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DOCTORAL THESIS

On the development and stabilisation of symmetrically unstable fronts

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Herman Melville

Abstract

Submesoscale fronts, with large geostrophically balanced horizontal density gradients and Rossby and Richardson numbers of $O(1)$, are common in the upper ocean. Here, destabilizing atmospheric forcing, can maintain a surface mixed layer with weak to vanishing stratification. This weak stratification often results in areas where the Ertel potential vorticity (PV) is of opposite sign to the Coriolis parameter, leading to regions prone to a hybrid convective–inertial perturbation known as symmetric instability (SI). Growing slantwise convection cells nearly aligned with isopycnals promote the transport of climate relevant tracers important for both the biology as well as energy transfers across scales, influencing both turbulence and the broader ocean circulation.

Submesoscale dynamics challenge traditional modeling approximations and remain unresolved in standard ocean models. Through a combination of linear theory and high-resolution idealised Large Eddy Simulations (LES), we investigate the role of (forced) symmetric instability in the potential vorticity budget. The focus is on the role of symmetric instability and ultimate restratification of the ocean column once the destabilising surface forcing has ceased. Comparisons between spin-down experiments with and without a strongly stratified thermocline below the surface mixed layer, as well as forced symmetric instability, suggest that without destabilising surface forcing, the PV flux from the interior is of minor importance. Furthermore, the main contributor to the restratification process is an SI-driven divergence of cross-frontal Reynolds stresses, which leads to a cross-frontal secondary circulation triggered by a modified thermal wind that stratifies the water column. Additionally, we show that the alternating vertical momentum fluxes associated with SI lead to frontogenesis and the formation of sharp fronts at the boundaries of the mixed layer. These non-geostrophic fronts are hot-spots for vertical potential vorticity fluxes and are where secondary Kelvin-Helmholtz instabilities (KHI) first appear. We show the complex influence of turbulence on the generation of symmetric and secondary Kelvin-Helmholtz instabilities.

This work enhances our understanding of how upper ocean fronts modulate energy transfer, with consequences for both the large- and small scale ocean dynamics as well as air-sea exchanges. The findings underscore the importance of SI in mixed layer energy dynamics and highlight implications for parameterising submesoscale processes in climate models.

Zusammenfassung

Submesoskalige Fronten in der ozeanischen Deckschicht sind oft im geostrophischen Gleichgewicht. Im Unterschied zu den mesoskaligen Fronten sind sie charakterisiert durch eine Rossby- sowie Richardson-Zahl der Größenordnung $O(1)$. Destabilisierender atmosphärischer Antrieb erhält die meist schwach geschichtete Deckschicht aufrecht. Die Kombination aus einer schwacher Schichtung und grossen horizontalen Dichtegradienten innerhalb der Fronten führt häufig zu einer Ertel'schen Potenziellen Vorticity (PV), die das entgegengesetzte Vorzeichen des Coriolis-Parameters aufweist. Dies begünstigt eine hybride Form aus konvektiver und Trägheitsinstabilität, bekannt als symmetrische Instabilität (SI). Anwachsende schräg verlaufende Konvektionszellen, die oft entlang der Isopyknen ausgerichtet sind, fördern hier den Transport klimarelevanter Tracer, die sowohl für biologische Prozesse als auch für den Energietransfer über verschiedene Skalen hinweg wichtig sind. Dies beeinflusst sowohl die Turbulenz als auch die großräumige ozeanische Zirkulation. Solche submesoskalige Dynamiken stellen traditionelle Modellierungsansätze vor Herausforderungen und werden in typischen Klimamodellen nicht aufgelöst.

Durch eine Kombination aus linearer Theorie und hoch aufgelösten, idealisierten Large Eddy Simulations (LES) untersuchen wir die Rolle der symmetrischen Instabilität auf das potentielle Vorticity-Budget. Der Fokus liegt dabei auf der Rolle von symmetrischer Instabilität bei der Restratifizierung der Deckschicht. Vergleiche zwischen Experimenten mit und ohne einer stark geschichteten Thermokline unterhalb der Deckschicht zeigen, dass die Bedeutung des PV-Flusses aus dem Inneren bei symmetrischer Instabilität ohne destabilisierenden Oberflächenantrieb geringer ist, als bisher angenommen. Den Hauptbeitrag zur Restratifizierung liefert eine durch SI hervorgerufene Divergenz der Reynolds-Spannungen, die zu einer quer zur Front verlaufenden sekundären Zirkulation führt. Diese Zirkulation lässt sich auf den durch Turbulenz modifizierten thermischen Wind zurückführen. Darüber hinaus zeigen wir, dass die mit SI verbundenen alternierenden vertikalen Impulsflüsse zu Frontogenese und zur Bildung scharfer Fronten an den Grenzen der Deckschicht führen. Diese nicht-geostrophischen Fronten sind Hotspots für vertikale PV-Flüsse und der Entstehungsort sekundärer Kelvin-Helmholtz-Instabilitäten. Wir zeigen den komplexen Einfluss von Turbulenz auf die Entstehung von symmetrischen

und sekundären Kelvin- Helmholtz-Instabilitäten und den damit verbundenen Energietransfer von geostrophischen Strömungen zu kleinskaliger Turbulenz.

Diese Arbeit verbessert unser Verständnis darüber, wie Fronten in der oberen Deckschicht den Energietransfer modulieren, mit Konsequenzen für sowohl groß- als auch kleinskalige ozeanische Dynamiken. Die Ergebnisse unterstreichen die Bedeutung der symmetrischen Instabilität auf den Energietransfer von großen zu kleinen Skalen und heben die Implikationen für die Parametrisierung submesoskaliger Prozesse in Klimamodellen hervor.

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List of Abbreviations

3-D	Three-Dimensional
AGSP	Ageostrophic Shear Production
BI	Baroclinic Instability
BP	Buoyancy Production
GSP	Geostrophic Shear Production
KE	Kinetic Energy
KHI	Kelvin Helmholtz Instability
LES	Large Eddy Simulations
ML	Mixed Layer
MLD	Mixed Layer Depth
N	Number of grid points
OSBL	Ocean Surface Boundary Layer
PE	Potential Energy
PV	Potential Vorticity (Ertel)
SI	Symmetric Instability
SML	Surface Mixed Layer
TKE	Turbulent Kinetic Eenergy

Physical Constants

Coriolis parameter	$f = 1.0 \times 10^{-4} \text{ s}^{-1}$
Density of seawater	$\rho_0 = 1025 \text{ kg m}^{-3}$
Earth's rotation rate	$\Omega = 7.2921 \times 10^{-5} \text{ rad s}^{-1}$
Gravitational acceleration	$g = 9.81 \text{ m s}^{-2}$
Saline contraction coefficient	$\beta_S = 7.6 \times 10^{-4} \text{ g}^{-1} \text{ kg}^{-1}$
Specific heat capacity of seawater	$C_p = 3990 \text{ J kg}^{-1} \text{ K}^{-1}$
Thermal expansion coefficient	$\alpha_T = 2 \times 10^{-4} \text{ K}^{-1}$

List of Symbols

A_h	horizontal eddy viscosity	$\text{m}^2 \text{s}^{-1}$
A_v	vertical eddy viscosity	$\text{m}^2 \text{s}^{-1}$
b	buoyancy	m s^{-2}
C	Smagorinsky constant	dimensionless
h	mixed layer depth	m
k	horizontal wave number	m s^{-1}
m	vertical wave number	m s^{-1}
L_x	horizontal domain size in the x-direction	m
L_y	horizontal domain size in the y-direction	m
L_z	vertical domain size in the z-direction	m
M^2	horizontal buoyancy gradient	s^{-2}
N^2	vertical buoyancy gradient	s^{-2}
Pr	Prandtl number	dimensionless
q	potential vorticity	$\text{m}^{-1} \text{s}^{-1}$
Ri	Richardson number (bulk)	dimensionless
Ri_0	Richardson number (balanced-initial)	dimensionless
Ri_b	Richardson number (balanced)	dimensionless
Ri_g	Richardson number (gradient)	dimensionless
Ro	Rossby number	dimensionless
u, v, w	velocity (x-, y-, z-direction)	m s^{-1}
x, y, z	spatial coordinate (x-, y-, z-direction)	m
κ	turbulent diffusivity	$\text{m}^2 \text{s}^{-1}$
λ	wavelength	m
ν	molecular/turbulent viscosity	$\text{m}^2 \text{s}^{-1}$
ρ	local density	kg m^{-3}
ρ_0	reference density	kg m^{-3}
ζ	relative vorticity	s^{-1}
ζ_a	absolute vorticity	s^{-1}

*For Ava, may this inspire you in your own journey of asking
the right questions...*

Chapter 1

Introduction

1.1 Background

Dynamical ocean processes encompass a vast range of scales, both in time and space, from large-scale circulation phenomena that influence climate over millennia and span entire ocean basins, to microscale dynamics where energy is dissipated. Mesoscale ($\approx O(10 - 100km)$) and microscale dynamics are relatively well understood. However, submesoscale processes, which lie between these scales remain less explored. Their rapid evolution, small horizontal scales and spatial heterogeneity make direct field observations inherently challenging (Shcherbina et al., 2015). As a result, much of our understanding of submesoscale dynamics has emerged from high-resolution numerical simulations (Capet et al., 2008) and idealised process studies (Boccaletti et al., 2007).

Mesoscale and submesoscale motions can be distinguished by the relative importance of the Earth's rotation. The ratio of the convective and Coriolis accelerations scales with the Rossby number, (Ro):

$$Ro = \frac{U}{fL} = \frac{\zeta}{f}, \quad (1.1)$$

where Ro is a dimensionless measure of rotational effects on the flow. Here, U is the characteristic velocity scale, L is the horizontal length scale, f is the planetary vorticity (given as: $2\Omega \sin \phi$, where Ω is the planetary angular frequency, and ϕ the latitude), and $\zeta = \partial v / \partial x - \partial u / \partial y$ is the vertical component of the relative vorticity.

Mesoscale dynamics are defined by a Rossby number ($Ro \ll 1$), where the dominant forces in the momentum equations are the horizontal pressure gradient and Coriolis acceleration, resulting in a flow that is approximately in geostrophic balance. Submesoscale dynamics on the other hand exhibit a Rossby number of order unity ($Ro \sim O(1)$), where the Earth's rotation is important but does not limit the motion as strongly as it does at larger scales (Molemaker et al., 2010).

Since $\zeta \approx U/L$ and $Ro = U/fL$, the length scale for submesoscales is given as $L = U/f$.

Following Thomas et al., 2008, U can be further defined by assuming thermal wind balance $U \approx \partial b_y H / f$ where buoyancy is given by $(b = -g(\rho - \rho_0) / \rho_0)$, and y is the direction of horizontal buoyancy gradient. Thus the submesoscale length scale can be given in terms of the lateral buoyancy gradient $L = M^2 H / f$ where $M^2 = \partial b / \partial y$. Submesoscale length scales can also be expressed in terms of the vertical buoyancy gradient. Since the vertical buoyancy gradient $N^2 = \partial b / \partial z$ scales with the lateral buoyancy gradient as $N^2 = M^4 / f^2$, thus $L = NH / f$, which is known as the Rossby radius. While this same definition holds for the mesoscale, in terms of submesoscales H is considered the mixed layer depth in contrast to the full water depth, and N is usually much smaller. With typical length scales for L in the range of 0.1 -10 Km.

Given that at submesoscale length-scales, $Ro \sim O(1)$, neither rotation nor stratification dominates, and with a departure from geostrophically balanced dynamics the evolution of ageostrophic circulation is permitted. This breakdown of the standard geostrophic balance introduces complexities that make submesoscale processes difficult to resolve in global and regional numerical models. Their effects on energy fluxes and mixing must often be parameterised (Bachman et al., 2017; Fox-Kemper et al., 2008).

In general however submesoscales are understood to consist of (1) frontal structures associated with potential- (PE) and kinetic energy (KE) (Thomas and Ferrari, 2008; Thomas et al., 2008), (2) a plethora of instabilities which develop and feed off the KE and/or PE generating further submesoscale motions, (3) Ro as discussed above, and (4) the ability to interact with and strongly influence other small-scale, high-frequency phenomena like Langmuir turbulence (Li et al., 2012) and near-inertial waves (Whitt and Thomas, 2013), facilitating a cascade of energy to smaller scales.

The global oceans in general play a significant role in regulating Earth's climate system as well as biogeochemical cycles. They are the largest active reservoir of heat and carbon on the planet, with the ocean interior having sequestered 30% of anthropogenic CO₂ emissions, in addition to storing 93% of the heat generated since the industrial revolution (Von Schuckmann et al., 2023). The upper ocean, characterized by a surface mixed layer (SML), is in direct contact with both the atmosphere and the ocean's interior. It is a critical component of the climate system, regulating the intense exchange of climate relevant tracers such as heat, momentum, carbon, nutrients, and pollutants between the atmosphere and the ocean interior (McWilliams, 2016; Thomas and Ferrari, 2008). As the most turbulent layer in the ocean (Fox-Kemper et al., 2022), the SML is maintained in a well-mixed state by energetic inputs primarily from wind stress, surface waves and atmospheric buoyancy fluxes (heating and cooling). This mixing generally results in weak vertical density stratification. Thus, traditional views of upper ocean dynamics have primarily focused on vertical processes such as the fluxes of momentum, heat, and freshwater, which work to

strengthen or weaken vertical stratification. However, lateral processes, which are closely tied to submesoscale dynamics, are often overlooked in climate models. Advances in satellite resolution (Fig. 1.1) and ocean modeling (Fig. 1.2) reveal that the SML is actually a highly complex region.

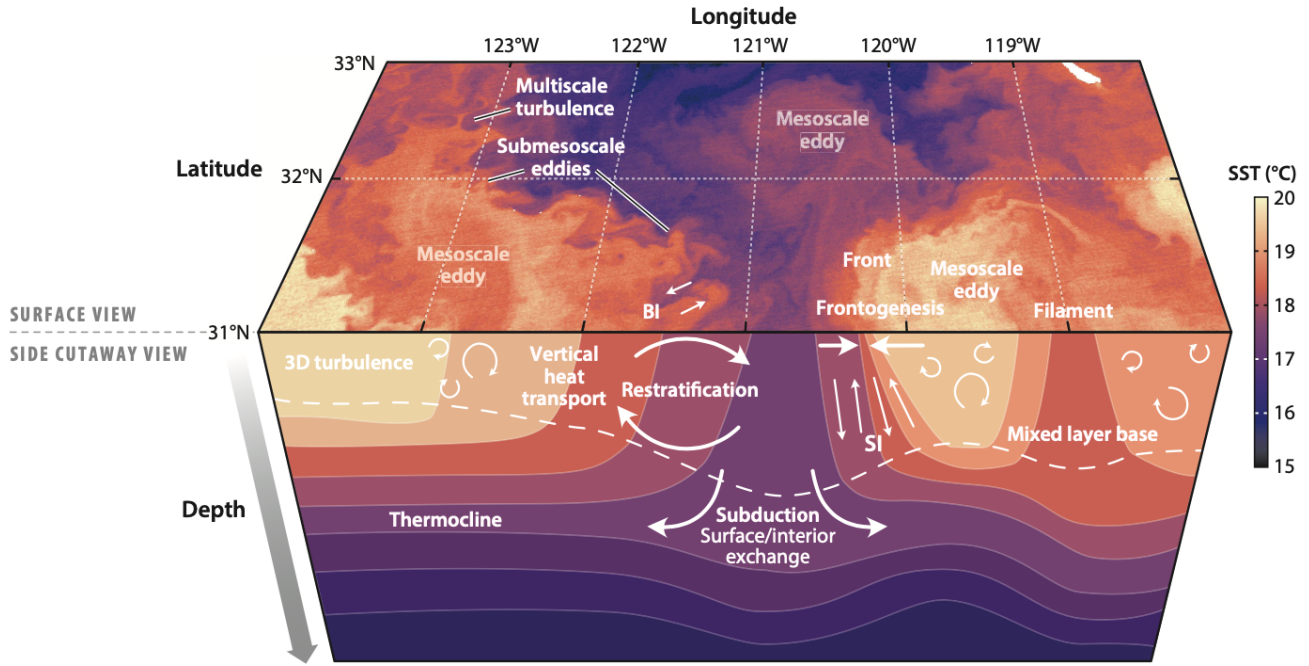


FIGURE 1.1: (Top, surface view) Sea surface temperature (SST) from NASA MODIS Aqua satellite on November 15, 2020. Data from <http://oceancolor.gsfc.nasa.gov>. (Bottom, cutaway view) Hypothetical temperature contours illustrating various submesoscale processes. The image is taken from (Taylor and Thompson, 2023).

Submesoscale currents, with horizontal scales of 0.1–10 km and lifetimes of hours to days, since the $Ro \approx 1$ the characteristic time-scale is $1/f \approx O(1)day$. This is much faster than the mesoscale and results in submesoscales playing a leading role in the evolution of the mixed layer in response to atmospheric forcing. At these scales one typically finds vortices, density fronts, filaments, and topographic wakes, especially in the upper ocean where lateral density gradients are prominent (Thomas et al., 2008; McWilliams, 2016). These near-surface features typically arise spontaneously in regions near mesoscale eddies and intense boundary currents, and are crucial for regulating air-sea exchanges and upper ocean dynamics. Since the SML is in direct contact with the atmosphere, submesoscale currents play an essential role in transporting the climate-relevant tracers between the oceans interior and the atmosphere. Furthermore due to the associated substantial vertical velocities, submesoscale dynamics are able to transport material across the SML within ~ 1 day, significantly coinciding with the response time for marine micro-organisms (Lévy

et al., 2012), thus helping to support the photosynthetic foundation of the food chain by moving nutrient-rich water from deeper layers up to the sunlit but otherwise nutrient-poor euphotic zone (Fig. 1.3).

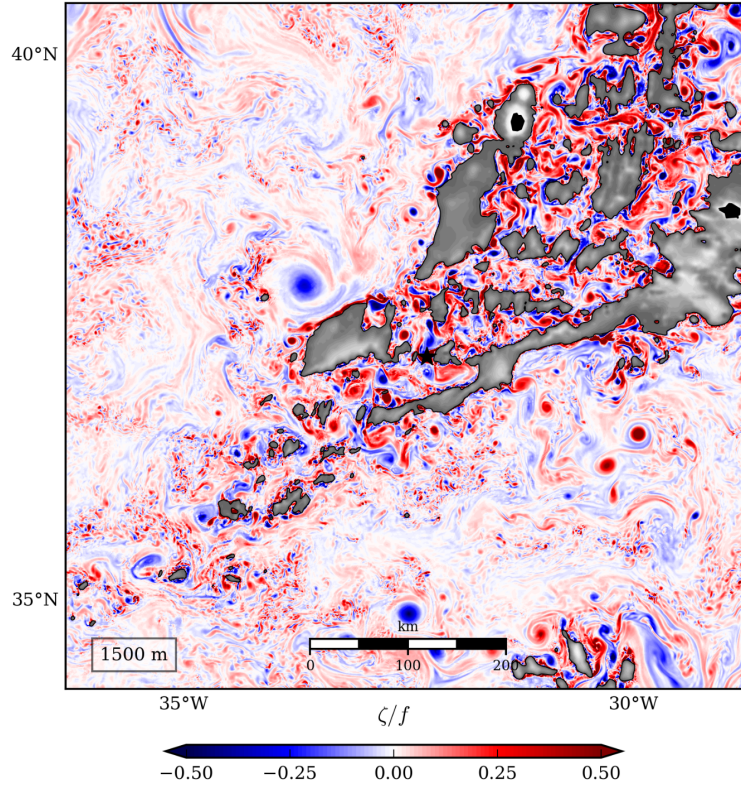


FIGURE 1.2: Snapshot of instantaneous relative vorticity ($\zeta = v_x - u_y$) non-dimensionalised by the local Coriolis frequency f , at a depth of 1500 meters across the Mid-Atlantic Ridge. Data derived from a numerical simulation with a horizontal resolution of = 750 meters. Image modified from Vic et al., 2018.

While air-sea exchanges and vertical mixing primarily drive changes in upper ocean stratification, lateral stirring becomes increasingly significant near density fronts (Ferrari and Rudnick, 2000). Extensive research has shown that turbulence in the SML can be significantly modified in frontal regions, where strong vertical shears serve as a major source of turbulent kinetic energy (TKE) through submesoscale processes (Sullivan and McWilliams, 2018). Fronts serve as reservoirs of mechanical energy, and can trigger a ‘zoo of dynamical instabilities’ during their restratification process (Thomas et al., 2008).

Among these instabilities is symmetric instability (SI), an ageostrophic instability that can develop when gravitational instability is modified by lateral buoyancy gradients in the presence of a frontal zone. Unlike baroclinic instability (BI), which evolves over longer timescales and draws its energy from available potential energy (APE), SI operates on much shorter timescales, extracting its energy from the kinetic energy (KE) associated

with the mean geostrophic shear through geostrophic shear production (GSP). This is a significant turbulent energy source within the ocean boundary layer, where its contribution reaches 34% of the total dissipation in winter and 17% in summer at the mid-depth of the boundary layer (Dong et al., 2024).

Further Dong et al., 2024 found that when considering the top two sources of global turbulent energy (latitudinal dependence), fronts make a leading-order contribution to ocean SML turbulence in many parts of the global ocean, with GSP being the most spatially extensive primary source, providing a contribution in 71% of the locations considered. This challenges traditional views of SML turbulence, which have largely overlooked the role of submesoscale processes. Since these motions drive energy cascades across both smaller and larger scales (Charney, 1971), ocean models tend to exhibit a bias in representing the mixed layer depth (MLD) (Fox-Kemper et al., 2008), the transition between the well-mixed surface layer and the more stratified ocean interior. Given their crucial role in regulating energy transfers and tracer distributions in the upper ocean, submesoscale dynamics and of relevance SI, must be properly accounted for in climate models.

