypothesis in which the warming initially dominates the moistening leading to a deeper MBL and higher LCL could also explain some of our findings. In that scenario, a higher LCL resulting from warming leads to moisture accumulation in the sub-cloud layer, which subsequently drives the LCL lower and initiates convection. We view this possibility as a potential subset of the original hypothesis rather than a separate process.

The latent-heat driven, deepening-warming decoupling process is a key instigator of the stratocumulus transition. The 2017 and 2018 cases represent two
slightly different manifestations of the transition. In the 2018 case, the latent heat flux gradient over the ENA behind the cold front is smaller than in the 2017 case, and the transition occurs further downstream at a lower latitude (see Figs. 4.3 and 4.4). The deepening-warming post-cold frontal transition that is evident in these simulations is one process in the continuum of transition processes that likely exist in the post-cold frontal environment. Images of the two simulated cases (Fig. 4.1) suggest a rich array of transitions occurring at different scales that do not follow a latitudinal pattern. While some of these transitions may be related to aerosol-cloud interactions, others may involve mesoscale instabilities inherent within the post-cold-frontal air mass, or other yet undiscovered instabilities. The transition continuum also likely includes processes that reverse the breakup and lead from partly cloudy conditions to solid or complex overcast. Future studies will hopefully address these other transition modes.

An important observation stemming from the WRF simulation experiments was that production and maintenance of clouds, specifically those at the wake of the cold fronts in both cases, proved particularly sensitive to the choice of the planetary boundary layer parameterization. Many test runs were conducted with UW PBL scheme (Bretherton and Park, 2009), and the prognostic TKE PBL schemes Mellor-Yamada Nakanishi and Niino Level 2.5 and 3 (MYNN2.5 and MYNN3) (Nakanishi and Niino, 2006, 2009), with only the latter capable of producing cloud structures that resembled the satellite images available at around the same time for both simulations. A series of studies by Nakanishi and Niino
(Nakanishi and Niino (2004); Nakanishi and Niino (2006); Nakanishi and Niino (2009)) used LES results to improve the second-order turbulence model of Mellor and Yamada (Mellor and Yamada, 1974), leading to a better representation of the planetary boundary layer (PBL) and marine fog in a mesoscale model. In the absence of a detailed comparison between the performance of these two PBL schemes, we can only assume that it may partly be due to the prescription of turbulent master length scale, $l$, by MYNN, that incorporates buoyancy length scale in the specification of $l$ proposed by Mellor and Yamada (1974), while the UW scheme follows the approach adopted by Mellor and Yamada (1974).

A basic answer to the broader question of the association between the deepening-warming hypothesis, mesoscale clusters of cumulus-coupled stratocumulus, and air-mass modifications is at least partially answered by the present analysis of the two simulations. The transition process, as depicted by these simulations, has at least three definable stages: the initiation of intrusions of unsaturated air (i.e. clear patches) at the beginning of the transition process, a period of chaotic cloudiness with disorganized and somewhat random patches of hybrid combinations of stratocumulus and cumulus, and a final configuration in which the chaotic cloudiness becomes organized into scattered patches of mesoscale cumulus-coupled stratocumulus that are organized. The exact relationship between the deepening and warming process and the development of mesoscale organization is not addressed by the current analysis, though answers may be discovered in future analyses of these simulations.
One element of this study that deserves special mention is the compatibility of the simulated cloud structure to the observations at the ENA site. Past comparisons of model results with detailed process-level observations have often suffered from limitations that prevented the regional scale cloud evolution to be studied in a manner consistent with observations that could be used to track the integrity of the model solutions. For example, LES simulations could not capture regional variability within an air mass and regional simulations that featured resolutions on the scale of tens of kilometers could not resolve convection and, accordingly, were unable to reproduce the observed mesoscale structure. The simulations presented herein are among the first to bridge this disconnect; cloud-scale solutions that can be evaluated at a specific site, but represent the regional variability.