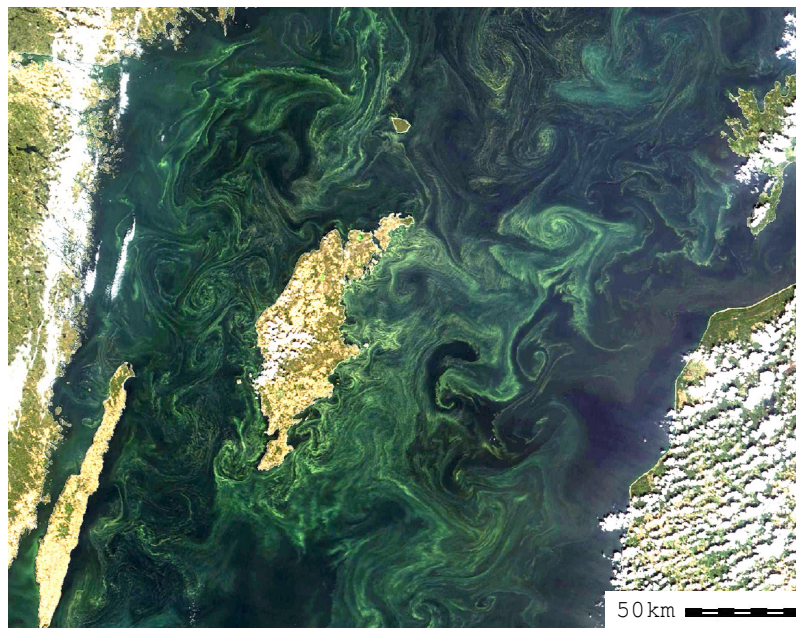


FIGURE 1.3: True-colour satellite image showing green phytoplankton tracers during a bloom in the Baltic sea highlighting submesoscale dynamics in the Eastern Gotland Basin. Photo provided by MODIS, figure adapted from (Leibniz-Gemeinschaft, 2021)

1.2 Governing equations

This section introduces the Reynolds-Averaged Navier-Stokes (RANS) equations as the fundamental governing equations before any further approximations or turbulence closures are applied. The importance of presenting these equations in their unclosed form is twofold:

1. **Physical Foundation:** The RANS equations describe the conservation of mass, momentum, and energy, and explicitly reveal the role of turbulent fluxes in modifying the mean flow. These fluxes appear as Reynolds stress terms in the momentum equations and as turbulent density fluxes in the density equation.
2. **Need for Closure:** The presence of unresolved terms in the RANS equations—such as the Reynolds stresses and turbulent fluxes—necessitates the introduction of a turbulence closure scheme to model these unknowns. In Chapter 3, we introduce a Smagorinsky closure, which parameterises these terms using a subgrid-scale viscosity model. The discussion of the unclosed RANS equations here serves to highlight the importance of turbulent fluxes for submesoscale dynamics. In order to address unresolved processes we use Large Eddy Simulations together with a Smagorinsky closure to resolve the sub-grid scale processes.

The Navier Stokes equations are a set of partial differential equations which describe the movement of viscous fluid. A branch of continuum mechanics, we can apply them to a rotating reference frame i.e. the Earth, and after several assumptions and simplifications, we arrive at a group of equations which aim to best describe the movement of the oceans and atmosphere. They are in essence the geophysical fluid dynamics counterpart of Newton's second law of motion. Thus, this section includes the governing equations which describe the system used in this thesis before the hydrostatic approximation and any sufficient closures are made. Given below are the Reynolds-averaged Navier Stokes equations (RANS). The equations are non-hydrostatic, meaning they do not assume hydrostatic balance in the vertical momentum equation. This allows for the explicit representation of vertical accelerations, which are important for small-scale processes like turbulence, internal waves, and submesoscale dynamics

The equations are Reynolds-averaged, meaning the flow variables (velocity, pressure, density) are decomposed into mean ($\bar{u}$) and fluctuating (i.e. u') components. The governing equations are then averaged, resulting in terms like the Reynolds stress and turbulent flux terms. The equations are without eddy closure, meaning that these Reynolds stresses and turbulent fluxes are not modelled or parameterised. Instead, they are left as unresolved terms that would require a closure to solve the system.

In this thesis, the fluid satisfies conservation of mass, momentum and energy. We make the Boussinesq approximation, which assumes that density variations ($\delta\rho$) are small, such that $\left(\frac{1}{\rho} \frac{d\rho}{dt}\right) \approx 0$, and primarily affect buoyancy - thus ρ only appears when it is multiplied by acceleration due to gravity (g).

1.2.1 Continuity - conservation of mass

We start from the continuity equation, since density variations are negligible, we assume the fluid is incompressible:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \quad (1.2)$$

where u, v, w are the velocity components in the x, y, z directions respectively.

1.2.2 Momentum equations (conservation of momentum)

Under the Boussinesq approximation, density variations are only significant in the buoyancy term, and only show up in the vertical momentum equation. The momentum equations under the traditional f-plane approximation (which assumes a constant $f = \Omega \sin \phi$) in full Cartesian coordinates are:

x-momentum equation

$$\frac{\partial \bar{u}}{\partial t} + \bar{u} \frac{\partial \bar{u}}{\partial x} + \bar{v} \frac{\partial \bar{u}}{\partial y} + \bar{w} \frac{\partial \bar{u}}{\partial z} = -\frac{1}{\rho_0} \frac{\partial \bar{p}}{\partial x} + f \bar{v} - \frac{\partial \overline{u'u'}}{\partial x} - \frac{\partial \overline{u'v'}}{\partial y} - \frac{\partial \overline{u'w'}}{\partial z} + \nu \nabla^2 \bar{u} \quad (1.3)$$

y-momentum equation

$$\frac{\partial \bar{v}}{\partial t} + \bar{u} \frac{\partial \bar{v}}{\partial x} + \bar{v} \frac{\partial \bar{v}}{\partial y} + \bar{w} \frac{\partial \bar{v}}{\partial z} = -\frac{1}{\rho_0} \frac{\partial \bar{p}}{\partial y} - f \bar{u} - \frac{\partial \overline{u'v'}}{\partial x} - \frac{\partial \overline{v'v'}}{\partial y} - \frac{\partial \overline{v'w'}}{\partial z} + \nu \nabla^2 \bar{v} \quad (1.4)$$

z-momentum equation

Since vertical motions are often large in submesoscale frontal zones the hydrostatic approximation used in their solution breaks down. Thus following Stone, 1970 consider the non-hydrostatic contributions such that:

$$\frac{\partial \bar{w}}{\partial t} + \bar{u} \frac{\partial \bar{w}}{\partial x} + \bar{v} \frac{\partial \bar{w}}{\partial y} + \bar{w} \frac{\partial \bar{w}}{\partial z} = -\frac{1}{\rho_0} \frac{\partial \bar{p}}{\partial z} - g \frac{\bar{\rho} - \rho_0}{\rho_0} - \frac{\partial \overline{u'w'}}{\partial x} - \frac{\partial \overline{v'w'}}{\partial y} - \frac{\partial \overline{w'w'}}{\partial z} + \nu \nabla^2 \bar{w} \quad (1.5)$$

where: $\bar{p}$ is the mean pressure, ρ_0 is the reference density of seawater, $\bar{\rho}$ is the mean density, ν is the kinematic viscosity and $\overline{u'_i u'_j}$, are the Reynolds stresses representing turbulent fluxes in velocity.

1.2.3 Density equation (conservation of density)

Using the conservation principles above, we can come up with the time rate of change of density in a fluid parcel that is moving with the flow:

$$\frac{D\rho}{Dt} = \frac{\partial\rho}{\partial t} + \mathbf{u} \cdot \nabla\rho \quad (1.6)$$

where D/Dt is the material derivative, $\mathbf{u} = (u, v, w)$ are the velocities in the (x, y, z) directions respectfully and $\nabla = (\partial/\partial x, \partial/\partial y, \partial/\partial z)$. If we consider the effects of diffusive processes we land up with the advection-diffusion equation for ρ :

$$\frac{\partial\bar{\rho}}{\partial t} + \bar{u}\frac{\partial\bar{\rho}}{\partial x} + \bar{v}\frac{\partial\bar{\rho}}{\partial y} + \bar{w}\frac{\partial\bar{\rho}}{\partial z} = \kappa\nabla^2\bar{\rho} - \left(\frac{\partial\overline{u'\rho'}}{\partial x} + \frac{\partial\overline{v'\rho'}}{\partial y} + \frac{\partial\overline{w'\rho'}}{\partial z} \right) \quad (1.7)$$

where κ is the molecular diffusivity of density (or heat/salt) and $\overline{u'\rho'}$, $\overline{v'\rho'}$, and $\overline{w'\rho'}$ are the turbulent density fluxes, representing the transport of density by turbulent motions. It is worth mentioning that one could add an additional term for any external sources or sinks of ρ . Furthermore these equations are often accompanied by an additional equation of state that describes ρ as a function of temperature, salinity, and pressure. However, this aspect will not be discussed in the current context.

1.3 Submesoscale fronts

Consider a basic schematic of the classic boundary layer vision of the ocean (Fig. 1.4(a)), where you have a horizontally homogeneous and vertically homogeneous mixed layer (ML), above some stratification, as thought of in a revolutionary paper by Haine and Marshall, 1998. If we apply cooling to the ML and decrease its temperature, the layer may entrain cooler water from below thus deepening the MLD. Conversely, heating the ML from above can increase its overall temperature, leading to expansion and potentially a shallowing of the mixed layer. Consider now if we apply stronger cooling/heating on one side of the domain and weaker cooling/heating on the other, we can set up a buoyancy gradient in the horizontal 1.4(b). Its still quite meaningful to have a definition of a ML, since this layer is still vertically mixed, however it is not necessarily horizontally mixed. Intuitively, one might think that this buoyancy distribution is unstable; denser fluid would naturally tend to sink below the more buoyant fluid, while the buoyant fluid would rise above the denser fluid continuing until the buoyancy gradient is entirely in the vertical.

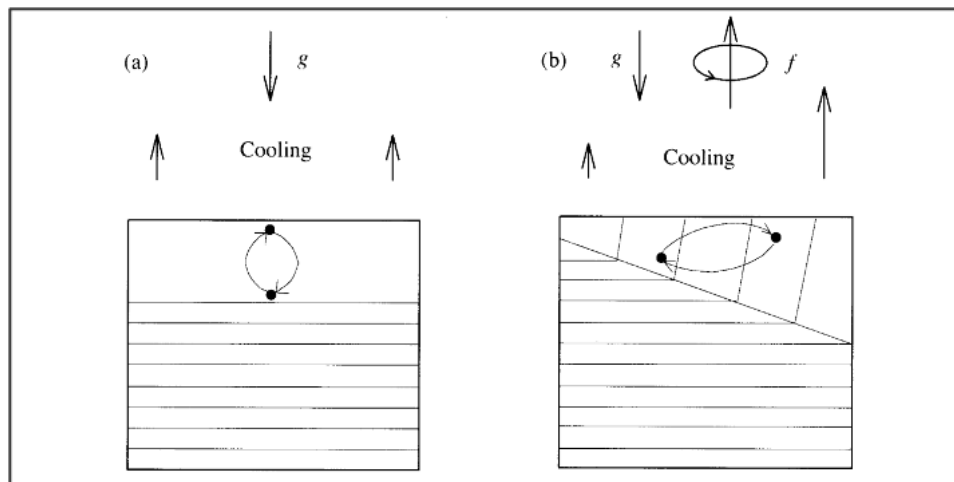


FIGURE 1.4: (a) The classic mixed layer scenario featuring a well mixed region of zero vertical stratification, as a result of surface cooling and consequent gravitational overturning. (b) Differential heating results in a lateral buoyancy gradient. When introduced in a rotating system, symmetric instability acts to reduce potential vorticity to near zero, resulting in weak stratification. This state promotes the formation of baroclinic waves, which facilitate horizontal buoyancy exchanges within the mixed layer. Image from Haine and Marshall, 1998

On a rotating planet however, the horizontal density gradient can be maintained due to the interaction between the buoyancy forces and the coriolis force. An example of

this in the atmosphere is the polar front, where cold polar air flows alongside warmer mid-latitude air. This resulting dynamic equilibrium state is usually unstable; that is the coriolis force can maintain the density distribution in the mean, but minor disturbances can disrupt the local balance, commonly leading to the emergence of instabilities. These instabilities that are not just disruptions to the flow, but play a critical role in transferring energy across scales, mixing fluids, driving local dynamics (i.e. weather) as well as the dynamics of Earth's climate and ecosystems. These processes can significantly modify the upper ML density structure by either increasing the vertical buoyancy gradient or acting to restratify it. Of interest here is how the associated instabilities interact with other small-scale motions that incite or regulate small scale turbulence (Taylor and Ferrari, 2009; Taylor and Ferrari, 2010). The interaction between the large-scale balanced dynamics and small scale unbalanced turbulence facilitates a process often described in the literature as a 'downward energy cascade', a mechanism whereby energy is transferred from larger to smaller scales (Taylor and Thompson, 2023).

1.3.1 Generation mechanisms

Fronts are defined as those regions where the horizontal scale in the along front direction is of the order of the deformation radius (NH/f), with the cross-frontal direction significantly smaller, presenting strong lateral buoyancy and velocity gradients (Hoskins, 1982). Semi-permanent or climatological fronts in the ocean occur in a variety of locations. They include western boundary currents, such as the Gulf Stream and the Agulhas current, which itself can shed rings (Lutjeharms and Van Ballegooyen, 1988) whose water mass properties may significantly differ from its surroundings (i.e. transient fronts), zonal currents such as the Antarctic circumpolar current (Sokolov and Rintoul, 2009), as well as the boundaries of water masses and the polar front (atmosphere). Fronts can also present as elongated filaments with sharp ρ -gradients at the sides, rather than developing as a ρ -step (McWilliams et al., 2009). However, strain-induced mesoscale fronts are not effective at transferring energy to smaller scales where it can be dissipated due to the balance imposed by large-scale quasi-geostrophic dynamics (Lévy et al., 2012).

Submesoscale fronts are formed by what is known as frontogenesis. The classical understanding is that favourably aligned surface horizontal buoyancy gradients, in a background horizontal deformation flow, are quickly intensified by a strain field which rapidly sharpens the local lateral density gradients (Fig. 1.1). Typically occurring at the surface and bottom boundaries, QG and the hydrostatic approximations now have the ability to break down, allowing various submesoscale instabilities to develop. Interestingly, it has been found that submesoscale fronts and dense filaments are the most effective agents for the

lateral spreading of materials on orders $10^{-2} - 10^{-4}m$ (McWilliams et al., 2009). However these types of fronts are more unpredictable in space and time owing to their continual formation, advection and eventual destruction.

1.3.2 Geostrophic adjustment, thermal wind and potential vorticity

If we think back to the thought experiment by Haine and Marshall, 1998, the set-up in Fig. 1.4(b) could have been created were a winter storm have passed through. The storm, homogenises the ML by removing any vertical gradients of salinity and temperature while leaving behind the horizontal gradients intact. The subsequent adjustment process to re-stratify the surface layer could take place in two ways, either surface heating from the sun warming the upper layers, or a gravitationally driven slumping of the nearly vertical isopycnals. Its the latter process that is of interest, which is driven by dynamical adjustment. Owing to the newly formed pressure gradient in the horizontal, water is driven from regions of high pressure to regions of lower pressure. As the water begins to move, the coriolis effect, induced by Earth's rotation, deflects the flow. Initially, the water may oscillate as it 'geostrophically adjusts' to the competing forces. Overtime the flow reaches a balanced state where the pressure gradient force is exactly counteracted by the coriolis force. In this equilibrium, known as geostrophic flow, the current flows parallel to isobars (lines of constant pressure), rather than directly along the pressure gradient. The fluid flows with the high pressure on its right (for the Northern hemisphere).

The equations for geostrophic balance which describes this are given as:

$$fu_g = -\frac{1}{\rho_0} \frac{\partial p}{\partial y} \quad (1.8a)$$

$$fv_g = \frac{1}{\rho_0} \frac{\partial p}{\partial x} \quad (1.8b)$$

Here f is defined as $f = 2\Omega \sin\phi$, where Ω is the Earth's angular velocity and ϕ is the latitude. u and v are the velocity components in the zonal (x) and meridional (y) directions respectively, while ρ_0 is the local density and p is the pressure.

If we now take the vertical derivative of Eq. 1.8 and combine it with the equation Eq. 1.5, we find the thermal wind relation such that the velocity of the flow varies with depth:

$$f \frac{\partial u_g}{\partial z} = \frac{g}{\rho_0} \frac{\partial p}{\partial y} \quad (1.9a)$$

$$f \frac{\partial v_g}{\partial z} = -\frac{g}{\rho_0} \frac{\partial p}{\partial x} \quad (1.9b)$$

This relation is possible due to horizontal changes in the density profile. The result implies that geostrophically balanced fronts can be sustained away from the gravitational equilibrium if lateral density gradients are linked vertical velocity shears. This results in a baroclinic flow meaning that velocity changes with depth (Cushman-Roisin and Beckers, 2011).

During the geostrophic adjustment process, the equilibrium state is generally unstable: the Coriolis force can maintain the density distribution in the mean, but any small disturbance will upset the balance locally, and the flow may locally oscillate between partially stable and unstable states. As a result, instabilities may arise depending on the background conditions of the flow and the mixed layer, with the role of local relative vorticity being a main player. To further understand the stability of a flow and why instabilities might occur, it is important to consider the role of potential vorticity (PV).

We start by defining relative vorticity, which is the curl of the velocity: $\zeta = \nabla \times \mathbf{u}$. By taking the curl of the full momentum equations (1.2.2) we find the change in relative vorticity for a baroclinic, incompressible, inviscid fluid. Making use of the mass continuity equation (1.2.1) we can now formulate an equation for Ertel's potential vorticity (PV, q):

$$q = \frac{(f\hat{\mathbf{k}} + \nabla \times \mathbf{u}) \cdot \nabla(\Phi)}{\rho} \quad (1.10)$$

where $\hat{\mathbf{k}}$ is the unit vector in the vertical, $\zeta_a = f\hat{\mathbf{k}} + \nabla \times \mathbf{u}$ is the absolute vorticity (the sum of the relative and planetary vorticity), and Φ is any conserved quantity. In this thesis we use buoyancy ($b = -g(\rho - \rho_0)/\rho_0$) as the tracer for the conserved quantity. Owing to incompressibility we can write 1.10 in the more recognisable form:

$$q = (f\hat{\mathbf{k}} + \nabla \times \mathbf{u}) \cdot \nabla(b) \quad (1.11)$$

PV is considered one of the most important dynamical variables in geophysical fluid dynamics. Here (an inviscid, adiabatic fluid in a rotating reference frame), it uniquely

combines the effects of rotation and stratification. Furthermore, it remains conserved under adiabatic and frictionless conditions. When strong horizontal or vertical gradients of density or velocity are present, such as during geostrophic adjustment, PV can vary significantly, triggering various instabilities when certain conditions are met. The potential instabilities that may arise are particularly important in submesoscale fronts where the interaction between stratification, rotation, and shear is pronounced.

1.4 Instabilities in submesoscale fronts

As previously discussed, geostrophic fronts motion often seeks an equilibrium or stable state defined by the balance of forces like pressure, gravity, and viscosity. In the ocean at the submesoscale, and under certain conditions, small perturbations can disrupt the stability of the system triggering a variety of instabilities which can grow exponentially (Thomas et al., 2008). By tapping into both potential energy (PE) reservoirs, set up by horizontal changes in buoyancy, and kinetic energy (KE) reservoirs, related to the vertically sheared thermal wind, instabilities can lead to complex flow structures and a down-scale energy transfer to more turbulent regimes (Taylor and Ferrari, 2009). The instabilities that develop differ in their names depending on whether the vertical vorticity, stratification, or baroclinicity of the fluid is responsible for the low PV. Yet despite the mechanism, the result is always the same, these processes act to modify the upper ocean's mixed layer density structure by either increasing the vertical buoyancy gradient or acting to restratify it, acting as the vessel by which an unstable flow adjusts to a stable state.

1.4.1 Baroclinic instability

Baroclinic instability (BI) was first discovered by Charney, 1947 and Eady, 1949 used to describe the evolution of mid-latitude weather systems. However, at the submesoscale $Ro \approx 1$, ageostrophic effects are more pronounced, and so growing perturbations might depart from the state of geostrophic balance that was initially assumed by Eady, 1949. Here, the instability which is sometimes referred to as 'mixed layer instability' when it occurs in the ML occurs at scales $O(1 - 10)$ km, nearly in thermal wind balance, with the wavelength of the most unstable perturbation given by (Eady, 1949) as:

$$\lambda \approx \frac{4NH}{f} \quad (1.12)$$

BI grows by converting available potential energy (APE), which is stored in the background stratification, from the basic state into perturbation KE. It does this by releasing the PE stored in the horizontal density gradients, rather than drawing energy from thermal wind shear, by fluxing buoyancy which carries lighter water up and denser water down (Stone, 1972). Thus BI can drive ML restratification and additionally plays a fundamental role in the generation of submesoscale eddies (Boccaletti et al., 2007; Fox-Kemper et al., 2008).

Baroclinic instability can be characterized by the along front velocity scale U and the length scale L associated with a disturbance developing along the front. The scales for the developing instability in terms of Ro are $L \approx U f^{-1} Ro^{-1}$ and $T \approx f^{-1} Ro^{-1}$. From a linear stability analysis first performed by Stone, 1966 for ageostrophic equations, we find that the fastest growing modes in the along front direction grow at a scale near the local deformation radius (Stone, 1966) such that: $NH/fL \approx 1$ where H is the vertical scale of the mode in question.

Following Boccaletti et al., 2007, unstable modes are linked to Ri in the following way:

$$\frac{N^2 H^2}{f^2 L^2} = Ro^2 Ri_b \approx 1 \quad (1.13)$$

1.4.2 Gravitational / convective instability

Gravitational (convective) instabilities develop when the background density gradient is unstable / negative i.e.

$$N^2 = \frac{\partial b}{\partial z} < 0 \quad (1.14)$$

For a basic state with no flow and an unstable density gradient, pure gravitational instability (GI) is generated that gains KE through buoyancy production:

$$BP = \overline{w'b'} \quad (1.15)$$

where the overline denotes, an ensemble average for example, and primes the deviation from that average. One can think of a scenario such as Fig. 1.4a, where an upper ocean (a homogenous ML lying above a stratified thermocline) is at rest, and subject to uniform cooling from above. If $N^2 < 0$ then the exchange of parcels occurs purely in the vertical and as such must release gravitational potential energy. Driven by these restoring buoyancy forces, fluid parcels continuously rearrange themselves extracting energy from the

APE stored in the vertical buoyancy stratification. The rate of this growth is given by $N^2 = -\frac{g}{\rho_0} \frac{\partial \rho}{\partial z}$.

1.4.3 Inertial instability

Consider the limit case where $N^2 = 0$ such that the mixed layer is uniform in density. Within this layer, let there be a horizontal velocity $u(y)$, where the rate of change of velocity in the horizontal, $\partial u / \partial y$, is constant. This setup now contrasts with gravitational instability, as here, energy exists solely in kinetic form. In this scenario, inertial instability can develop via lateral shear production and effectively extracting KE from the laterally sheared geostrophic current.

According to parcel theory (Haine and Marshall, 1998), energy release occurs when $\partial u / \partial y > f$, leading to the onset of inertial instability. This type of instability arises when the vertical component of the absolute vorticity of the flow is negative i.e. $\zeta_k < 0$. The growth rate is given by

$$\omega^2 \leq f(u_y - f) = -f\zeta_k \quad (1.16)$$

illustrating the direct relationship between the lateral shear and the effects of the Earth's rotation.

1.4.4 Symmetric instability

Symmetric Instability (SI), an ageostrophic instability that can develop when regular gravitational instability is modified due to the lateral buoyancy gradients associated with the presence of a frontal zone. The buoyancy perturbations associated with SI modes are typically small, and develop faster than their BI counterpart (Stone, 1966).

A formal linear stability analysis shows that different types of instabilities can arise when

$$q = (f\hat{\mathbf{k}} + \nabla \times \mathbf{u}) \cdot \nabla b < 0 \quad (1.17)$$

indicating that the potential vorticity (PV) within a fluid volume has the opposite sign to the coriolis parameter (Hoskins, 1974). In this thesis, we set $f > 0$, conditions found in the northern hemisphere. Hence negative potential vorticity satisfies the instability criterion and is equivalent to $f q < 0$.

Following Thomas et al., 2013, the instability criterion for SI becomes more obvious if we assume a thermal wind balance and decompose PV into two distinct components: q_ζ , which relates to the relative vorticity, and q_b which is associated with baroclinicity:

$$q = \underbrace{(f + \zeta)N^2}_{q_\zeta} - \underbrace{M^4/f}_{q_{bc}} \quad (1.18)$$

The equation highlights the role of lateral buoyancy gradients in setting up conditions for instability. Particularly, when the destabilizing influence of these gradients is strong enough to overcome the stabilizing effects of vertical stratification and rotation, it pre-conditions the flow for SI (Taylor and Ferrari, 2009). As a result, increased baroclinicity (M^4/f) becomes a dominant factor potentially driving fq below zero.

In an initially stable front ($fq > 0$), low baroclinic PV is balanced by high vortical PV. If the upper ML's stratification is mixed and N^2 is reduced, ultimately leading to an overall decrease in q_ζ , conditions may arise that lead to the destabilisation of the front. However, in the absence of a significant frontal buoyancy gradient (i.e. $M^2 = 0$), inertial instability can occur when $N^2 > 0$ and $f + \zeta < 0$. Thus, for SI to exist, the condition $(f + \zeta)N^2 > 0$ and an M^4 that is sufficiently large enough such that $fq < 0$ is met. Since $fq < 0$ is a necessary but not sufficient condition for SI.

Given the complexity of the relationship between gravitational, inertial and symmetric instabilities, identifying the dominant instability can prove challenging, particularly when strong fronts exist and the above mentioned instabilities can all produce slantwise motion for $fq < 0$. Under these conditions, the dominant instability that develops can be summarised by the Thomas angle (Thomas et al., 2013) and will be discussed in a more relevant setting in Chapter 6.

Much of the ocean is stably stratified such that fN^2 is positive, dominating q (1.18) and thus stable to SI. However, frictional stresses, or diabatic fluxes can lead to conditions where $fq < 0$. Thus, the criterion for SI can be satisfied through surface cooling (Haine and Marshall, 1998), which leads to buoyancy loss, or by an Ekman buoyancy flux (EBF). The latter arises from the transportation of cooler water above warmer water as a result of cross-frontal Ekman transport. This occurs when down-front winds blow along the direction of the frontal jet (Thomas and Lee, 2005; Thomas and Taylor, 2010), and is discussed in detail in Chapter 6). Consequently, SI unstable flows are typically observed in the surface and bottom boundary layers of the ocean (Thomas and Lee, 2005).

Various prior numerical studies have explored the non-linear evolution of SI under various conditions. Most of these investigations have centred on a single value of the

non-dimensional horizontal buoyancy gradient. Likewise, we follow a similar approach, concentrating on a single value of the non-dimensional gradient Richardson number Ri_g :

$$Ri_g = N^2 / [(\frac{\partial u}{\partial z})^2 + (\frac{\partial v}{\partial z})^2] \quad (1.19)$$

This is because an alternative criteria for the growth of symmetric instability can be given in terms of the balanced Richardson number Ri_b (Taylor and Ferrari, 2009; Thomas et al., 2008; Stamper and Taylor, 2017) where Ri_b is given as:

$$Ri_b = \frac{f^2 N^2}{M^4} \quad (1.20)$$

This provides a more intuitive way of thinking about SI in terms of competing effects of stratification. If the geostrophic flow features negligible vertical relative vorticity (ζ) then 1.18 becomes

$$fq = f^2 N^2 - M^4 \quad (1.21)$$

Now, $Ri_b < 1$ becomes the sufficient condition for SI to develop (Stone, 1966; Taylor and Ferrari, 2009).

In contrast to gravitational instability which extracts energy from APE, SI predominately grows by extracting mean KE from the geostrophic shear at a rate given by the geostrophic shear production:

$$GSP = \overline{\mathbf{u}'_h w'} \cdot \overline{\frac{\partial \mathbf{u}_g}{\partial z}} \quad (1.22)$$

SI itself is not responsible for the dissipation as its length scale is much larger than that of the dissipation scale. So while SI may act to indirectly drive energy downscale, it is generally understood that energy dissipation is a result of the associated secondary instabilities (Kimura, 2024). Taylor and Ferrari, 2009 found that secondary Kelvin–Helmholtz instabilities that develop from the primary SI bands cure the instability by either entraining nearby fluid with $PV > 0$ or inducing stabilizing viscous/diffusive fluxes of PV at the sea surface. This represents an energy transfer towards turbulent motions (Taylor and Ferrari, 2009; Thomas et al., 2013).

1.4.5 Kelvin-Helmholtz instability

Kelvin–Helmholtz instability (KHI) is an instability that occurs when there is velocity shear in a single continuous fluid or a velocity difference across the interface between two fluids thus making it relevant in the discussion of submesoscale fronts. Its classical billow structures were first observed in the ocean by Woods, 1968, but this instability is dynamically important in the evolution of internal wave breaking (Howland et al., 2021) and exchange flows (Hogg and Ivey, 2003) as a saturation mechanism. KHI can also occur as a secondary instability saturating the growth of symmetric instability (Taylor and Ferrari, 2009). The well-known necessary but not sufficient condition given by the Miles–Howard theorem states that there is potential for KHI to grow somewhere in the flow if the gradient Richardson number $Ri_g < 1/4$.

It is suggested that the final step towards the scales at which 3-D turbulence and dissipation is bridged by secondary KHI (Taylor and Ferrari, 2009). It has been found that finite-amplitude SI develops secondary KHI along bands of enhanced shear, which then break down into smaller-scale turbulence. Consequently KHI will be the secondary instability saturating the growth of SI in this thesis.

1.5 Thesis outline and structure

1.5.1 GSP prevalence and the role of SI

Following destabilizing events, such as strong winds or cooling, restratification of the SML is essential for restoring vertical stability in the upper ocean.

Traditionally, BI instability has been identified as a key mechanism in this process. However, recent studies suggest that on shorter time scales the role of SI in the restratification of submesoscale fronts may be downplayed.

From observations, it is indeed confirmed that large scale ocean fronts are close to a state of thermal wind balance (Rudnick and Luyten, 1996), and that this balance is a good approximation for motions at the mesoscale or larger, where $R_0 \ll 1$. However, challenges emerge when an ocean model’s resolution tries to resolve the submesoscales ($R_0 \approx 1$), where perturbations might depart a geostrophically balanced state and non-geostrophic submesoscale instabilities like SI may develop but are left unresolved. Parameterisations must be introduced (i.e. Bachman et al., 2017), making sure to neither out-compete the resolved eddies for energy (Henning and Vallis, 2004) nor count the effects of the eddies more than once (Delworth et al., 2012).

In order to stabilize the flow to SI, a source of higher-PV fluid is required. Picture the ocean's ML, where a mixed layer that is unstable to SI might overlies a thermocline whose higher stratification makes it stable to SI. It is generally believed the increase in mixed-layer PV appears to be associated with the KHI (Taylor and Ferrari, 2009).

Contrary to this, we find that the exact mechanism that drives the energy exchange and where this required PV flux injection might take place may not be as trivial as expected. This leads us to ask what role PV fluxes from the ocean's interior play in the dynamics of SI, particularly in the context of restratification? Furthermore, how do initial conditions, such as stratification and turbulence, affect the development, saturation, and eventual decay of SI, and what role do secondary KHI play in the picture?

Along with understanding the development of SI, it is the restratification mechanism and associated increase in PV that is largely the motivation behind this work. We further ask what the key mechanisms driving the restratification process in SI-unstable submesoscale fronts might be, and how do these mechanisms vary under different environmental conditions? How might the situation change when external forcing is applied? That is how does SI contribute to the restratification of the ocean's SML following destabilizing events?

We take a bottom-up approach to studying the development, equilibration and restratification of submesoscale fronts by symmetric instability. By using an LES in an Eady type setup, we can break down the problem into its most simplistic form, and then compare the results to more realistic scenarios as we increase the complexity of the model, ultimately concluding with a more realistic setup involving forcing.

1.5.2 Structure

Chapter 2 provides a theoretical foundation of the linear theory associated with vertically-bounded SI in horizontally homogeneous frontal zones. It also provides insight into the dependence on the maximum growth rate of SI for different values of the balanced Ri_b and ν_t .

In Chapter 3, we outline the type of model employed and the underlying equations governing its construction. Here we already provide an analysis into the effect that resolution plays on the growing symmetric modes, as well as the minimum resolution required to resolve any secondary features associated with them. This is then used to justify the experimental setups employed, where we distinguish between the various initial conditions, background conditions, model resolution, and parameters used. The chapter also provides a section on model robustness by simply comparing the total flux of PV

within one of the model runs to the sum of its components. The chapter concludes with a comparison of the model output to what we expect to find from linear theory.

Chapter 4 explores the development of SI within the most basic setup, providing insights into how the frontal system evolves through a series of spin-down experiments that vary in nature through their initial stratification. Increasing the complexity to a two-layer model, we address the current school of thought as to how PV fluxes might change within the domain by adding an attached interior region of highly stratified fluid. The energetics are also explored.

Chapter 5, ties to its predecessor by investigating what the key mechanisms that drive the restratification process and pv fluxes are. The chapter consists of three sub-sections, the first of which provides an analysis of optimal initial conditions for SI growth. The second subsection discusses the impact that turbulence has on SI growth. The third subsection contrasts how fluxes from the boundaries might change SI development, as well as the role SI plays in initiating restratification within a convectively formed ML.

Chapter 6 provides an analysis on the evolution of a symmetrically unstable front that has been spun-up using storm forcing, with the results compared and contrasted against the preceding model runs. This chapter is then succeeded by a general discussion and conclusion and some insight into how these results may be incorporated into future research is provided.

Chapter 2

Linear Theory

2.1 Introduction

Fronts are prone to various linear instabilities that drive submesoscale motions. While BI plays a key role in releasing the potential energy stored within horizontal density gradients, SI grows by extracting KE from the geostrophic shear. Here KHI, an important shear-driven instability, can occur as a secondary instability and saturate the growth of SI, eventually leading to enhanced small-scale dissipation and mixing.

Consider a flow which is initially in hydrostatic and geostrophic balance in an infinite domain. Here, the hydrostatic limit relies on the fact that the horizontal scale (L) of ocean basins are much larger than the ocean depth (H). This assumption leads to a small aspect ratio $\delta = H/L \ll 1$, meaning that vertical accelerations are much smaller compared to gravitational forces. We can now neglect all the terms except pressure gradient and gravity force in the vertical momentum equation, and is termed the hydrostatic approximation.

The growth rate (σ), obtained from normal mode solutions of the form $u' = Ue^{ikx+imz-\sigma t}$, is given by (e.g. Bachman and Taylor, 2014):

$$\sigma = \left[\frac{M^4}{N^2} - f(f + \zeta) - N^2 \left(\frac{k}{m} - \frac{M^2}{N^2} \right)^2 \right]^{1/2} \left(1 + \frac{k^2}{m^2} \right)^{-1/2} - \nu_t(k^2 + m^2) \quad (2.1)$$

Here, N^2 and M^2 are the vertical and horizontal buoyancy gradients, respectively. The cross-frontal horizontal wave number is denoted as k and the vertical wave number is given by m . $\zeta = \partial_x v - \partial_y u$ is the vertical component of the relative vorticity, and f is a constant Coriolis parameter. The above form assumes a Prandtl number of one so that the turbulent viscosity (ν_t) equals the turbulent diffusivity, which are both considered as constant. If the isopycnal slope $s_b = (M^2/N^2) \ll 1$, SI modes develop in a hydrostatic regime with $m \gg k$. As discussed in Taylor and Ferrari, 2009 and Bachman and Taylor, 2014, the growth rate in the non-viscous hydrostatic limit, i.e. $\nu_t = 0$, is then given by the

term in the angle brackets. In such a limit the fastest growing modes are aligned with the isopycnal surfaces, so that $k/m = M^2/N^2$. The factor $\left(1 + \frac{k^2}{m^2}\right)^{-1/2}$ gives the contribution from non-hydrostatic dynamics, which tends to decrease the maximum growth rate. Finally, the last term shows that turbulent friction stabilises the shortest modes and acts to slightly reduce the slope of the most unstable mode (Taylor and Ferrari, 2009).

2.2 Hydrostatic limit

We now focus on an infinite horizontal domain with $\zeta = 0$. In the vertical, the domain is considered to be finite with a vertical scale H , for example the surface mixed layer depth. In a viscous ocean the fastest growing modes will develop at the largest possible scale, the vertical wave number (m) of the the fastest growing mode is then given by $m = 2\pi/H$. Using Eq. 2.1 we are now able to calculate the growth rate and horizontal wave length of fastest growing mode using the initial conditions for N^2 , M^2 , f , H , and some estimate of ν_t .

In the hydrostatic limit, i.e. $N^2 \gg M^2$ and $m \gg k$, Eq. 2.1 then reduces to

$$\sigma = \left[\frac{M^4}{N^2} - f^2 \right]^{1/2} - \nu_t \left(\frac{2\pi}{H} \right)^2 \quad (2.2)$$

The root of Eq. 2.2 gives the upper bound of turbulent viscosity allowing unstable SI modes to grow:

$$\nu_t^{max} \approx \frac{H^2}{4\pi^2} f \sqrt{\left(\frac{1}{Ri_0} - 1 \right)} \quad (2.3)$$

Here, $Ri_0 = N^2 f^2 M^{-4}$ is the initial bulk Richardson number. For example, taking $H = 50m$, $f = 1 \times 10^{-4}$, and $Ri_0 = 0.4$ leads to $\nu_t^{max} = 0.0078 m^2 s^{-1}$. Note, that in a non-hydrostatic regime ν_t^{max} will be smaller. As this study focuses on conditions with a very weak stratified mixed layer, most of our experiments will encounter such a non-hydrostatic regime. The maximum growth rates according to linear theory for several non-hydrostatic conditions are given in Fig. (2.1). In general the maximum growth rate decreases with larger Ri_0 . For a given f , smaller Ri_0 represent a larger isopycnal slope s . Larger s_b allows SI modes to grow, i.e. the growth rate (σ) is positive, for relatively large values for the turbulent viscosity.

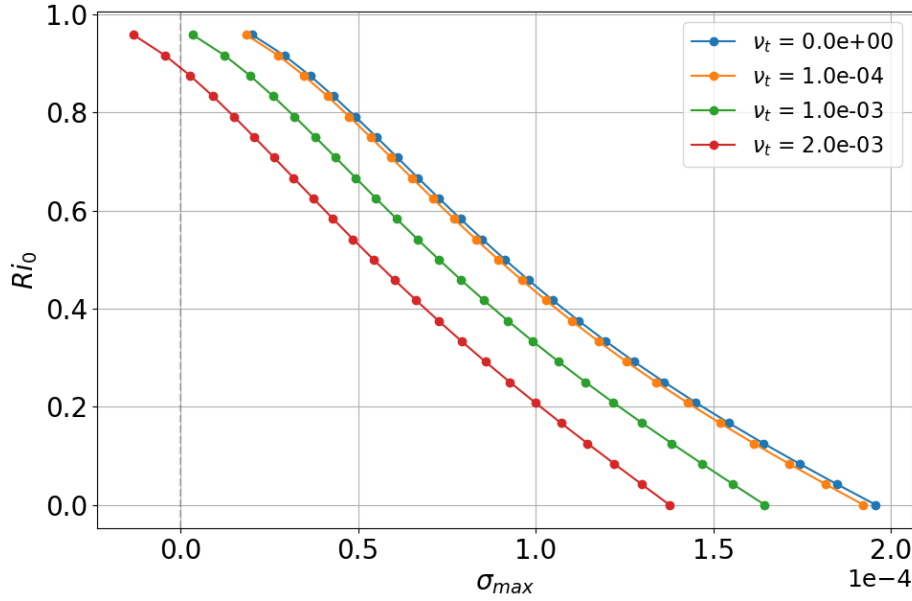


FIGURE 2.1: Maximum growth rates for different values of the initial Richardson number Ri_0 and the turbulent viscosity ν_t . All growth rates are given for $f = 1 \times 10^{-4} s^{-1}$, $M^2 = 4.3 \times 10^{-8} s^{-2}$, $H = 50m$ and a vertical wave number given by $m = 2\pi/H$. Ri_0 is varied by varying N^2 . The angles $\alpha = \tan(s)$ between the isopycnal slopes $sb = (M^2/N^2)$ and the horizontal ranging from $\alpha = 90^\circ$ in case of $Ri_0 = 0$ to $\alpha = 13.75^\circ$ for $Ri_0 = 0.95$.

2.3 Interplay between SI and KHI

Growing SI modes will increase the vertical shear, so that they become unstable to Kelvin-Helmholtz instabilities (KHI) (Taylor and Ferrari, 2009). KHI transfer energy from the SI modes to turbulence, preventing further growth. The growth of KHI depends on the stratification and the vertical shear of the horizontal velocities. In the simplest form of adjacent shear layer the growth rate of KHI is given by Smyth and Carpenter, 2019 as:

$$\sigma_{KH} = \pm \sqrt{\frac{1}{4} \Delta u^2 m^2 - \Delta b m} \quad (2.4)$$

where Δu and Δb are the difference in the horizontal velocity and buoyancy between both layers, respectively. Here σ_{KH} is associated with SI, thus it scales with the vertical wave number (m) of the SI modes (Wienkers et al., 2021). According to linear theory, the largest shear in the SI modes is normal to the wave number direction and in the middle of a vertically bounded domain (Wienkers et al., 2021). Only the vertical projection of that

shear is responsible for driving KHI. The impact of SI on draining energy from a given front in thermal wind balance, i.e. for given M^2 , N^2 and f , is therefore a complex interplay between the growth of SI and KHI modes, modified by the (pre-)existing turbulence (ν_t).

2.4 Discussion

In large-scale oceanic flows, where the aspect ratio $\delta = H/L \ll 1$, the hydrostatic approximation is valid, ensuring that pressure and gravity dominate vertical momentum balance. However, in submesoscale regions with weak stratification and significant vertical motion, vertical accelerations can no longer be ignored, leading to a breakdown of the hydrostatic assumption. Consequently, non-hydrostatic effects become relevant, particularly in mixed-layer processes where SI growth occurs.