To the extent that these two cases represent different cold front climatology and produce transitions at different latitudes, they suggest a sensitivity to changing post-cold-frontal air mass characteristics in a warming climate. Warming in Northern Canada and an increasingly ice-free Arctic are likely to produce less impressive cold air outbreaks during summer and, at least initially, potentially smaller gradients of latent heat flux across the ENA. A reduction in the gradient of the latent heat flux in this region suggests that the stratocumulus transition might occur at lower latitudes than at present until the warming of the ocean, which takes longer, potentially offsets the process. In any event, a near-term reduction in the gradient, which seems quite feasible given the current amplitude and speed of the Arctic warming, could produce (or is already producing) a
decoupling-induced, negative cloud feedback during the summertime.

Holistically, WRF simulations combined with observations from the ENA surface site is a potent research combination. The model provides hints at the specific data and process combinations that might reveal a much more statistically defensible modus operandi for the transition region when applied to a longer term record from the ENA site. Future combined observational and modeling studies are recommended to further clarify the connection between the surface fluxes, decoupling, and cloud transitions.
Appendix A

WRF Settings

Here, the namelist file used to run the 2018 simulation is presented, along with detailed explanations of variables not addressed in the “WRF Parameterizations” section, with the aim of assisting replication of simulations used in this study. The 2017 WRF simulation had identical settings, except for the start and end dates of the simulation. Important namelist options in each section that required further explanations are discussed in the following sections.

A.1 Time Control

interval_seconds: Refers to the interval between input files produced by WPS. Since the initial and boundary condition FNL data obtained had intervals of three hours, the preprocessed input data by WPS (metgrid files) are also 3-hourly.

history_interval: Indicates the intervals at which WRF will write out the simulation data. For the parent and child domains, intervals of 60 and 30 minutes, were used in our simulations, respectively.

frames_per_outfile: We chose a high enough number for this variable, because it was more manageable in this case when all the output intervals are written
in a single file. The output files for the second domain for both simulations are about 1 TB, which did not pose any memory restraints for us.

**restart:** We experienced difficulty using the “restart” option, which in essence allows one to segment the simulation into different runs, so that when the program encounters an error, previous simulations prior to that time would not be lost. The problem with using this option in our case was that the model would crash after only a few time steps when using a restart file. It must be noted here that a lot of debugging went into making sure that the model would run without any error for the entirety of the simulation run, which lasted about 9 hours for a 72-hr simulation.

### A.2 Domains

**eta_levels:** The eta levels were obtained using WRF Domain Wizard software, version 2.84 (NOAA, 2013), which is a very useful tool to easily set up a domain. The eta levels were estimated using hyperbolic tangential stretching option, that creates uniformly spaced layers in the PBL, allowing them to gradually stretch apart to maximum distance at mid-levels (around 700 hPa), and then compresses them further aloft. The vertical spacing between the lowest levels were set to start at 15 m.

**feedback:** This setup determine a two-way or one-way nested run. In the former scenario, the values of the variables in the coarse domain are overwritten by those in the nest at points located at the intersection of the two domains, when
this function is activated. Otherwise, the nesting process will be referred to as “one-way”. A two-way nested run will be more computationally expensive, but ultimately more accurate than a one-way one. In our simulations, we benefited from this setting.

**wif_input_opt**: This option was activated to enable processing of Water/ice-friendly aerosol input from metgrid, used in the Thompson aerosol aware micro-physics scheme (mp.physics = 28).

**nproc_x & nproc_y**: WRF offers three different configurations at the time of compiling the model in order to take advantage of parallel computing; MPI or Distributed-Memory Parallelism (DMPar) where each parallel process is allocated its own memory space, OpenMP (Open Multiprocessing) or Shared memory Parallelism (SMPar) meaning that all processors share the same memory space, and hybrid build with both MPI and OpenMP (DMPar + SMPar). Computational and Information Systems Lab (CISL) recommends using MPI configuration for optimizing the performance of WRF. WRF decomposes the domain into several regions and assigns each MPI task to one of these regions. The total number of compute tasks are equal to \( nproc_x \times nproc_y \), where \( nproc_x \) and \( nproc_y \) are the number decompositions, hence compute processors, along the \( x \) and \( y \) axes, respectively. Usually, a larger value is assigned to \( nproc_y \) than the \( nproc_x \).