In submesoscale fronts, the transition from hydrostatic to non-hydrostatic behaviour occurs when vertical velocities approach horizontal velocities in magnitude, typically at scales where the aspect ratio δ is no longer small. This is particularly relevant in the mixed layer, where stratification is weak, and instabilities like SI generate significant vertical motions. Consequently, resolving these dynamics in numerical models requires a non-hydrostatic framework to capture the full range of instability-driven turbulence

The main findings from normal mode linear theory provide a foundational understanding of the results obtained in the numerical experiments discussed in Chapters 4 and 5. A key takeaway is that only a relatively large eddy viscosity (ν_t) has a significant influence on the growth rate (σ), emphasizing that smaller values of eddy viscosity have minimal damping effects on instability development. In the inviscid case, the growth rate (σ) for a front in thermal wind balance is determined exclusively by the orientation of the wave number vector (k/m). Additionally, the emergence of secondary KHI plays a crucial role in halting the further growth of SI. The onset and evolution of KHI are themselves governed by the vertical wave number (m) of the SI modes, highlighting an intricate coupling between these instability types that regulate energy transfer and the eventual equilibration of the system. These theoretical principles offer critical context for interpreting the numerical simulations, particularly in understanding how energy cascades and instabilities interact under varying conditions.

Chapter 3

Numerical Methods

3.1 Numerical simulations of SI unstable fronts

In this thesis, we use an large eddy simulations (LES) model to perform non-linear three-dimensional numerical simulations of a ML front to complement and validate the linear theory of chapter 2.

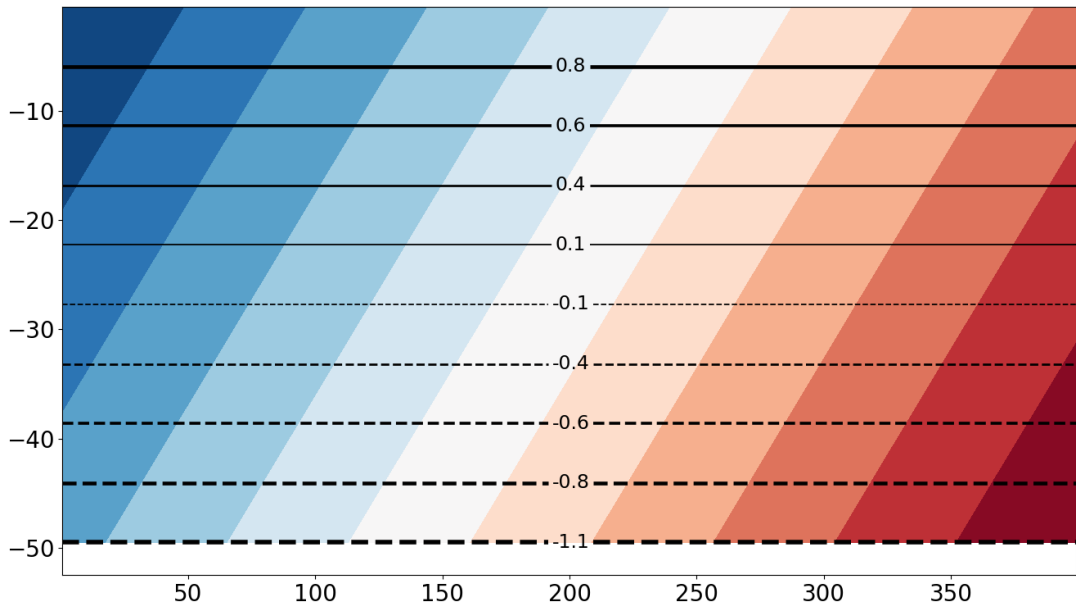


FIGURE 3.1: Frontal region highlighting the across front density variation b_b with contours of the background velocity $\bar{u}_b$ (cm s^{-1}) whose magnitude is represented by line thickness. The across front stratification is balanced by thermal wind shear in $\bar{u}_b$ which varies only in the vertical, while the buoyancy is a linear function of y and z .

We consider an Eady type model which consists of fluid with initially uniform potential vorticity between two rigid horizontal boundaries, which can be viewed as an idealised

representation of a ML front (Eady, 1949). The physical setup in its most basic form is represented in Fig. (3.1). In this area, the geostrophically balanced velocities are considered to be horizontally constant, i.e. $\zeta = 0$ in the balanced flow.

The LES model makes use of the integrated non-hydrostatic Boussinesq- momentum equations:

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} + f \mathbf{k} \times \mathbf{u} = \frac{1}{\rho_0} \nabla p + \mathbf{k} b + \mathbf{F} \quad (3.1)$$

Here, $\mathbf{U} = \mathbf{u}_b + \mathbf{u}$, $\mathbf{k}$ is the vertical unit vector, f is a constant Coriolis parameter, and $\mathbf{F} = \nabla \cdot \nu \nabla \mathbf{u}$ gives the non-conservative frictional force, with eddy viscosity $\nu(x, y, z, t)$ provided by the LES closure. The model calculates the deviations from steady background velocity $\mathbf{u}_b$. We consider a background velocity in zonal direction which is in thermal wind balance, so that $\partial_z u_b = M^2/f$. M^2 denotes a meridional gradient $M^2 = \partial_y b_b$ in the steady background buoyancy b_b . For the sub-grid closure, we use the approach of Smagorinsky, 1963 with $\nu = C^2 \Delta^2 |S|$. S is the rate-of-strain tensor, Δ the grid size, and C the Smagorinsky constant, which is $C = 0.14$ in our runs. In tensor notation S is given by $S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$. The pressure is solved by using an efficient pseudo-spectral method (Pekurovsky, 2012).

The buoyancy equation is given by:

$$\frac{\partial b}{\partial t} + (\mathbf{u} + \mathbf{u}_b) \cdot \nabla(b) + v M^2 + w N_0^2 = \mathcal{D} \quad (3.2)$$

, where $N_0 = \partial_z b_b$ is the initial and constant background Brunt-Väisälä frequency, and $\mathcal{D} = \nabla \cdot \kappa \nabla b$. The turbulent diffusivity is given by $\kappa = \nu/Pr$, where a Prandtl number of $Pr = 1$ is applied. In the horizontal we use cyclic boundary conditions, while the vertical boundaries are rigid. Here, the vertical velocity (w) is zero and no-flux boundary conditions are applied for buoyancy and momentum.

By fixing a background M^2 , we can investigate the evolution and neutralisation of SI-unstable fronts by varying the initial balanced Richardson number (Ri_0) through N^2 . Spin down simulations see restratification as an increase in overall Ri_b , which can be achieved by either an increase in N^2 , a decrease in M^4 , or even a decrease in N^2 which is offset by a larger decrease in M^4 (Bachman et al., 2017). In comparison, Wienkers et al., 2021 fix N^2 and instead vary their setup based on M^2 , through what they define as frontal strength, $\Gamma \equiv M^2/f^2$. The variation of frontal strength provides insight into the role of SI in extracting momentum from the geostrophic shear under differing frontal conditions.

The experiments conducted are summarised in Table 3.1. They simulate a ML with a

vertical scale H set to $50m$. In all experiments, the Coriolis parameter $f = 1 \times 10^{-4} s^{-1}$ and the meridional background buoyancy gradient $M^2 = -4.3 \times 10^{-8} s^{-2}$, thus all runs share the same vertical geostrophic shear. The meridional domain size is $L_y = 4 \times \lambda$, with λ being the wavelength of the fastest growing mode according to Eq. (2.1). In these simulations, submesoscale instabilities that exhibit along-front structures, such as BI might grow and confound the results after a few inertial periods. To avoid this, we select an along-front domain size that is smaller than these BI waves but still larger than the typical turbulence correlation length scale. The velocity fields in all runs in this section are initialised with a white noise perturbation of amplitude $10^{-4} ms^{-1}$.

3.2 Effects of resolution

The improvement of resolution in climate models naturally allows for the description of a broader range of the energy spectrum (Capet et al., 2008). As a consequence there have been considerable contemporary advancements in understanding oceanic submesoscale dynamics. However, in these particular models, dissipation continues to be primarily influenced by numerical limitations rather than physical ones. As computational cost increases with the higher resolution simulations, ocean models often do not have the sufficient resolution to capture these small scale processes. Thus parametrisations (Bachman et al., 2017) might be introduced to make models more affordable. However they come at the cost of potentially failing to accurately capture all of the physics. We find that secondary-instabilities associated with SI, whose roles will be discussed in Chapter (5), require a resolution of at least $2m$ to be fully captured within our runs.

The experiments conducted in this section are summarised in Table 3.1. They simulate a front in thermal wind balance that can be modelled using a basic Eady type spin down setup. Here the vertical is fixed representing a ML with a vertical scale H set to $50m$. The horizontal domain is infinite with cyclic boundary conditions such that $\zeta = 0$. In all experiments the Coriolis parameter $f = 1 \times 10^{-4} s^{-1}$, the meridional background buoyancy gradient $M^2 = -1.0 \times 10^{-7} s^{-2}$, and the vertical buoyancy gradient are kept constant $N^2 = 5.0 \times 10^{-7} s^{-2}$. Thus all runs share the same vertical and horizontal geostrophic shear with an applied initial Richardson number $Ri_0 = 0.5$, where $Ri_0 = N^2 f^2 / M^4$ and sets the initial frontal conditions.

Experimental names indicate the resolved resolution, i.e. the suffix ‘_8’, indicates a model resolution of $8m$. The meridional and zonal domain sizes are fixed at $L_y = 800m$, $L_x = 800m$ respectively. These model runs do not include an attached stratified interior beneath the mixed layer. Thus the vertical domain size remains fixed at $L_z = 50m$. The variation between model runs is applied through the number of grid points (N), with

$N_z = 50$ fixed throughout. Thus the only isotropic run is ‘RI05_1’, with a resolution of 1m in both the horizontal and vertical i.e. $L_{x;y;z}/N_{x;y;z} = 1m$. In these runs we apply an initial noise of amplitude of $B_0 = 10^{-7} s^{-1}$.

Name	Ri_0	$\nu_{sgs}[m^2s^{-1}]$	$N_{mix}^2 [s^{-2}]$	α	$N_{x,y}$	$L_{x,y}$	Res [m]
RI05_8	0.5	Smag	5.0 e-7	11.3°	100	800	8
RI05_4	0.5	Smag	5.0 e-7	11.3°	200	800	4
RI05_2	0.5	Smag	5.0 e-7	11.3°	400	800	2
RI05_1	0.5	Smag	5.0 e-7	11.3°	800	800	1
RI04_high	0.4	Smag	7.40 e-8	30.2°	26.6°	16.5	0.25

TABLE 3.1: Summary of the configuration details of each numerical simulation involved in the resolution comparison. Ri_0 is the initial Richardson number, ν_{sgs} the turbulent viscosity for the sub-grid scale. ‘Smag’ indicates $\nu_{sgs}(x, y, z, t)$ is given by the Smagorinsky closure. N_{mix}^2 is the initial stratification in the mixed layer, α gives the angle of the isopycnal slope with the horizontal, i.e. $\tan \alpha = M^2/N^2$. Res indicates the resolution calculated as the horizontal domain length (L) over the number of grid points (N) i.e. $Res = L_{x,y}/N_{x,y}$

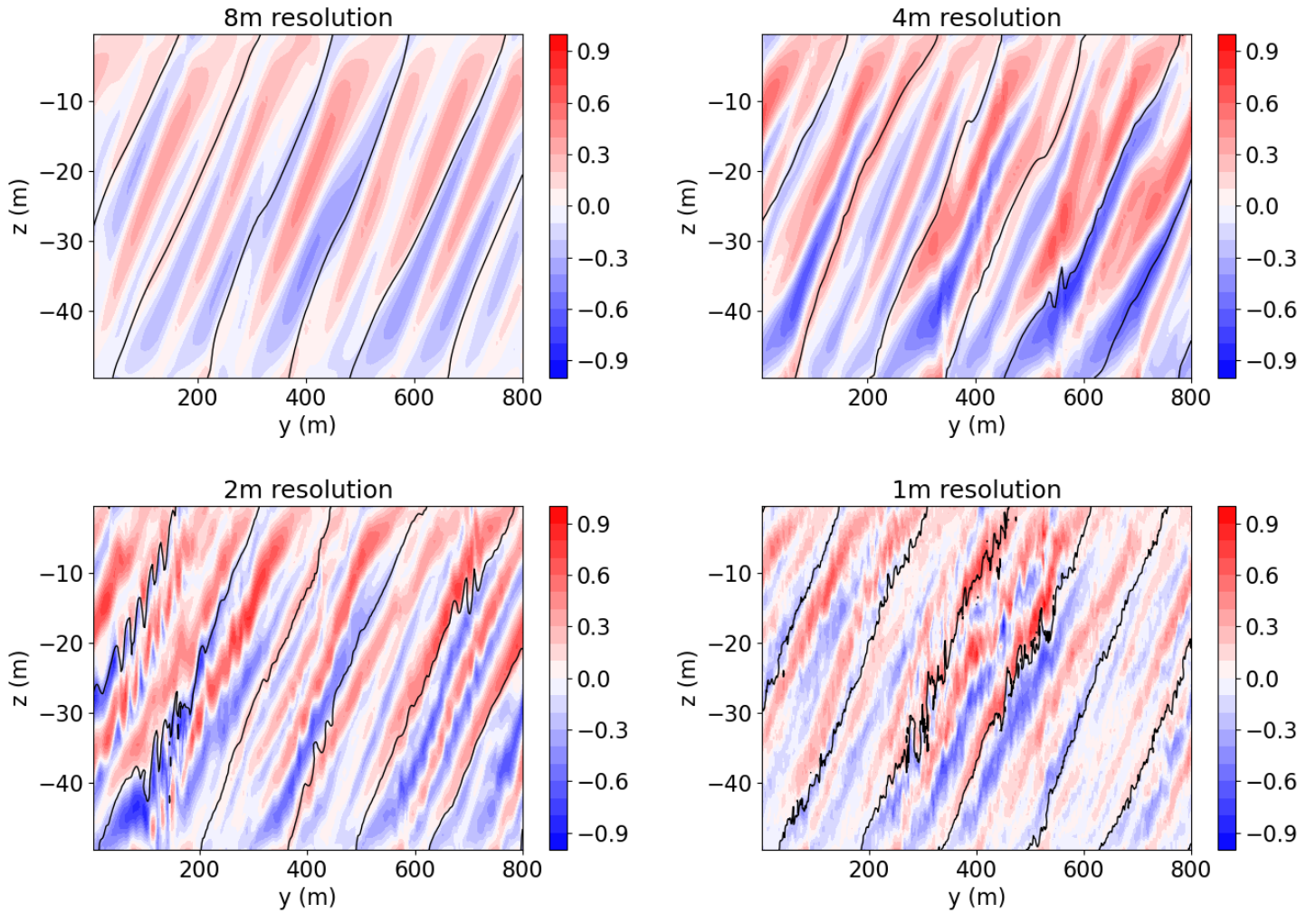


FIGURE 3.2: The appearance of SI convection cells in the cross-frontal velocity field (cm s^{-1}) snapshots at 35h, for various resolutions of the runs ‘RI05_’ as indicated in Table 3.1. Contours indicate zonally averaged isopycnals. At higher resolutions KH-instabilities are evident, acting on the shear layers between the SI cells.

Figure 3.2 shows SI modes in the cross-frontal velocities after 35h of run time. The first figure in the upper left corner, corresponds to a model resolution of 8m. A growing symmetric mode is evident in the snapshot. The cells are almost aligned with the isopycnals. In the higher resolution run of 2m, it is evident that as the magnitude of the local shear grows at the edges of the symmetric instability cells, secondary small-scale KH instabilities appear. These features of the flow are not resolved at resolutions less than 2m. This is significant as the lower resolution runs might smooth out or entirely miss important small-scale dynamics like KH-instabilities, which are crucial for accurately representing the submesoscale processes. Consequently this may have an effect on energy dissipation and the restratification process for example. The resolved secondary instabilities seen in the higher resolution runs have consequences for the isopycnal slopes. Qualitatively, their

alignment with the SI cells does not seem to change with resolution. However as the resolution increases and smaller secondary instabilities are resolved, so too do the isopycnals contort and break up, indicative of mixing. At 1m resolution it seems that some of the regions have already broken down into isotropic turbulence.

The alternating positive-negative signal seen in the cells also highlights the cross-frontal flow. That is, positive cross-frontal velocities at the surface of the domain and negative cross-frontal velocity at the bottom. This is in accordance with the work of Taylor and Ferrari, 2009, and it too will be discussed in further detail in Chapter (5). It is worth noting that we already see the higher vertical modes in the higher resolution runs, which trigger KHI earlier as seen in the linear instability analysis.

3.3 Model Robustness

3.3.1 PV diagnostic

In this sub-section, we assess the robustness of the LES model by analysing the consistency between the total PV) flux and the sum of its individual components. This approach ensures that the model accurately resolves the physical processes contributing to the evolution of PV, and that the numerical methods used maintain proper conservation and balance.

We know that in an inviscid, adiabatic fluid in a rotating reference frame, PV is conserved by the fluid motion. We can write the PV in this setup as follows:

$$q = (f\hat{k} + \nabla \times u) \cdot \nabla(b + b_b) \quad (3.3)$$

where b_b is the background buoyancy. This can then be rewritten in terms of the absolute vorticity ω_a , with the evolution written in flux form as follows:

$$q = \omega_a \cdot \nabla(b + b_b) \quad \Rightarrow \quad \frac{\partial q}{\partial t} = -\nabla \cdot J \quad (3.4)$$

where J is given by:

$$J = (u + u_b)q + \nabla b \times \mathbf{F} - \omega_a \mathcal{D} \quad (3.5)$$

Here $\mathbf{F}$ is a frictional or non-conservative frictional force and $\mathcal{D}$ is as defined in Eq. 3.2. If we take horizontal averages we land up with the following equation for the vertical PV fluxes

$$\overline{J_z} = \overline{w'q'} + \overline{(\nabla_h(b + b_b) \times \mathbf{F}_h) \cdot \mathbf{k}} - \overline{(\zeta + f\hat{k})\mathcal{D}} \quad (3.6)$$

where the terms on the r.h.s. represent the advective flux (J_{adv}) - which describes the transport of PV by the resolved flow, the frictional flux (J_{fric}) - related to momentum dissipation due to frictional forces, and the diabatic PV flux (J_{dia}) - which represents changes in due to non-conservative processes like heat exchange. In figure 3.3, we compare J_z directly against the sum of the fluxes from each of these components.

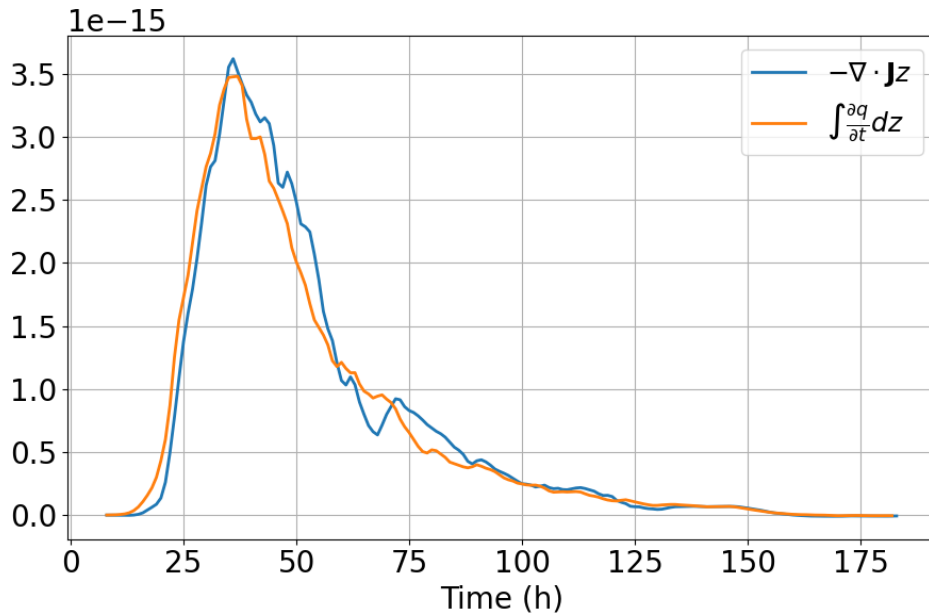


FIGURE 3.3: Time series comparison between the rate of change of PV flux (LHS) and the vertical PV flux divergence (RHS) of equation 3.4 for RI052 ($m s^{-4}$). The evolution of PV flux divergence is set by the vertical pv fluxes J_z which are largely accounted for by the advective (J_{adv}), frictional (J_{fric}), and diabatic fluxes (J_{dia}).

The figure reveals a close agreement between the total PV flux and the sum of its components throughout the simulation period. This agreement is essential, as it confirms that the model is accurately capturing all contributing processes to the PV budget without introducing significant numerical errors which ensure no artificial fluxes of PV are introduced, or that there are no unaccounted-for sources of flux. Any discrepancies between the total flux and the summed components would indicate potential issues in the representation of subgrid-scale processes or in the flux calculation methods used. This is

essential as the stability of the setup to SI is governed by the PV criterion. PV is notoriously difficult to diagnose, with this test validating our ability to accurately calculate the pv fluxes.

3.3.2 Comparison with linear theory

Using Eq. 2.1 from Bachman and Taylor (2014), we plot the maximum growth rates from linear theory for various initial Richardson numbers, Ri_0 , by determining the wavenumber k that maximizes the growth rate. The bisection method was employed to find the optimal wavenumber.

The maximum growth rates derived from the LES output are calculated from GSP (Fig. 4.8) as follows:

$$\frac{d\text{GSP}/dt}{\langle \text{GSP} \rangle} \quad \text{where} \quad \langle \text{GSP} \rangle_i = \frac{\text{GSP}_i + \text{GSP}_{i+1}}{2} \quad (3.7)$$

This approach allows for a direct comparison between the theoretically predicted growth rates of SI and those observed in the LES. The LES captures both the low-resolution and high-resolution simulations, which are presented in Fig. 3.4.

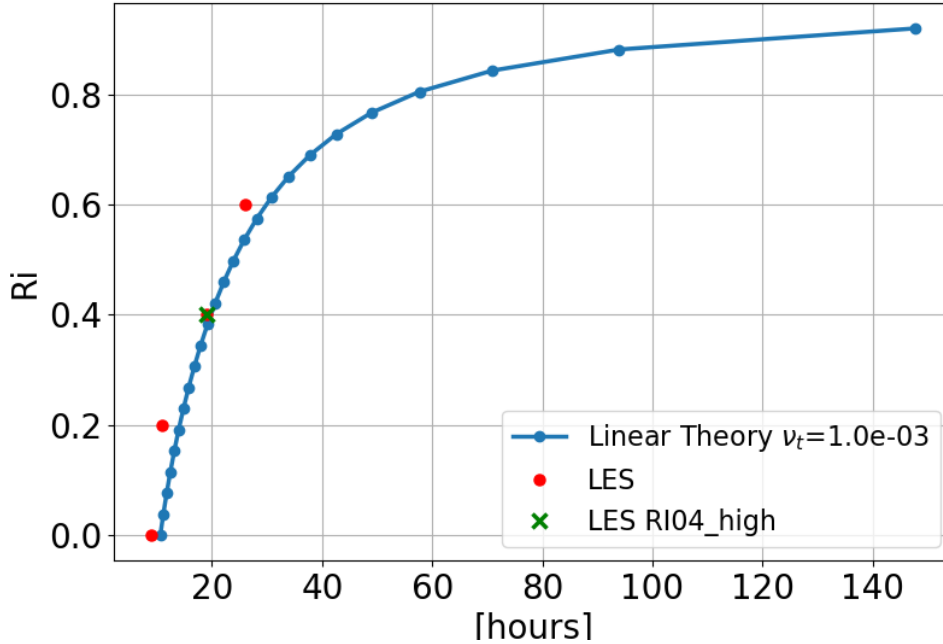


FIGURE 3.4: Comparison of τ_σ (h) of the fastest growing mode from linear theory for $\nu_{sgs} = 1.e^{-3}m^2s^{-1}$ and LES output for ‘RI00-RI06’ (red dots) and ‘RI04_high’ (green cross).

We find strong agreement between the linear theory predictions and the LES output for the maximum growth rates across different Ri_0 , for both the low-resolution ($2m$) and the

high-resolution ($0.25m$) LES runs. Linear theory predicts that the maximum growth rate of SI decreases with increasing Ri_0 , which we observe in both the theoretical curve and the LES output. This indicates that the simulations successfully capture the dynamics of SI even at different levels of resolution, further supporting the robustness of the model in accurately representing the dynamics at these scales.

The slight deviations between the LES results and the linear theory curve could be attributed to several factors. In particular how the subgrid-scale parameterizations are handled. The use of different subgrid-scale viscosities in the LES, particularly in the low-resolution runs, may introduce small discrepancies, especially where the turbulent dynamics are less well resolved. Furthermore as the simulations progress, nonlinearities and secondary instabilities such as KHI, may modify the SI growth rates beyond what is predicted by linear theory. While linear theory captures the early stages of SI, the nonlinear evolution of the flow may result in slight departures from the theoretical predictions.

Despite these potential discrepancies, the strong agreement between the linear theory and LES output validates the ability of the LES to resolve the onset of SI, including the development of secondary instabilities that are not captured by linear theory alone. Since the LES plays a crucial role in capturing the nonlinear dynamics that follow, we can explore late time dynamics associated with the fully developed state of SI to really understand its role in the equilibration and restratification of the system.

Chapter 4

Modelling SI

Destabilizing atmospheric forcing can maintain a surface layer with weak to vanishing stratification. In the presence of a geostrophically balanced horizontal density gradient, such weak stratification often results in areas where the Ertel potential vorticity (PV) is of opposite sign to the Coriolis parameter, making these regions prone to symmetric instability (SI). In this chapter, we use idealised large eddy simulations (LES) to explore the growth and saturation of symmetric instability (SI) within a frontal zone using the Eady model framework. Our objective is to understand how SI-driven energy transport and the long-term dynamics evolve in response to variations in the initial frontal conditions, which are set through Ri_0 .

In their study, Stone, 1966 used asymptotic expansions to analyse the linear stability of normal mode perturbations, showing that symmetric instability occurs only when $Ri_b < 1$. For the basic state in the Eady model, this condition, is equivalent to $f q < 0$. In Eady's original work, which considered only geostrophic perturbations, baroclinic instability emerged only when $Ri_b > 0.84$ Eady, 1949. In contrast, Stone's analysis incorporated ageostrophic perturbations, allowing for the development of growing baroclinic modes.

4.1 Model setup and configurations

The experiments conducted in this chapter can be broken down into two categories, and are summarised in Table 4.1. The first section 4.2 simulates a ML with a vertical scale H initially set to $50m$ as graphically represented in 3.1. The second section 4.3 involves model runs with an attached stratified interior of $N^2 = 1 \times 10^{-6} s^{-2}$ beneath the mixed layer, with run names including an '_int' suffix. In these runs the vertical domain size then increases from $L_z = 50m$ to $120m$, which is graphically represented in figure 4.1. The time step is fixed at $dt = 0.5s$. In order to prevent reflection of internal waves in runs with an attached interior, velocities are damped in a sponge layer in the lower $20m$.

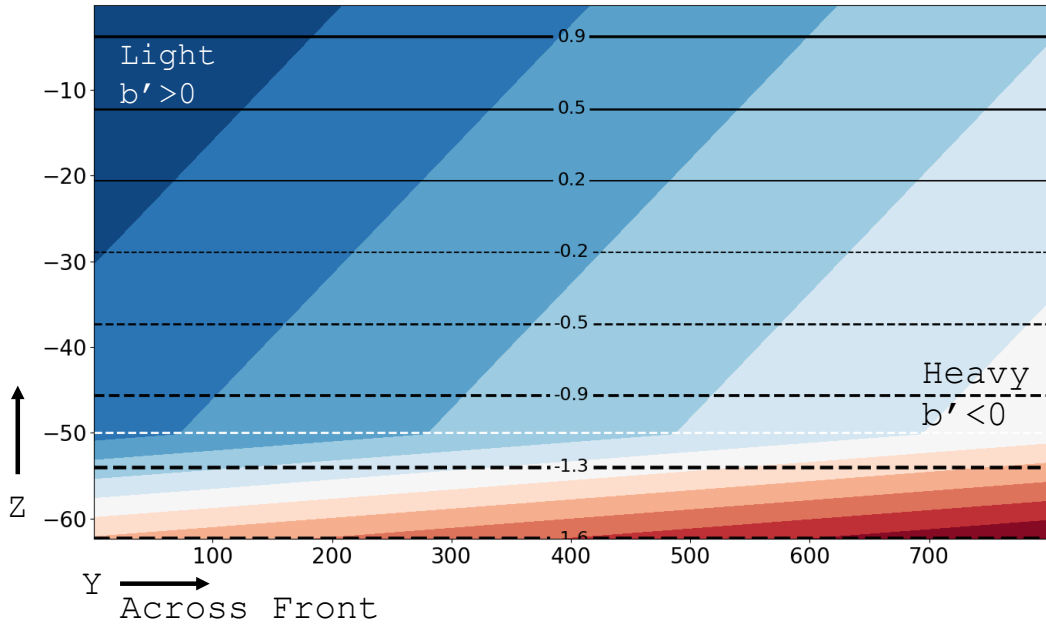


FIGURE 4.1: Frontal region highlighting the across front density variation b_b with contours of the background velocity $\bar{u}_b$ ($cm\ s^{-1}$) whose magnitude is represented by line thickness. The across front stratification is balanced by thermal wind shear in $\bar{u}_b$ which varies only in the vertical, while the buoyancy is a linear function of y and z . Here the full depth representing runs labelled 'RI_int_' has been limited for graphical purposes. The white dashed line represents the mixed layer depth and limit in those runs without an attached interior.

In all experiments the Coriolis parameter $f = 1 \times 10^{-4} s^{-1}$ and the meridional background buoyancy gradient $M^2 = -4.3 \times 10^{-8} s^{-2}$, thus all runs share the same vertical geostrophic shear. Experimental names indicate the applied initial Richardson number, Ri_0 . As with the previous runs, to prevent reflection of internal waves within the attached interior, velocities are damped in a sponge layer in the lower 20m. The meridional domain size is $L_y = 4 \times \lambda$, with λ being the wavelength of the fastest growing mode according to Eq. (2.1). We use an isotropic grid with a resolution of $\Delta = 1m$. Additionally we run simulations with a higher resolution using an isotropic grid of $\Delta = 0.25m$. Due to computational costs, $L_y = 2 \times \lambda$ in the high resolution runs. The velocity fields in all runs are initialised with a white noise perturbation of amplitude $10^{-4} ms^{-1}$.

4.2 Eady model - one layer

This section explores the development and implications of simulations with $Ri_0 < 1$ on the dynamics of SI and KHI. We aim to understand how these instabilities evolve, their impact

Name	Ri_0	$N_{mix}^2 [s^{-2}]$	α	β	$\tau_\sigma [h]$	$\lambda [m]$
RI00	0.0	0	90°	47.3°	9.1	46
RI02	0.2	3.70 e-8	49.3°	36.0°	12.1	69
RI04	0.4	7.40 e-8	30.2°	26.6°	16.5	100
RI06	0.6	1.11 e-7	21.2°	20.2°	23.4	136
RI00_int	0.0	0	90°	47.3°	9.1	46
RI02_int	0.2	3.70 e-8	49.3°	36.0°	12.1	69
RI04_int	0.4	7.40 e-8	30.2°	26.6°	16.5	100
RI06_int	0.6	1.11 e-7	21.2°	20.2°	23.4	136
RI04_high	0.4	7.40 e-8	30.2°	26.6°	16.5	100
RI04_int_high	0.4	7.40 e-8	30.2°	26.6°	16.5	100

TABLE 4.1: Summary of the configuration details of each numerical simulation. α gives the angle of the isopycnal slope with the horizontal, i.e. $\tan \alpha = M^2/N^2$. The latter three rows corresponds to linear theory using Eq. (2.1) for $H = 50m$, $\nu_t = 1 \times 10^{-4} m^2 s^{-1}$, and $m = 2\pi/H$. β gives the angle of the wave number vector with the horizontal, i.e. $\tan \beta = k/m$, τ_σ is the period, and λ the wave length of the fastest growing mode, respectively.

on the restratification of the ML, and their the associated energetic processes. To facilitate a straightforward comparison with linear theory, we limit L_z to $50m$ and maintain uniform initial PV throughout the domain. This setup allows us to examine the fundamental dynamics of these instabilities under controlled conditions.

4.2.1 SI

We start by analysing the ‘RI04’ simulation, which is initialised with a white noise perturbation of amplitude $10^{-4} m s^{-1}$. Figure 4.2 provides snapshots of cross-frontal velocities at various stages of SI-induced restratification. The evolution of the flow field demonstrates the transition from an early, well-organized SI structure to more complex turbulent dynamics as time progresses.

The early stage of SI growth (Fig. 4.2a) shows a relatively ordered flow structure, consistent with the initialized mode. The cross-frontal velocities exhibit periodic patterns in the across front or meridional direction, aligned with the tilt of the isopycnals (shown by the black contours), both of which are relatively steep. The velocity field indicates the characteristic wave-like structure associated with SI, with alternating regions of positive (red) and negative (blue) velocities. At this stage, the isopycnal slopes are still pronounced, with the flow dominated by linear SI growth. By 24 hours (Fig. 4.2b), the SI mode continues to grow, with the wavelength of the instability clearly visible in the cross-frontal velocity field. The amplitude of the velocities has increased, showing stronger

positive and negative regions, indicative of intensified SI activity. The tilt of the isopycnals remains much the same compared to the previous snapshot, suggesting no change in the restratification. At this point, the flow is still relatively organized, with the instability maintaining a coherent structure, and the wavelength that develops is in accordance with the linear theory.

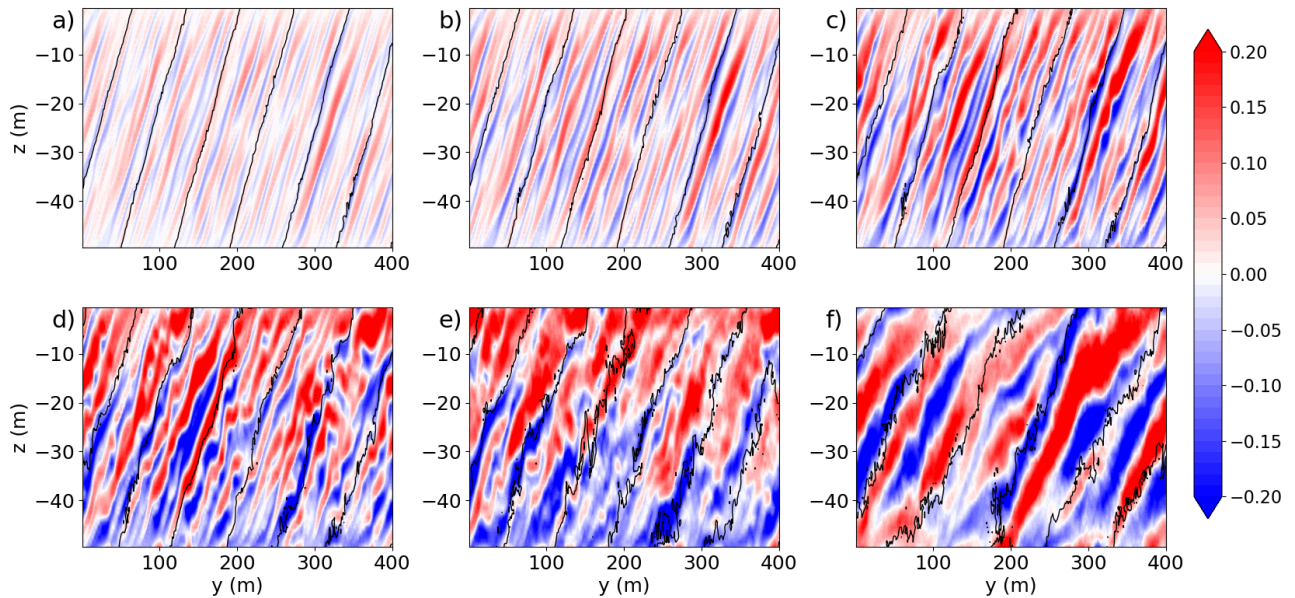


FIGURE 4.2: Cross-frontal velocities (cm s^{-1}) during different stages of SI induced restratification from ‘RI04’. Shown are snapshots from meridional sections after a model integration of a) 22h, b) 24h, c) 26h, d) 28h, e) 30h, and f) 40h. Contours indicate zonally averaged isopycnals.

More noticeable changes are evident by 26 hours (Fig. 4.2c). There is a significant broadening of the velocity structures, with the cross-frontal velocities appearing more diffuse. The isopycnal slopes maintain their angle once more. However, nonlinear effects begin to emerge, as some secondary instabilities start to develop in the velocity field as the shear along the isopycnals grows in certain localised areas. These instabilities are likely the precursors to more complex processes such as KHI, which typically arises in the later stages of SI development. Despite these changes, the flow still retains a significant amount of its wave-like structure, though with increased irregularity. It is not until 28 hours (Fig. 4.2d), that the system has entered a non-linear regime, yet the isopycnals maintain their initial angle, while the cross-frontal velocities display irregular and mixed patches of positive and negative values. This is a clear indication of secondary instabilities beginning to develop into KHI, as seen in the broadening and tilting of the velocity streaks. These instabilities are beginning to roll up, causing the once-linear SI mode to transition into a more turbulent state. The presence of coherent KHI billows can be inferred from

the swirling velocity patterns, marking the onset of turbulent mixing. By 30 hours, (Fig. 4.2e), the KHI billows have further developed and are now in the process of rolling up into vortical structures, leading to enhanced mixing and turbulence. The cross-frontal velocity field shows clear signs of nonlinear breakdown, with large patches of alternating velocities becoming more disordered. We find that this maintains for the next 8-10 hours, until (Fig. 4.2f), where we see a new SI mode developing, with a different wavelength compared to the initial SI wavelength. Finally it is first here that we see a flattening of the isopycnals, albeit smooth. This period marks the beginning of a new cycle of instability and restratification, with modified characteristics due to the turbulent nature of the flow.

4.2.2 Impact of Ri_0

We can determine the stability of the system at various stages by analysing the evolution of Ri_0 overtime. Figure 4.3 shows a comparison for the runs ‘RI00 - RI06’. As expected there is an overall increase in Ri_b over time in each simulation. Given that M^2 is held constant, the evolution is indicative of ever increasing stability of the flow, an increase in N^2 and consequently a flattening of the isopycnals. We also see that there is a clear dependence in the time it takes for Ri_b to tend towards 1 (or an equilibrium value), on Ri_0 . That is the time taken for the system to stabilize is inversely proportional to Ri_0 . Furthermore its clear that the exponential growth of Ri_b is more rapid in runs with low Ri_0 evident when comparing the curves’ steepness between $Ri_0 = 0$ through to $Ri_0 = 0.6$. This is indicative of intense SI growth until SI is most likely suppressed. Finally we see the impact of inertial oscillations for all the simulations with timescales close to the inertial period $2\pi/f \approx 17.5h$, the effects or amplitudes of which most pronounced in the runs with low Ri_0 .

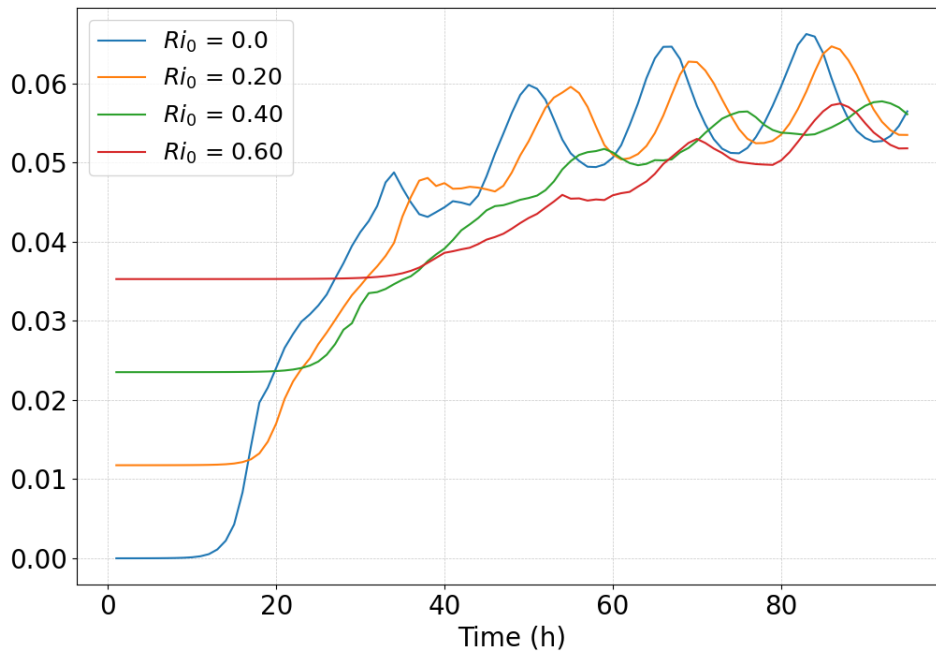


FIGURE 4.3: Time series of domain averaged Ri_b over time for runs from RI00 to RI06 as indicated in the legend. Since M^2 is held constant, the evolution is in essence an increase in N^2 over time.

4.2.3 Potential vorticity (PV) changes

The hovmöller plots represent the evolution of PV in the vertical domain over time for varying Ri_0 (Fig. 4.4). For all cases, PV starts from negative values, conditions favourable for SI development. For the weakly stratified cases where $Ri_0 = 0.0$ and 0.2 , we observe early and significant changes in PV, highlighted by the positive (red) regions. While there is still noticeable PV increase in the $Ri_0 = 0.4$ and 0.6 cases, the evolution is more gradual and distributed more evenly throughout the water column suggesting that the restratification process in these higher Ri_0 acts more gradually and milder in intensity.

This notion is seen more clearly in slope of the time series (Fig. 4.5) during its exponential growth. Over time, all runs become more stable, with PV tending toward zero with rate of stabilization depending heavily on Ri_0 . Here we can see the direct influence of stratification in suppressing or amplifying the mixing processes.