Arriving at the optimal decomposition was one of the biggest challenges we faced when running the simulations. It is closely dependent on the total number of computational nodes, size of the domains, and the output intervals designated
to each domain. After many trial and errors, we arrived at the decompositions specified in the namelist. We used a total number of 150 compute nodes, \((150 \times 36\) cores), dedicating \(75 \times 60\) to computation and the rest, \(75 \times 12\) to the I/O tasks, explained in “Namelist Quilt” section.

## A.3 Physics

**use_aero_icbc**: This option is used with aerosol-aware Thompson scheme with water- and ice-friendly aerosol climatology, and when set to “True”, allows the model to use climatological aerosol input from WPS.

**icloud_bl**: Activating this option allows subgrid-scale clouds from the PBL scheme to be coupled to the radiation schemes. This options is specific to MYNN2.5 and MYNN3 PBL schemes.

**bl_mynn_cloudpdf**: In order to represent subgrid-scale clouds, three probability distribution functions (PDF) are provided. Rather than resorting to multiple schemes to classify and represent different cloud types, which is a complex approach and normally does not lead to smooth cloud transitions, statistical methods using PDFs based on turbulence closure schemes (Mellor (1977); Sommeria and Deardorff (1977)) can be used to arrive at a unified scheme to represent all types of clouds. Kuwano-Yoshida et al. (2010) proposed an improved cloud PDF scheme based on the assumption of joint-Gaussian probabilities for the liquid water potential temperature and total water content, with standard deviations
estimated from the Mellor-Yamada level-2 turbulence scheme, and improved turbulence closure parameters and mixing length. Because it is a diagnostic second-order turbulence scheme that relies on resolved gradients, rather than higher order moments, it is computationally efficient, and results in improved representation of marine boundary layer clouds (Kuwano-Yoshida et al., 2010).

**bl_mynn_mixlength:** An improved, scale-aware mixing length formulation for MYNN proposed by Ito et al. (2015) has been used that takes into account the cloud-specific mixing length, as well. This scheme is designed with the aim of resolving turbulent eddies that are on the order of the model grid resolution (∼1 km), and has demonstrated improved performance in comparison to the MYNN3 scheme (Ito et al., 2015).

**icloud:** This option controls whether the effect of clouds is considered on the optical depth calculations in shortwave and longwave radiation, as well as the representation of cloud fraction in the model. The method proposed by Xu and Randall (1996) has been adopted here, which takes subgrid-scale cloud amounts into account by using statistical distribution of cloud water and cloud ice on the subgrid-scale, rather than threshold approaches that give either 0 or 1 values for cloud fraction.

**o3input:** When set equal to “2”, this option inputs climatological Ozone data adapted from the Community Atmosphere Model (CAM) radiation scheme, as well as aerosol data for RRTMG radiation scheme. In contrast to the default Ozone data used in the scheme that is only a function of height, this Ozone
dataset has additional latitudinal and temporal (monthly) variations.

### A.4 Dynamics

**w_damping:** Vertical velocity damping has been activated to ensure the model remains numerically stable throughout the run, and avoid CFL errors due to locally large vertical velocities.

**dampcoef** A Rayleigh damper with damping coefficient (inverse damping time scale) of 0.2 is used in the top 5 km to damp spurious waves in the stratosphere.

**use_theta_m:** Activating this option incorporates the effect of moisture on pressure in small intervals.

### A.5 Namelist Quilt

**nio_tasks_per_group & nio_groups:** Quilting enables dedicating compute cores specifically to the task of writing out the simulation data at output intervals. This options works with MPI configuration. The total number of I/O tasks is equal to

\[ nio_{\text{tasks}}_{\text{per}}_{\text{group}} \times nio_{\text{groups}} \]

where \( nio_{\text{tasks}}_{\text{per}}_{\text{group}} \) is the number of processors used for I/O quilting per I/O group which is specified by \( nio_{\text{groups}} \). According to Balle and Johnsen (2016), \( nio_{\text{tasks}}_{\text{per}}_{\text{group}} \) cannot be greater than \( nproc_{\text{y}} \), and ideally \( nproc_{\text{y}} \) should be an exact multiple of \( nio_{\text{tasks}}_{\text{per}}_{\text{group}} \). This I/O configuration, together with the compute task configuration (\( nproc_{\text{x}} \) and \( nproc_{\text{y}} \)) gave the best results in terms of reducing the output overheat at
each output interval, and balancing I/O and compute resources.

A.6 WRF Namelist

&time_control
start_year = 2018, 2018,
start_month = 07, 07,
start_day = 28, 28,
start_hour = 00, 00,
start_minute = 00, 00,
start_second = 00, 00,
end_year = 2018, 2018,
end_month = 08, 08,
end_day = 01, 01,
end_hour = 00, 00,
end_minute = 00, 00,
end_second = 00, 00,
interval_seconds = 10800,
input_from_file = .true.,.true.,
history_interval = 60, 30,
frames_per_outfile = 2000, 2000,
restart = .false.,
restart_interval = 8000,
io_form_history = 2
io_form_restart = 2
io_form_input = 2
io_form_boundary = 2
debug_level = 0
/
nocolons = .true.

&domains

time_step = 15,
time_step_fract_num = 0,
time_step_fract_den = 1,
max_dom = 2,
e_we = 751, 1051,
e_sn = 751, 1051,
e_vert = 82, 82,
eta_levels = 1.0000, 0.9978, 0.9955, 0.9933, 0.9910, 0.9888, 0.9866, 0.9844, 0.9822, 0.9799, 0.9776, 0.9751, 0.9724, 0.9696, 0.9665, 0.9633, 0.9598, 0.9560,
p_top_requested = 5000,
sfcp_to_sfcp = .true.,
extrap_type = 1,
lowest_level_from_sfc = .true.,
interp_theta = .false.,
num_metgrid_levels = 32,
num_metgrid_soil_levels = 4,
dx = 4050, 1350,
dy = 4050, 1350,
grid_id = 1, 2,
parent_id = 0, 1,
i_parent_start = 1, 201,
j_parent_start = 1, 201,
parent_grid_ratio = 1, 3,
parent_time_step_ratio = 1, 3,
feedback = 1,
smooth_option = 1,
rh2qv_method = 2,
wif_input_opt = 1,
num_wif_levels = 30,
nproc_x = 60,
nproc_y = 75,
/

&physics
mp_physics = 28, 28, 28,
use_aero_icbc = .true.,
ra_lw_physics = 4, 4, 4,
ra_sw_physics = 4, 4, 4,
sf_sfclay_physics = 5, 5, 5,
sf_surface_physics = 2, 2, 2,
bl_pbl_physics = 6, 6, 6,
icloud_bl = 1,
bl_mynn_cloudpdf = 1,
bl_mynn_cloudmix = 1, 1,
bl_mynn_edmf = 1, 1,
bl_mynn_edmf_part = 1, 1,
bl_mynn_edmf_mom = 1, 1,
bl_mynn_edmf_tke = 1, 1,
bl_mynn_tkebudget = 1, 1,
bl_mynn_tkeadvect = .true., .true.,
bl_mynn_mixlength = 2,
cu_physics = 0, 0,
icloud = 1,
isfflx = 1,
isnow = 1,
swint_opt = 1,
radt = 1, 1,
bldt = 0, 0,
num_soil_layers = 4,
num_land_cat = 21,
sf_urban_physics = 0,
iz0tlnd = 1,
isftcflx = 0,
grav_settling = 0,
o3input = 2,
scalar_pblmix = 1,
aer_opt = 3,
/