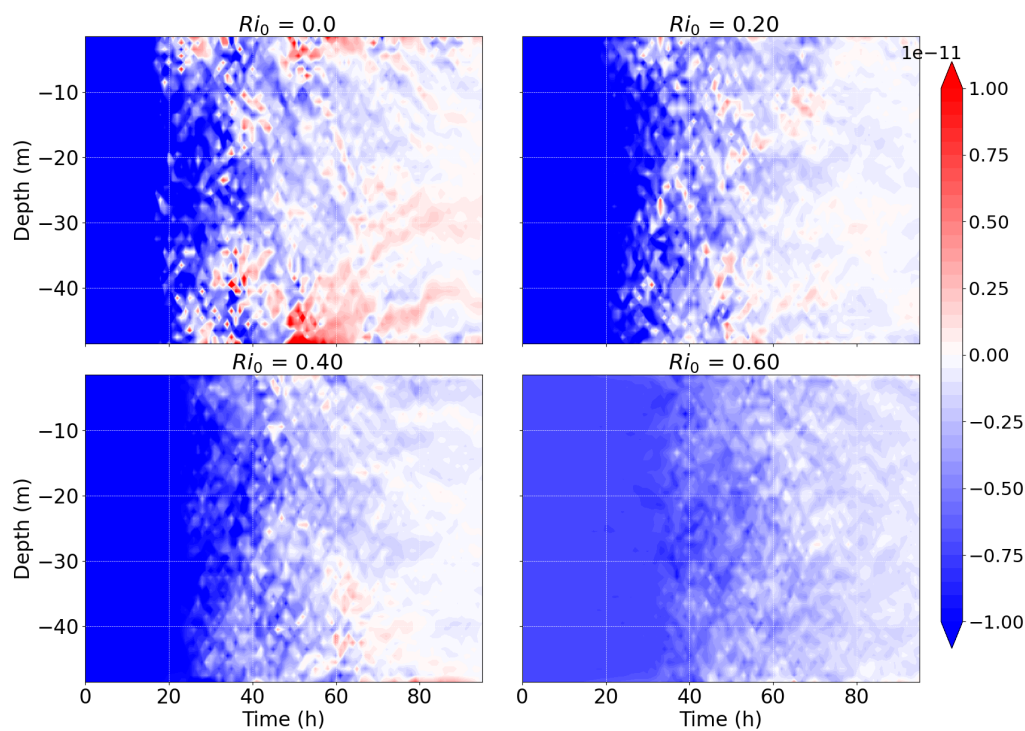


FIGURE 4.4: Comparison of hovmöller plots of horizontally averaged potential vorticity (PV) over time for experiments ‘RI00 - RI06’ (s^{-3}).

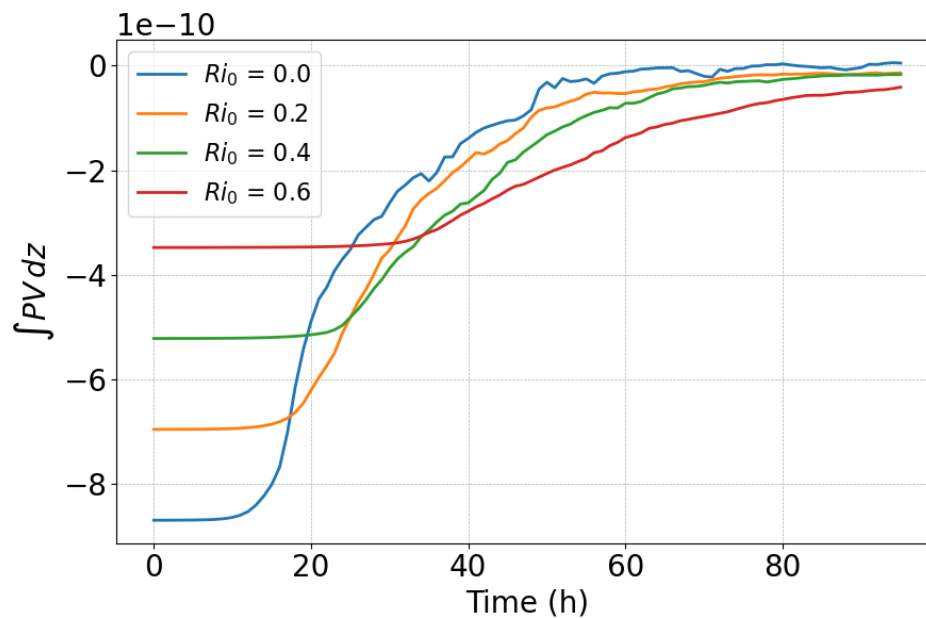


FIGURE 4.5: Time series of vertically integrated PV over time for experiments ‘RI00 - RI06’ (ms^{-3}). A filter has been applied over the inertial period.

4.2.4 Energetics of SI

SI has the potential to play a prominent role in the forward energy cascade. In order to find the sources and sinks of turbulent kinetic energy (TKE) we start with a Reynolds decomposition, expressing deviations from the thermal wind component of the velocity, $\mathbf{u}_g = M^2/f\hat{k}$, by splitting $\mathbf{u}$ into a mean part (represented as a horizontal domain average, denoted by an overbar) and fluctuations from the mean. Thus, $\mathbf{u}$ is written as:

$$\mathbf{u} = \mathbf{u}_g(z)\hat{i} + \bar{u}\hat{i} + \mathbf{u}' \quad (4.1)$$

We can then obtain an equation for the turbulent kinetic energy (TKE):

$$\text{TKE} \equiv \frac{1}{2} \left(\overline{u'^2 + v'^2 + w'^2} \right) \quad (4.2)$$

with its evolution given by:

$$\frac{\partial}{\partial t} \text{TKE} = \underbrace{-\overline{\mathbf{u}'_h w'} \cdot \frac{\partial \mathbf{u}_g}{\partial z}}_{\text{GSP}} - \underbrace{\overline{\mathbf{u}'_h w'} \cdot \frac{\partial \mathbf{u}}{\partial z}}_{\text{AGSP}} + \underbrace{\overline{w' b'}}_{\text{BP}} + \epsilon \quad (4.3)$$

The first two terms on the r.h.s together represent the total shear production (P), converting energy from the mean flow into TKE. Specifically, the along-front contribution (P_i) is split into a geostrophic shear production term (GSP), energised by the thermal wind shear, and an ageostrophic part (AGSP). The other potential source of TKE comes from buoyancy production (BP), represents the transfer of energy from potential energy into TKE. Finally, ϵ represents dissipation of TKE.

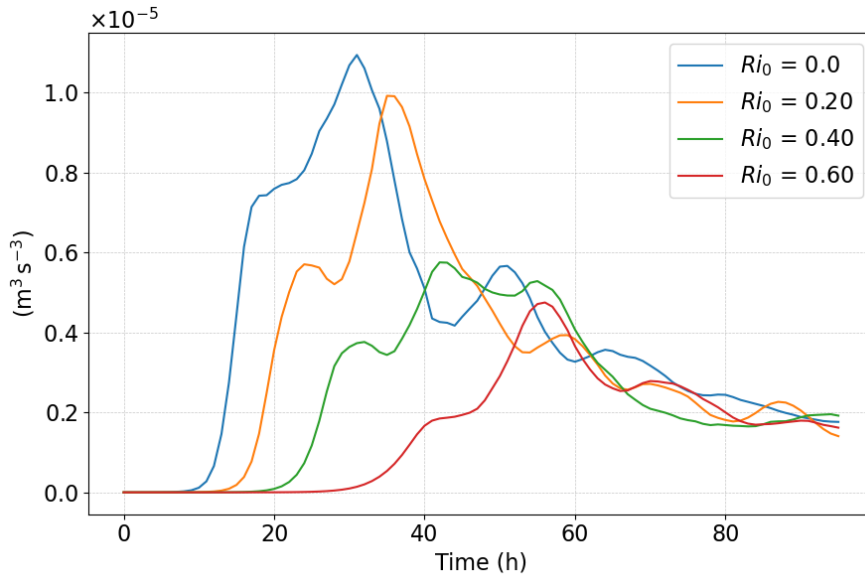


FIGURE 4.6: Time series of vertically integrated TKE over time for runs from Ri_0 : RI00 to RI06 as indicated in the legend ($m^3 s^{-3}$).

In figure 4.6, we see the dependence of TKE on Ri_0 . At lower values of Ri_0 , SI modes have more time to develop, and that we see that they are able to remove far more energy from the thermal wind shear before KHI develop. We also see that in all simulations there is a small dip in TKE, before a second boost of energy is injected.

Fig.4.7 provides the evolution of the relevant terms in the TKE budget for ‘RI04_high’. It is seen that the transfer of GSP from the balanced flow occurs predominantly in the middle of the domain from about $-40m$ to $-10m$ (Fig. 4.7a). After $t=32h$, the GSP shows a slump in its growth to $t=42h$, this is associated with a transfer from the smaller SI modes towards turbulence, seen graphically in snapshots of cross-frontal velocities during the evolution of SI induced restratification (Fig. 5.4b,d). At $t=42h$ the small scale turbulence ceases and GSP grows once more. This second round of growth is due to the evolution of SI around the second vertical mode with $\lambda = 50m$ (Fig. 5.4e). We find that the time integrated GSP was the dominant energy source for all simulations and that the two latter terms (AGSP & BP) play a less significant role in the TKE budget.

It is known that GSP serves as a mechanism through which SI extracts KE from the background geostrophically balanced mean flow (Thomas et al., 2013). The amount of GSP extracted by SI varies greatly with the initial stability of the stratified shear flow, this can be quantified by using Ri_0 . It is seen that GSP decreases with increasing Ri_0 (Fig. 4.8). This is due to the proportion of the thermal wind mixed down by SI, a factor dependent on frontal strength (Wienkers et al., 2021).

We see that at very low values of Ri_0 , the weak stratification associated with strong

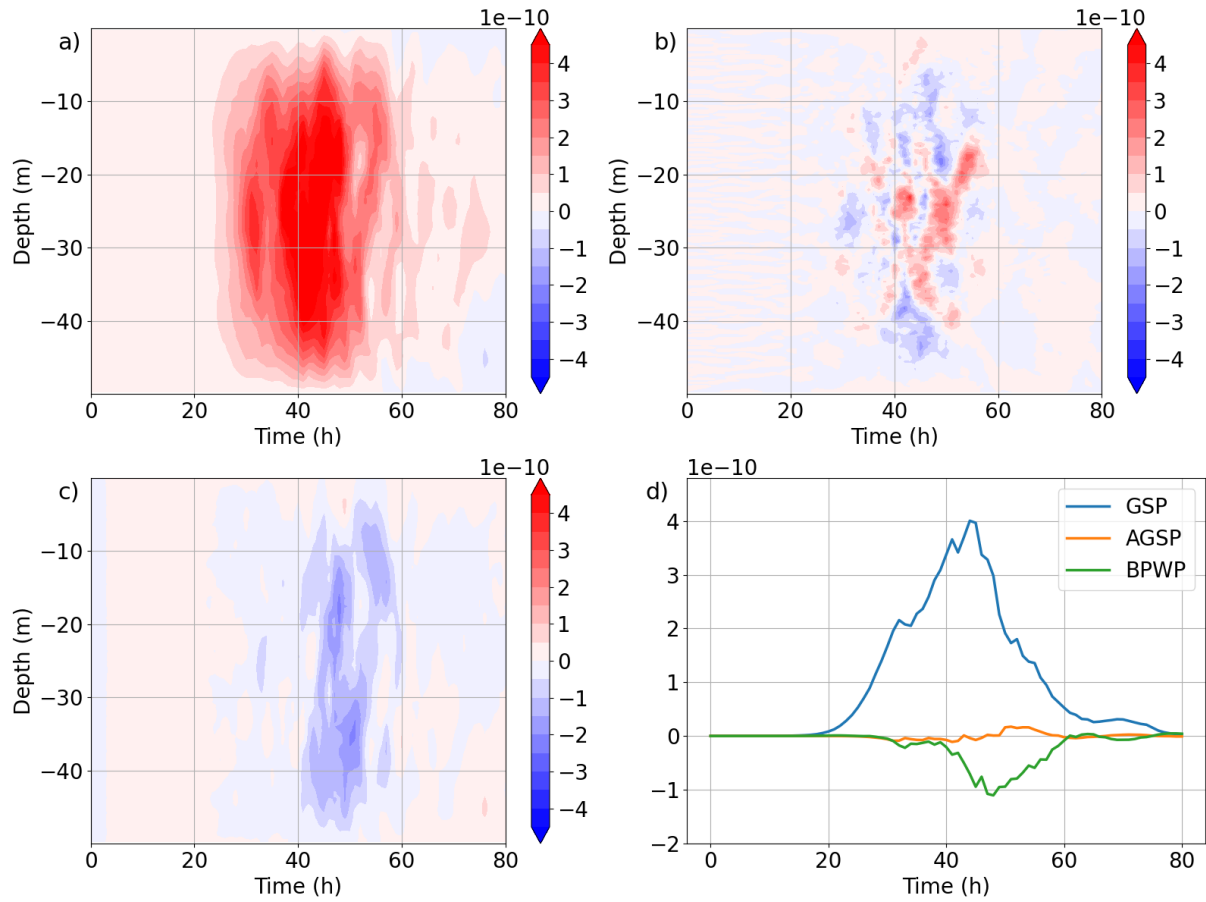


FIGURE 4.7: Horizontally averaged (a) geostrophic shear production (GSP), (b) ageostrophic shear production (AGSP) and (c) buoyancy production (BP) for experiment 'RI04_high' ($m^2 s^{-3}$). In (d) the associated horizontally averaged and vertically integrated time evolution ($m^3 s^{-3}$).

fronts leaves the system more prone to SI. The GSP peaks sharply and attains its maximum value, suggesting that SI occurs more vigorously, leading to a higher rates of KE extraction from the geostrophic flow. It is evident that after sometime a second round of SI develops, with slightly less rates of GSP. As Ri_0 increases, the peaks in GSP become lower and broader. This indicates a reduction in the intensity and efficiency of SI, resulting in a less pronounced extraction of KE. In weaker fronts, the increased stratification provides a stabilizing effect, dampening the SI and thus reducing the GSP. At high Ri_0 , the GSP is minimal and the curves are relatively flat suggesting that the stratification is strong enough to largely suppress the occurrence of SI. Furthermore we see the time dependency of SI growth on Ri_0 , that is for lower values of Ri_0 , SI development occurs earlier and reaching a neutral state quicker. This is all in agreement with the linear theory.

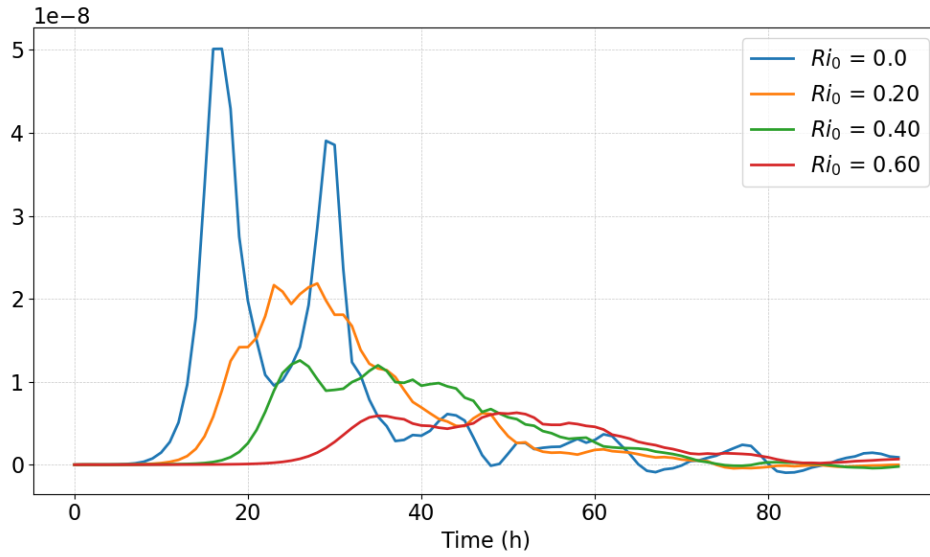


FIGURE 4.8: Time series of vertically integrated GSP $\left(\overline{u'w'} \cdot \frac{\partial \overline{u_g}}{\partial z}\right)$ varied by initial Richardson number (Ri_0) , $(m^3 s^{-3})$. The colors correspond to each simulation from RI00 to RI06 as indicated in the legend. SI ultimately extracts KE from the background through GSP, until the system is stabilised and rates of GSP tend to zero.

4.3 Eady Model - Two-Layer

The two-layer Eady Model builds on the previous single-layer framework by adding a highly stratified layer beneath the 50m deep mixed layer, extending the total depth to 120m (see Table 4.1). The stratified lower layer, with a thickness of 70m, serves to explore how a stable region influences the development of SI, and the associated PV flux. This setup is motivated by a desire to probe deeper into the dynamics of PV injection, which, according to literature, is critical for stabilizing SI-unstable flows. As discussed earlier, in the case of the ocean's ML, turbulent pv fluxes due to KHI are thought to be the main mechanism to neutralize SI. Specifically, overturning SI cells are believed to penetrate into the thermocline entraining higher-PV fluid (Taylor and Ferrari, 2009).

The two-layer model employed here aims to reveal more about how the ML interacts with the thermocline during SI development, particularly regarding PV injection into the ML. In this context, our goal is to uncover whether PV flux indeed originates from the thermocline, as the prevailing theory suggests, or if other, more complex dynamics are at play and whether the existing literature adequately captures the nuanced energy exchanges that govern restratification.

4.3.1 SI and RI

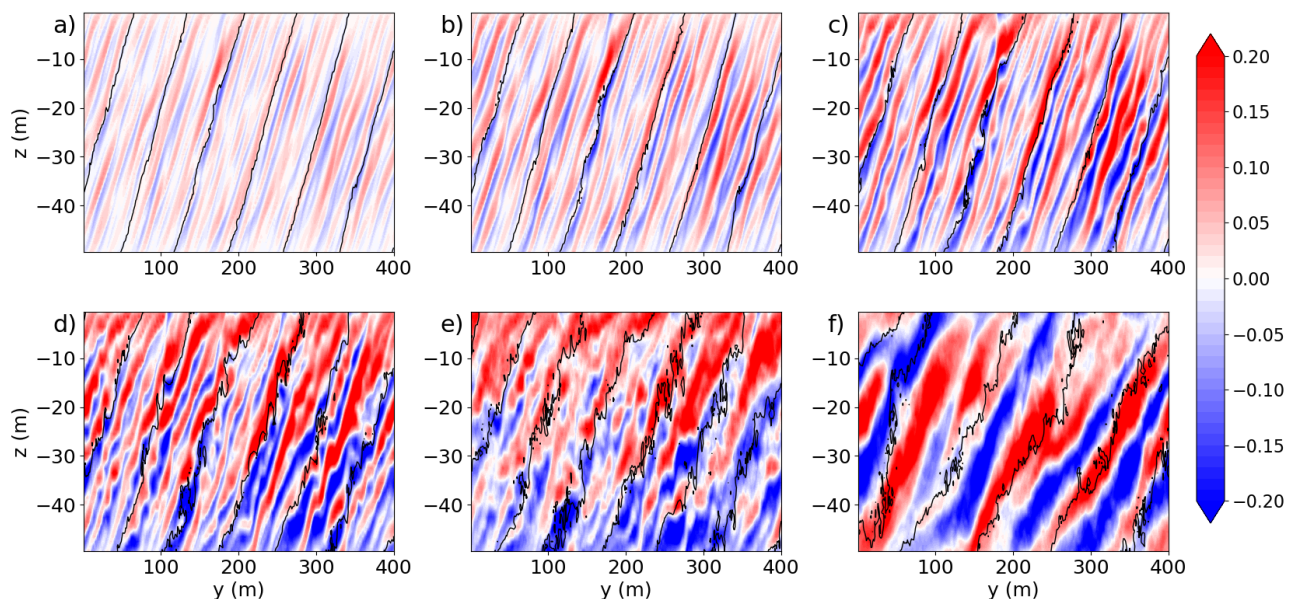


FIGURE 4.9: Cross-frontal velocities (cm s^{-1}) during different stages of SI induced restratification from ‘RI04_int’. Shown are snapshots from meridional sections after a model integration of a) 22h, b) 24h, c) 26h, d) 28h, e) 30h, and f) 40h. Contours indicate zonally averaged isopycnals.

We start the analysis by once more looking at snapshots of the evolution of cross frontal velocities from the run ‘RI04_int’ (Fig. 4.9). The evolution of the flow field again demonstrates the transition from an early well-organised SI modes which grow in their structure, to more complex turbulent dynamics over time. Comparing the progression of SI-induced restratification with its equivalent run ‘RI04’ (Fig. 4.2), which has no attached interior, we see that the progressions of the two setups are very much aligned with one another, such that the analysis provided in 4.2.1, applies here as well. To note is that once more we find a new SI mode developing (Fig. 4.9f), with a different wavelength compared to the initial SI wavelength. We can assess the development of the cross-frontal velocities (v) over time by taking horizontal averages (Fig. 4.10A(a) & B(a)). Upon closer examination, while the overall structure between the two setups appears largely similar, there are some subtle but potentially significant differences in terms of the energy exchanges and flow dynamics. The hovmöller plots, calculated for ‘RI04’ and ‘RI04_int’ show alternating bands of positive (blue) and negative (red) velocities highlighting the initial wavelength of SI, which remains constant in both runs for the initial around $t = 20$ hours. It is clear that after this SI attains a new wavelength, evident once more in both runs. This transition from an initial SI mode to a different wavelength is quite similar in both cases, suggesting that

the interior stratified region does not seem to influence the initial SI wavelength selection significantly.

The time series' for both Ri and N^2 do not show drastic differences between the two runs, indicating that the interior region does not significantly alter the overall stability profile at the surface. This might explain why the SI characteristics are so closely aligned. However, slight variations in the magnitude of N^2 at later times could suggest that the interior region affects the underlying stratification more subtly, potentially influencing the longer-term evolution of the flow.

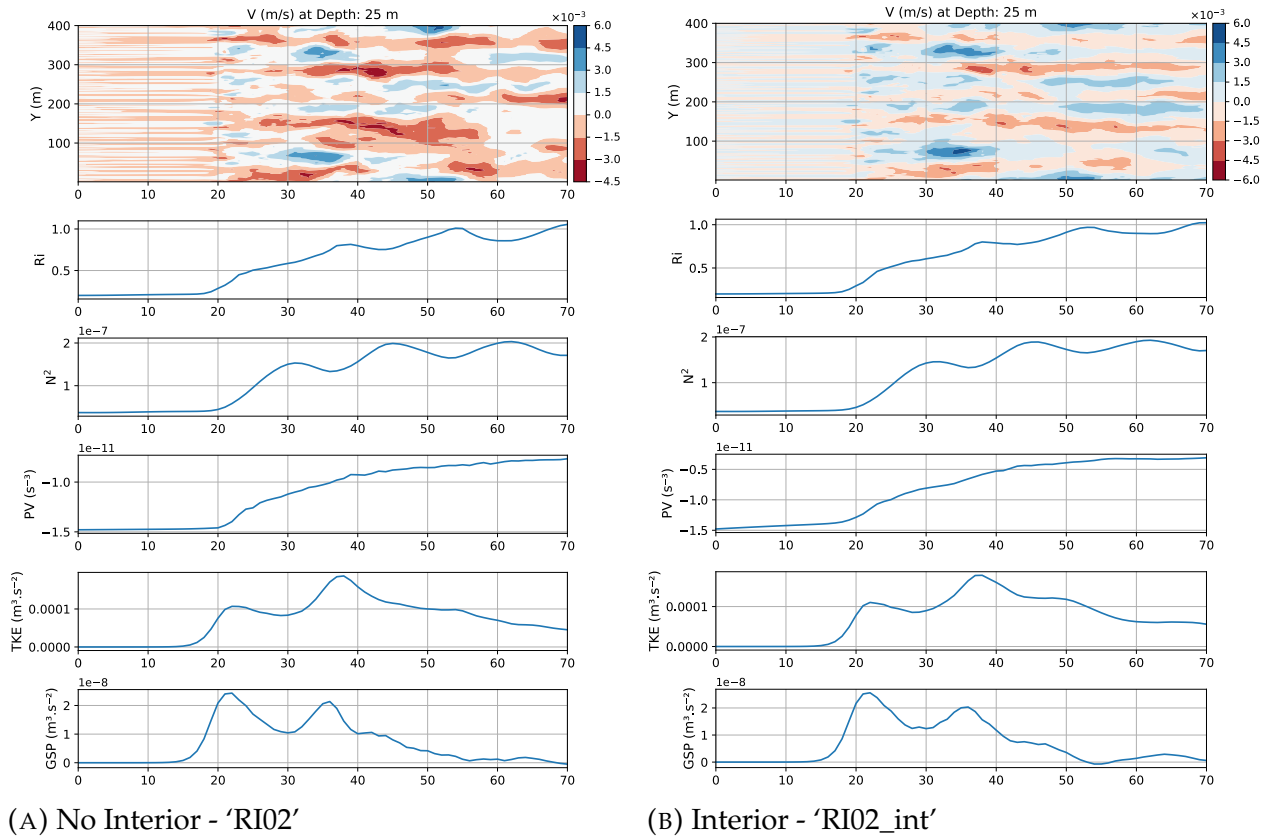


FIGURE 4.10: The evolution of cross-frontal velocities, Ri , $N^2(s^{-2})$, PV , TKE , and GSP in the presence and absence of a stratified interior for $Ri_0 = 0.2$. All time-series have been spatially averaged, and any smoothing applied has implemented a box-car on over 20 grid points.

In both cases, there is a clear increase in PV over time. In the interior case (B), we see PV attain a value larger in magnitude than the run without an interior (A), which shows a more gradual increase in PV . This aligns with the hypothesis that the interior might serve as a source of high- PV fluid in the stratified region, however the source of this PV is not immediately evident.

The near-identical profiles of TKE and GSP across both setups are particularly striking. TKE shows a similar trend, peaking around the same time in both runs, implying that the turbulent energy production mechanisms are unaffected by the presence of the interior. Likewise, GSP does not exhibit any notable deviation between the two cases, suggesting that the interior layer may not immediately translate into large-scale differences in energy production or dissipation.

The absence of a significant difference in GSP and TKE could imply that the energy dynamics are largely independent of the lower stratified region, and that the PV exchange might occur through a more subtle mechanism that doesn't strongly impact these particular metrics. Thus it is worth exploring how the evolution of PV across different stages of the simulations, for different Ri_0 values, occurs. Note, it is worth mentioning that the density profile of our ML to the interior is rather small when compared to typical values found in the real ocean.

4.3.2 PV and PV fluxes

As previously discussed, it is expected that the mean PV within the ML becomes positive overtime. However the dependence of SI on a materially conserved quantity such as PV, creates a paradox. That is rearranging fluid parcels within an unstable region does not restore stability to the flow. Thorpe and Rotunno, [1989](#) explored several potential explanations for this dilemma. Later, Taylor and Ferrari, [2009](#) proposed that secondary KHI arising from the primary SI bands help to resolve the instability. These secondary instabilities either mix in fluid of positive PV (i.e. entraining fluid from the well stratified thermocline below), or generate stabilizing viscous and diffusive PV fluxes at the ocean surface, leading to the shutdown of SI as the sign of PV within ML becomes positive (Thomas et al., [2013](#)).

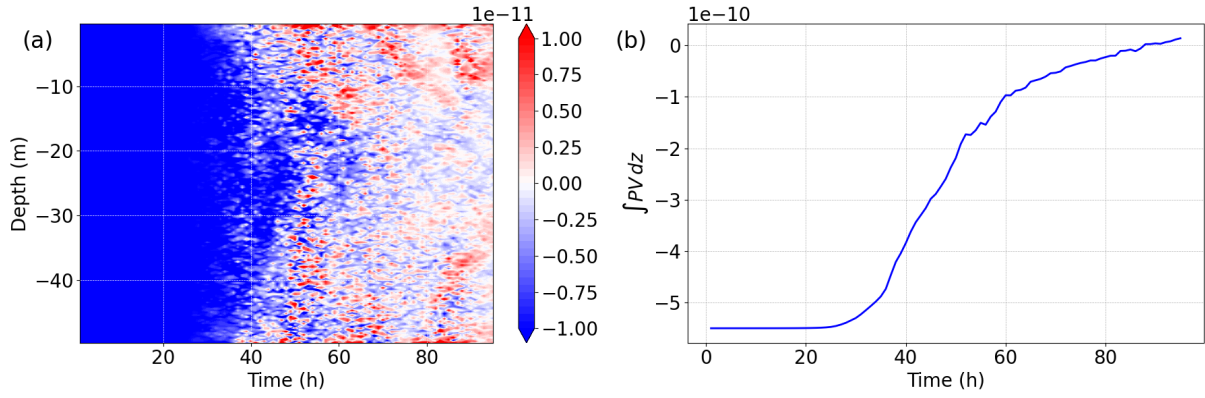


FIGURE 4.11: (a) Hovmöller plot of horizontally averaged potential vorticity (PV) over time for experiment 'RI04_int_high' (s^{-3}). (b) Time series of vertically integrated PV ($s^{-3}m$).

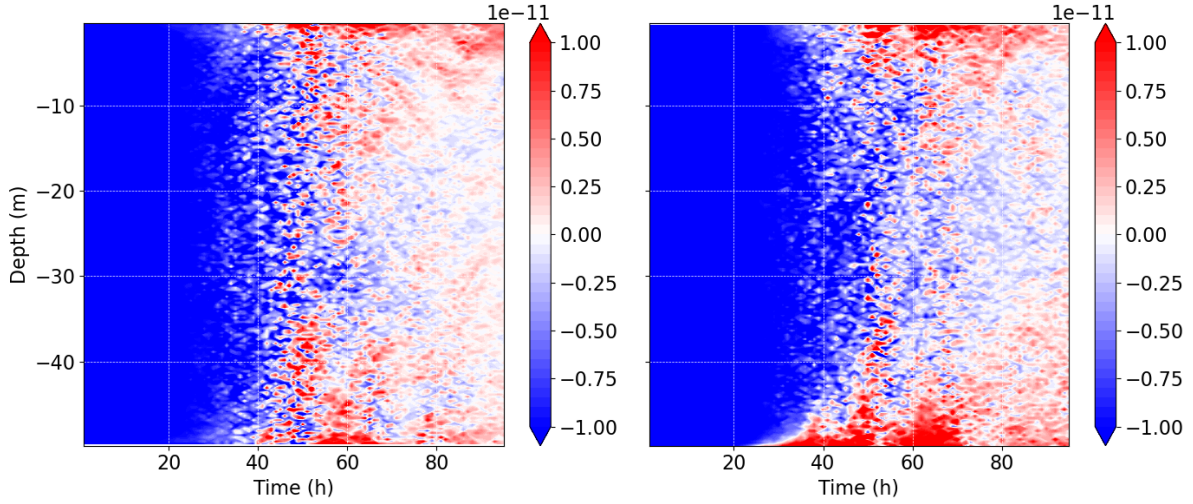


FIGURE 4.12: Hovmöller of horizontally averaged PV (s^{-3}) from the high resolution model runs RI04_high & RI04_int_high where $Ri_0 = 0.4$. The contrast between PV flux entrainment in the setup without an attached interior (left) and with (right) is highlighted.

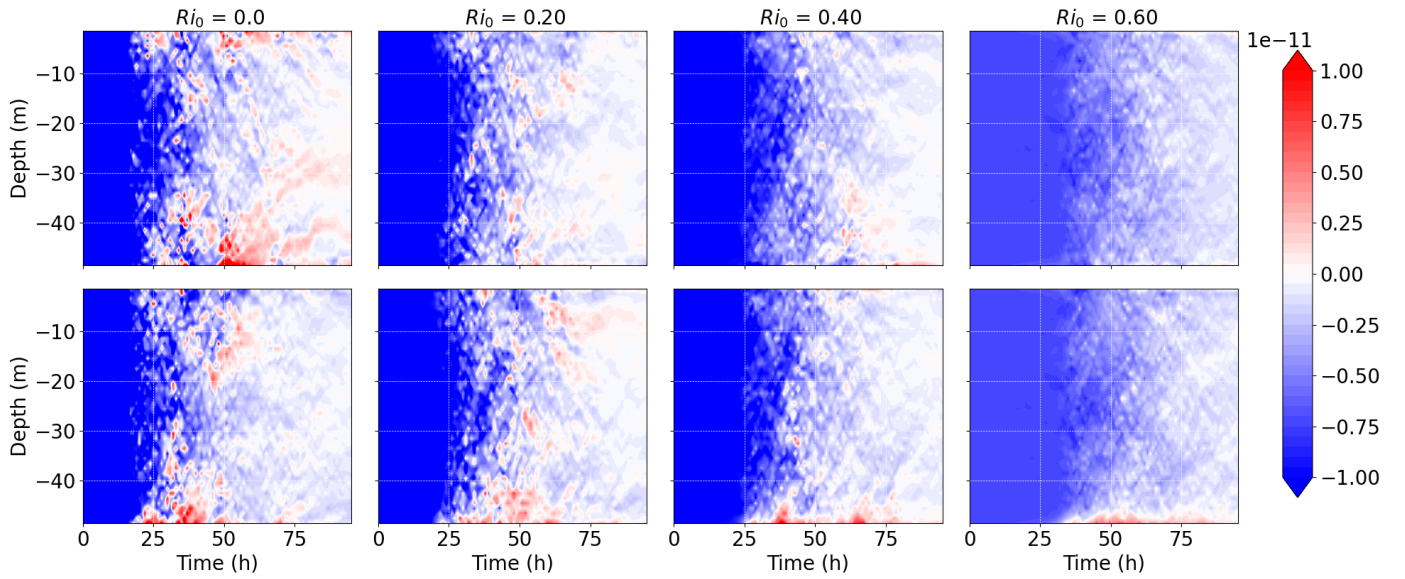


FIGURE 4.13: Hovmöller of horizontally averaged PV (s^{-3}) varied by Ri_0 , highlighting PV entrainment from below. The top row includes simulations without an attached interior (RI00-RI06) while the bottom row are those with an attached interior (RI00_int-RI06_int).

Figure 4.13 shows the evolution of the horizontally averaged PV for experiments ‘RI00’ to ‘RI06’ and ‘RI00_int’ to ‘RI06_int’. In agreement with the expectations from linear theory, experiments with smaller Ri_0 have faster growth rates and reach a neutral state earlier. PV values are somewhat higher towards the boundaries. However, for the mean mixed layer, PV fluxes from an attached interior do not play a dominant role in the restratification. It is seen that the depth of the PV entrainment is limited to the lower few meters. Furthermore in instances without an attached interior, the PV in the upper 40m of the domain is comparable to the runs without an attached interior. We find that restratification takes place regardless of whether there is an attached interior or not. Note that we have chosen a relatively small jump in the stratification, with a low value for the thermocline of $N^2 = 1 \times 10^{-6} s^{-2}$. Experiments with $N^2 = 1 \times 10^{-4} s^{-2}$ show even less impact.

The limited influence of the attached interior served as the primary motivation for running a high-resolution model as the resolution of 1m may prove insufficient for resolving the eddies responsible for entrainment. However, we find that the high resolution comparison leads to similar results (4.12). In the run without an attached interior, the increase in PV should be largely accounted for by the frictional and diffusive flux components, however owing to the difficulty in calculating these quantities at the boundaries, the analysis is computed between $-5m$ and $-45m$. Away from the boundaries, the advective fluxes should dominate.

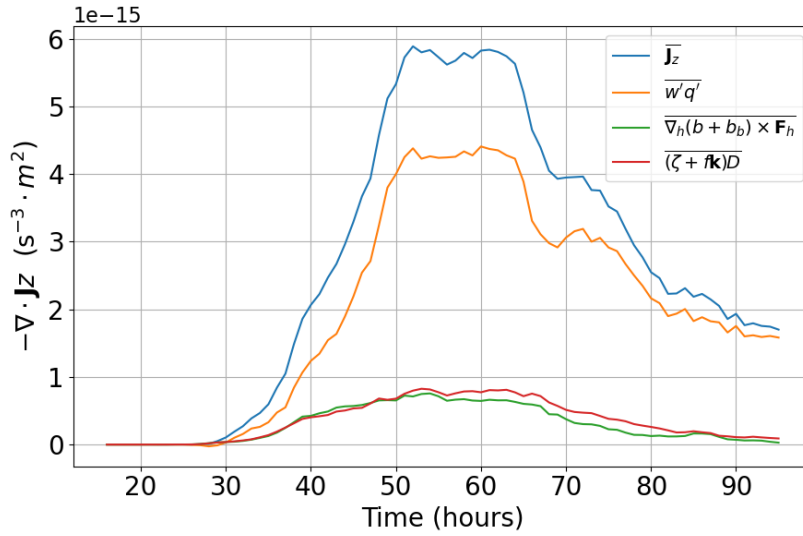


FIGURE 4.14: Time series of the net fluxes between -5 m and -45 m, smoothed over the inertial period using a moving average filter. The figure shows the total PV flux ($\overline{J_z}$), along with its components: advective flux ($\overline{w'q'}$), frictional flux ($\overline{(\nabla_h(b + b_b) \times \mathbf{F}_h) \cdot \mathbf{k}}$), and diabatic flux ($\overline{(\zeta + f\mathbf{k})D}$). All fluxes are shown in units of $\text{s}^{-3} \cdot \text{m}^2$.

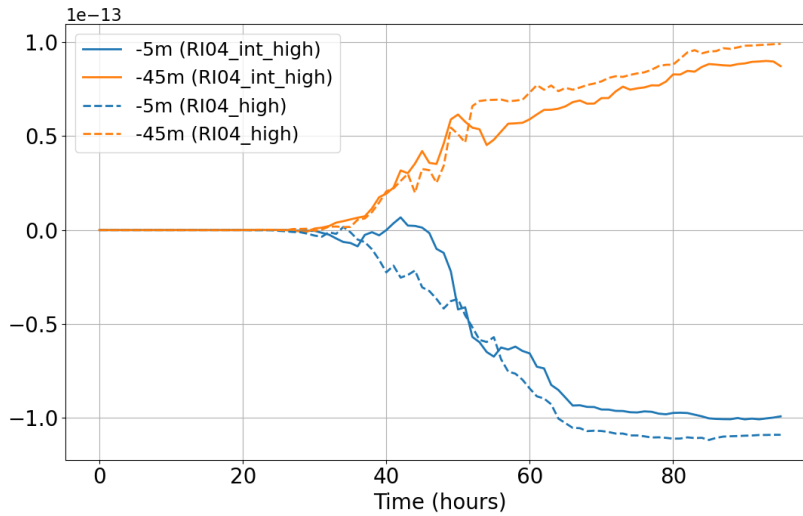


FIGURE 4.15: A comparison between the integrated advective PV flux $\int_t^{t_0} \overline{w'q'} dt$ between -5m and -45m , smoothed over the inertial period using a moving average filter, from experiments RI04_high and RI04_int_high (s^{-2}m^2).

In general, we find that the surge in PV is largely driven by advective processes (Fig. 4.14). It is seen that these advective fluxes are relatively symmetric with similar contributions from both boundaries (Fig. 4.15). While the RI04_int_high setup shows a slightly

more pronounced change in the PV flux, indicating stronger advective processes compared to the RI04_high case, the fundamental symmetry and the relative magnitudes remain consistent across both setups. The significance of the symmetric nature of the advective PV fluxes indicates a balanced vertical exchange of PV between the surface and deeper layers. Thus the advective flux contributes to the overall PV budget but without creating any net gains or losses vertically. However the advective PV fluxes cannot explain the PV increase in the domain, as using the applied boundary conditions, no advective fluxes directly at the boundaries are possible. Note: A detailed discussion on the remaining fluxes is provided in Chapter 5.

4.3.3 Energetics - GSP

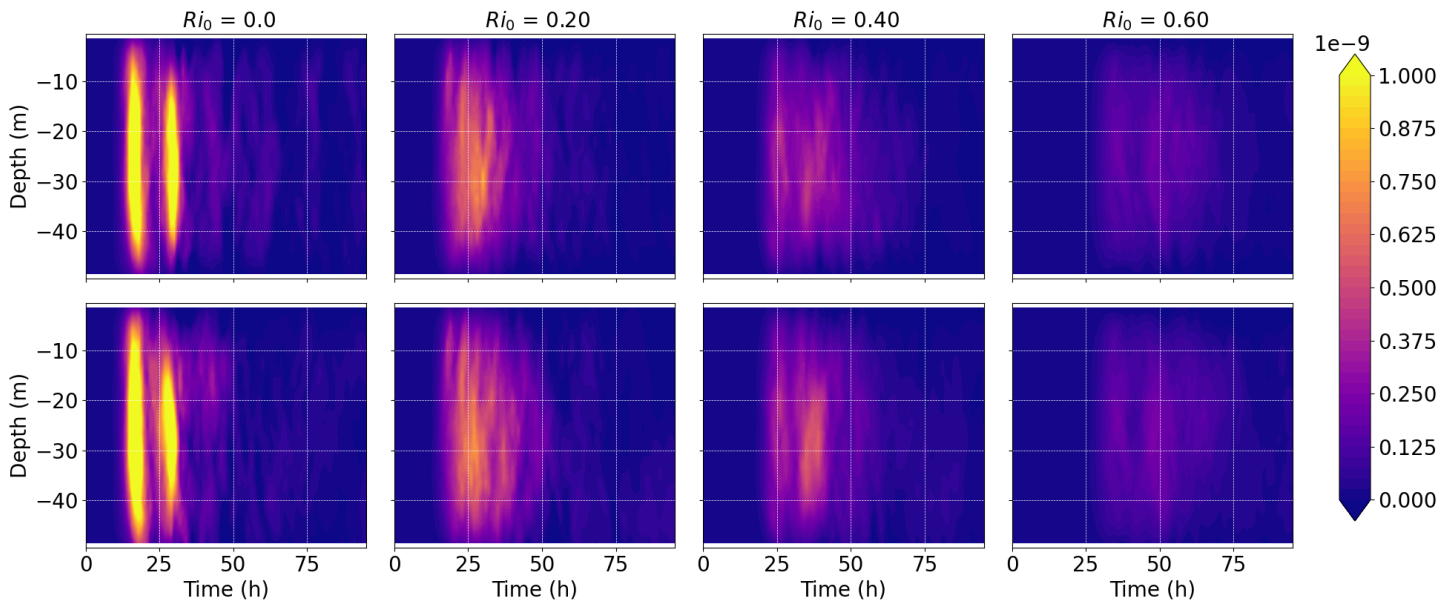


FIGURE 4.16: Hovmöller of horizontally averaged GSP varied by Ri_0 for experiments: RI00 to RI06 (top row) and RI00_int to RI06_int (bottom row) ($\text{m}^2.\text{s}^{-3}$)

Similar to the entrainment of PV, we find that the energetics and in particular GSP are indifferent to whether there is a source of high PV water underlying the ML or not, acting predominantly within the middle of the ML. This remains the case when moving to higher resolutions at the base of the ML, and is also unchanged at larger more realistic values of N^2 . That is, restratification occurs irrespective of the presence of an attached interior (Fig. 4.16).

We want to clarify, that the situation might change with a permanent PV flux out of the ocean due to destabilising atmospheric forcing. In such cases an SI layer develops below

the convective layer. Positive PV injection into the SI layer should then originate at the lower boundary (Taylor and Ferrari, 2010).