&fdda
/

&dynamics
w_damping = 1,
diff_opt = 2, 2, 2,
km_opt = 4, 4, 4,
diff_6th_opt = 2, 2, 2,
diff_6th_factor = 0.12, 0.12, 0.12,
base_temp = 300.
damp_opt = 3,
zdamp = 5000., 5000., 5000.,
dampcoef = 0.2, 0.2, 0.2,
h_mom_adv_order = 5, 5, 5,
h_sca_adv_order = 5, 5, 5,
v_mom_adv_order = 3, 3, 3,
v_sca_adv_order = 3, 3, 3,
non_hydrostatic = .true., .true., .true.,
moist_adv_opt = 4, 4, 4,
scalar_adv_opt = 4, 4, 4,
chem_adv_opt = 2, 2, 2,
tke_adv_opt = 4, 4, 2,
momentum_adv_opt = 3, 3, 3,
gwd_opt = 0,
use_theta_m = 1,
use_q_diabatic = 1,
epssm = 0.2, 0.2, 0.2,
emdiv = 0.01, 0.01, 0.01,
smdiv = 0.1, 0.1, 0.1,
/

&bdy_control
spec_bdy_width = 5,
spec_zone = 1,
relax_zone = 4,
specified = .true., .false.,
nested = .false., .true.,
/

&grib2
/

&namelist_quilt
nio_tasks_per_group = 75,
nio_groups = 12,
/
Appendix B

FLEXPART-WRF Settings

FLEXPART-WRF comes with different options available for choosing the input wind field (WIND_OPTION), PBL parameters such as friction velocity ($u^*$), surface sensible heat flux, and PBL height (SFC_OPTION), PBL turbulence parameterization (TURB_OPTION), and land-use schemes (LU_OPTION). All trajectory simulations have been conducted with the following configuration:

**WIND_OPTION**: There are four options available in FLEXPART-WRF for input vertical wind velocity; option 0 uses instantaneous vertical velocity ($W$) on Cartesian coordinates that is the default output from WRF, option 1, the time-averaged wind, option 2, the instantaneous mass-weighted time derivative of sigma levels as vertical velocity ($\dot{\sigma}$), and option -1, a divergence-based vertical wind velocity which determines vertical velocity with mass-conservation and hydrostatic assumptions. WRF needs additional settings to output the instantaneous and time-averaged vertical wind velocity on sigma levels. According to Brioude et al. (2012a), $W$ from option 0 produces the largest uncertainties when the orography of the domain is complicated, whereas instantaneous and time-averaged $\dot{\sigma}$ give better results. Also, even though the conditions required for computing vertical velocity from the last option do not necessarily hold at the mesoscale, it leads to
much smaller uncertainties than option 0. Given that the only output available from our WRF simulations was instantaneous $W$ on geometric vertical coordinate, the last option (-1) was opted to optimize the trajectories despite its higher computational cost, even though most of the domain is located on the Eastern North Atlantic ocean where almost no complex orography exists, which would have justified using option 0.

**TURB\_OPTION:** Four options are available for parameterizing the turbulent wind field in the PBL; option 0 completely ignores turbulence, option 1 uses the Hanna scheme Hanna et al. (1982) for the PBL turbulent mixing, and option 2, the prognostic turbulent kinetic energy (TKE) from WRF. Option 3 is similar to option 2, but partitions TKE obtained from WRF such that turbulent energy production and dissipation are equal. Brioude et al. (2013) found that options 2 and 3 cannot keep the tracer well-mixed in the planetary boundary layer. They found out that when the Hanna scheme for turbulence parameterization is used in conjuction with skewed turbulence (rather than Gaussian) in the convective boundary layer (activated by the swtich CBL = 1), the tracer particles are almost homogenously well-mixed throughtout the depth of the convective boundary layer. They recommend this setting and it is what we used in all trajectories in this article.

**SFC\_OPTION:** Two options exist in FLEXPART\_WRF for computing PBL height. It is either derived directly from the WRF output PBLH (option 1), or estimated by FLEXPART-WRF using a Richardson number threshold Brioude
et al. (2013) (option 0). Here, option 0 has been chosen to characterize the boundary layer, in order to be more in line with the choice of TURB_OPTION described above.

**LU_OPTION**: In this study, the same land-use scheme used in WRF has been implemented in FLEXPART-WRF with option 1.
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