4.4 Discussion

In summary, this series of snapshots from the ‘RI04_high_op’ simulation illustrates the progressive development of SI from linear growth through nonlinear breakdown to fully developed turbulence. The cross-frontal velocities evolve from a well-organized, wave-like structure in the early stages to increasingly chaotic patterns as secondary instabilities (KHI) and turbulence emerge. By 40 hours, restratification has flattened the isopycnals, but new SI modes are beginning to form, demonstrating the cyclical nature of the instability in response to the underlying geostrophic shear.

While the runs with an attached interior show slightly more PV entrainment in the low- Ri cases (0.0 and 0.2), the differences diminish as Ri_0 increases and in general remain confined to the lower 10m. This supports the idea that the influence of the interior stratified layer might be more prominent in weakly stratified flows, but has limited impact when the flow is more strongly stratified. Thus, while entrainment exists, it has minimal influence on the overall restratification process. The results suggest that SI is capable of restratifying the mixed layer effectively, regardless of the interior, challenging previous assumptions about the critical role of thermocline entrainment.

In light of this, it becomes clearer that the presence of the interior layer might subtly enhance PV entrainment in specific cases but doesn’t lead to dramatic changes across all configurations. This is in line with the lack of significant differences seen in the energy metrics (GSP, TKE), since the entrainment of PV is so minimal, it barely influences the flow’s overall energy balances, with this notion holding across all Ri_0 values. This suggests that the energy exchange mechanisms driving SI are not directly influenced by the presence of an interior layer, confirmed by GSP acting predominantly in the middle of the ML domain.

The PV fluxes in both setups are largely symmetric, dominated by advective processes. The flux contributions from both boundaries are similar, and no significant vertical asymmetry is found. Higher-resolution runs show consistent results, reinforcing that PV fluxes remain largely unaffected by the presence of the interior. Thus a natural question to ask is where the increase in PV comes from which neutralises SI and how this then restratifies the frontal system. In Chapter 5 we look to address these questions before moving on to a more realistic setup.

Chapter 5

SI Induced Restratification

In this chapter, we use a set of three-dimensional (3-D) numerical simulations of the Eady model that span a range of low $Ri(0 - 0.6)$ to understand the physical processes that lead to the development, saturation and eventual restratification of SI-unstable fronts under various initial conditions. In particular we aim to further understand the impact of varying initial conditions on the development and characteristics of SI, the role of PV fluxes from the boundaries and ocean interior in the restratification of the ML and how secondary instabilities affect the stability and structure of the ML.

In Section (5.1), we outline the model setup employed and its construction. A host of model experiments are introduced, where we distinguish between the various initial conditions, background conditions, model resolution, and parameters used. Section (5.2) consists of three sub-sections, the first of which provides an analysis of optimal initial conditions for SI growth. The second subsection discusses the impact that turbulence has on SI growth. The third subsection contrasts how fluxes from the boundaries might change SI development, as well as the role SI plays in initiating restratification within a convectively formed ML. In the final Section (5.3), we present our conclusions and provide insight into how these results may be incorporated into future research.

5.1 Model setup and configurations

Using an Eady type setup, model consists of fluid with initially uniform potential vorticity between two rigid horizontal boundaries. The physical setup is represented in Fig. (4.1). In this area, the geostrophically balanced velocities are considered to be horizontally constant, i.e. $\zeta = 0$ in the balanced flow.

Unlike the previous runs where the velocity fields are initialised with a white noise perturbation of amplitude $10^{-4} m s^{-1}$, the high resolution experiment ‘RI04_high_op’, in this chapter starts with an optimal perturbation of two wavelength of the most unstable waves in the buoyancy anomaly, i.e. $b_{ini}(y) = B_0 \sin(4\pi y/L_y)$. We apply a very small amplitude of $B_0 = 10^{-8} s^{-1}$. Its worth noting that all previously cited studies use a white

noise perturbation and a resolution of 1m. In contrast our resolution is much higher at 0.25m.

Name	Ri_0	$N_{mix}^2 [s^{-2}]$	$\nu_{sgs} [m^2 s^{-1}]$	α	β	$\tau_\sigma [h]$	$\lambda [m]$
RI04_high	0.4	7.40 e-8	smag	30.2°	26.6°	16.5	100
RI04_int_high	0.4	7.40 e-8	smag	30.2°	26.6°	16.5	100
RI04_high_op	0.4	7.40 e-8	smag	30.2°	26.6°	16.5	100
RI04_int_high_v1	0.4	7.40 e-8	1.0 e-3	30.2°	26.6°	16.5	100
RI04_int_high_v2	0.4	7.40 e-8	1.0 e-4	30.2°	26.6°	16.5	100

TABLE 5.1: Summary of the configuration details of each numerical simulation. Ri_0 is the initial Richardson number, ν_{sgs} the turbulent viscosity for the sub-grid scale. ‘Smag’ indicates $\nu_{sgs}(x, y, z, t)$ is given by the Smagorinsky closure. N_{mix}^2 is the initial stratification in the mixed layer, α gives the angle of the isopycnal slope (s_b) with the horizontal, i.e. $\tan \alpha = M^2/N^2$. The latter three rows corresponds to linear theory using Eq. (2.1) for $h = 50m$, $\nu_t = 1 \times 10^{-4} m^2 s^{-1}$, and $m = 2\pi/H$. β gives the angle of the wave number vector with the horizontal, i.e. $\tan \beta = k/m$, τ_σ is the period, and λ the wave length of the fastest growing mode, respectively.

5.2 Results

5.2.1 Optimal growth

We first discuss the high resolution experiment ‘RI04_high_op’, which is initialised with buoyancy anomalies representing two wavelengths of the fastest growing mode. Fig. 5.1 gives the cross-frontal velocities during varying stages of SI induced restratification. The SI mode grows at the initialised wavelength. In the early stages, after 17h, the difference between s_b and the wave number, i.e. between the angles α and β , is visible (Fig. 5.1a). This is in agreement with linear theory (see Table 5.1). In Fig. 5.1(d) we see the first sign of evolving secondary KHI. At this stage the isopycnal slopes are already considerably reduced (An explanation is provided in subsection b.). In Fig. 5.1(e) the roll-up of the KHI-billows is in the final stage. Here m has changed from a first vertical mode in (a) - (c) to an approximate second mode in (d) and (e). By 28h, Fig. 5.1(f), these billows have already broken up into full three dimensional turbulence. The averaged PV and Ri now suggest that the system is stable with respect to SI (not shown).

Our discussed linear theory does not account for vertical boundaries, apart from the maximum possible vertical wave length. Wienkers et al., 2021 included vertical boundaries in their linear stability analysis which shows a decrease in growth rate at the lowest

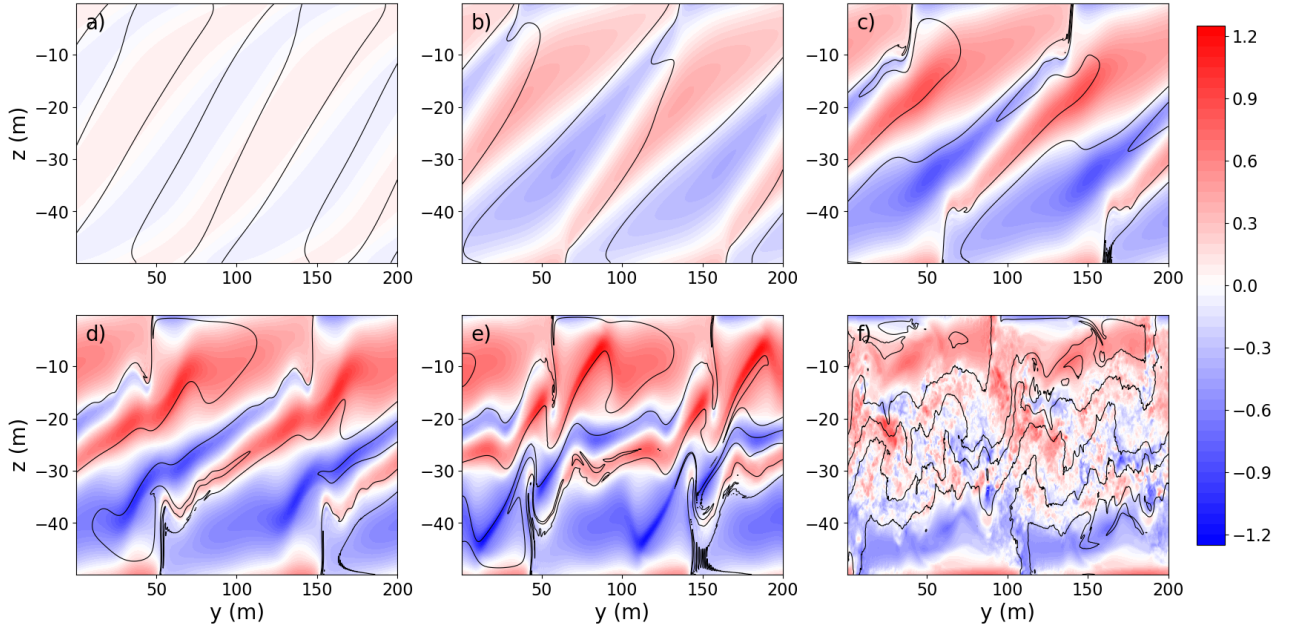


FIGURE 5.1: Cross-frontal velocities ($cm\ s^{-1}$) during different stages of SI induced restratification from ‘RI04_high_op’. Shown are snapshots from meridional sections after a model integration of a) 17h, b) 21h, c) 23h, d) 24h, e) 25h, and f) 28h. Contours indicate zonally averaged isopycnals.

possible wave number. However, linear theory does not account for non-linearities or pv fluxes at the boundaries.

The up- and downwards flux of meridional momentum leads to areas of convergence and divergence at the boundaries. Consequences for the isopycnal slopes are already evident in Fig. 5.1a. For example, negative velocities lead to strong isopycnal slopes, whereas positive velocities increase the stratification. This leads to frontogenesis with two strong ageostrophic fronts at each vertical boundary (Fig. 5.1b-e). Convective instabilities can be seen at each dense (cold) side of the surface fronts and on the buoyant (warm) side of the fronts at the bottom. The appearance of the first KHI-billows are also associated with the sharp gradients both within and below the fronts. It is worth noting that diapycnal fluxes resulting from a finite region that is unstable to SI have also been observed in Grisouard, 2018. Frontogenesis as a driver for restratification is discussed in Thomas and Ferrari, 2008.

In order to reach a state where the front is stable to SI, a flux of positive PV is necessary. However due to the “impermeability theorem” of Haynes and McIntyre, 1987, which states that PV fluxes are not possible across isopycnal surfaces, this positive PV flux has to come from the boundaries. A reminder that the evolution of the vertical PV flux (3.6) is given by $\overline{J_z} = \overline{w'q'} + \overline{(\nabla_h(b + b_b) \times \mathbf{F}_h) \cdot \mathbf{k}} - \overline{(\zeta + f\mathbf{k})\mathcal{D}}$. Since J_{adv} is zero at our rigid surfaces, the two remaining fluxes J_{dia} and J_{fric} have to be responsible for the necessary

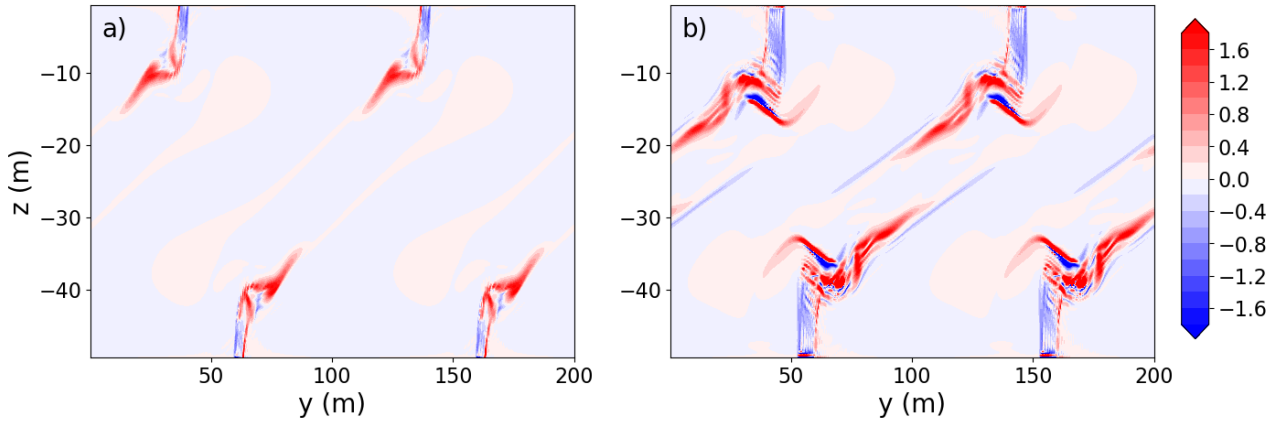


FIGURE 5.2: Zonally averaged Ertel potential vorticity anomalies ($\times 10^{-11} s^{-3}$) after a model integration of a) 21h and b) 23h. Note, that the initial negative $PV(t = t_0)$ is removed prior to plotting. The evolution corresponds to Fig. 5.1c and Fig. 5.1d.

positive PV injection. Owing to the cyclic boundary conditions, all mean horizontal gradients vanish, meaning that only ‘primed’ correlations from deviations of the horizontal mean are possible. However, quantifying the J_{fric} and J_{dia} directly on the boundaries of a staggered numerical grid is challenging, if not outright impossible.

Figure 5.2 shows the zonally averaged PV anomalies for two different stages corresponding to the cross-frontal velocity figures Fig. 5.1c and Fig. 5.1d. We can identify negative PV anomalies in the convective region associate with the fronts. We also see the injection of the necessary positive PV associated with the fronts. The sharp gradients directly at the boundaries seem to support the demanded ‘primed’ correlations in the gradient terms of the frictional and diabatic PV fluxes. In fact, the frictional and diabatic PV fluxes are responsible for the positive PV intrusion along the sharp fronts. These fluxes show enhanced values reaching 10m into the interior along these fronts (not shown).

The evolution of vertically integrated budgets of GSP and BP for ‘*RI04_high_op*’ are given in Fig. 5.3a, with the GSP from ‘*RI04_high*’ included for comparison.

GSP grows exponentially, roughly in accordance with the growth period of $\tau_\sigma = 16.5h$ as given in Table 5.1. The growth is far quicker than that of the ‘*RI04_high*’ experiment, which sees far more linear growth in its initial stages. We find that GSP dominates over BP in all our experiments. Initially BP is a source for TKE, which is associated with the convective frontogenesis regions. At later stages both stratification and TKE increase throughout the domain, so that BP becomes a sink for TKE. Due to KHI, both BP and GSP show strong fluctuations after transitioning to turbulence at $t=24h$. As the vertical gradient in the geostrophic velocity ($\partial_z \bar{u}_b$) is constant, the evolution of GSP is given by the zonal Reynolds stresses. The Reynolds stresses are shown for $t=21h$ in Fig. 5.3b. At this stage,

near pure growth of the SI mode (Fig. 5.1b) and ideal correlation between u' and w' is obtained. Such optimal growth is only possible with an initialisation that matches the fastest growing mode.

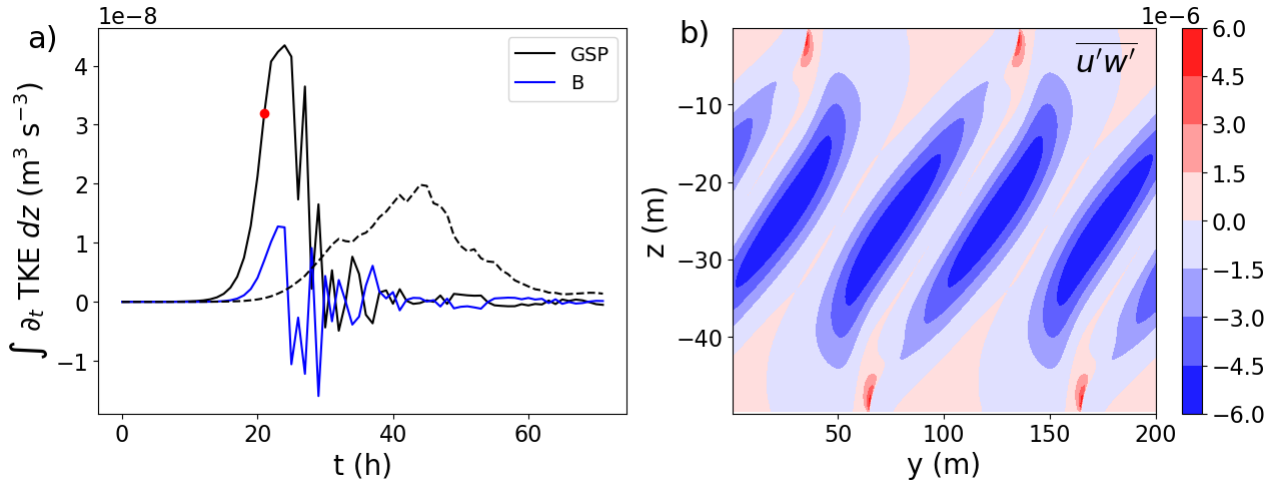


FIGURE 5.3: a) Horizontally averaged and vertically integrated geostrophic shear production (GSP) and buoyancy production (BP) for experiment ‘RI04_high_op’. The dashed line gives GSP for experiment ‘RI04_high’. The red dot marks the time at which b) shows a section of the zonal Reynolds stresses $\overline{u'w'}$ ($\text{m}^2 \text{s}^{-2}$).

5.2.2 Turbulent growth

In this section, we discuss the impact of initial turbulence on the evolution of SI. The velocity is initialised with white noise with an amplitude of $1 \times 10^{-4} \text{ms}^{-1}$, representing a low initial levels of turbulence. This initialization sets the stage for understanding how SI evolves under weak initial turbulence conditions and how secondary KHI develops as part of the SI lifecycle.

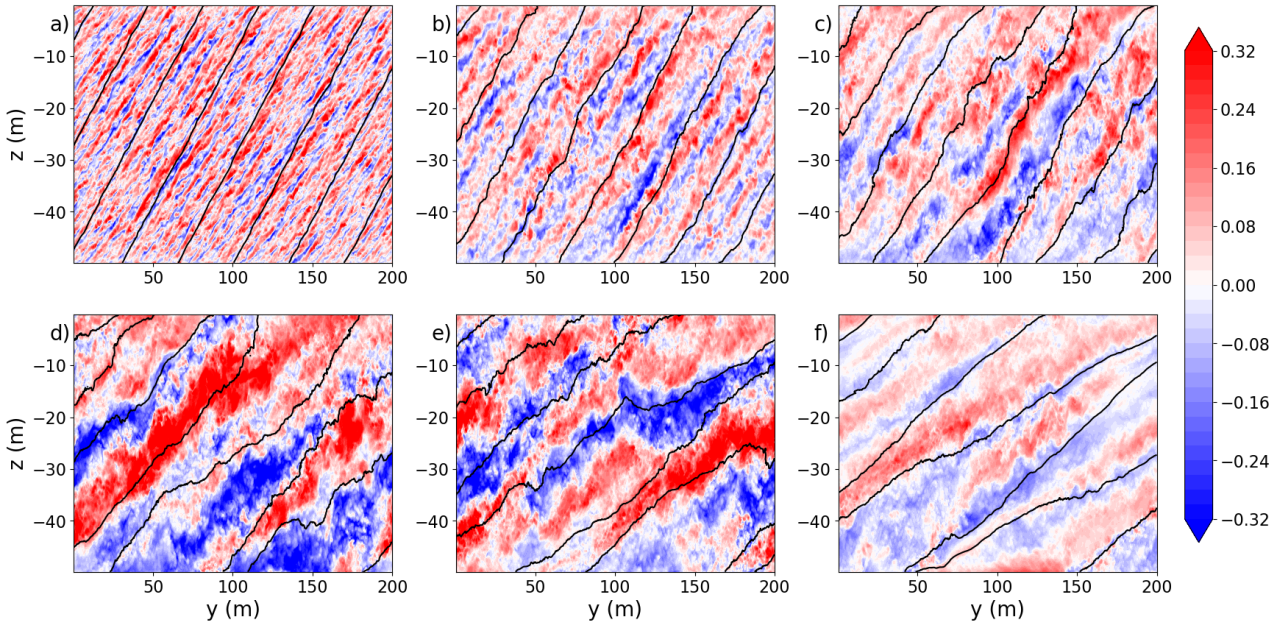


FIGURE 5.4: Cross-frontal velocities (cm s^{-1}) during different stages of SI induced restratification for experiment ‘RI04_high’. Shown are snapshots from meridional sections after a model integration of a) 18h, b) 25h, c) 30h, d) 40h, e) 52h, and f) 76h. Contours indicate zonally averaged isopycnals. Due to the small amplitudes in the early stages, the velocities are multiplied by a factor of 10 in a) and by a factor of 2 in b).

The cross-frontal velocities during varying stages of SI for the high resolution experiment ‘RI04_high’ are shown in Fig. (5.4). The observed evolution differs somewhat from the predictions of linear theory. According to Eq. 2.1 turbulence (resolved or parameterised by the eddy viscosity) damps smaller SI modes, such that the largest possible wave, given here with $m = 2\pi/H$, determines the fastest growing mode. However much smaller wavelengths with higher vertical modes are observed. The associated diapycnal mixing shifts the growing SI to smaller vertical modes Fig. 5.4(b) - (e).

SI itself is not responsible for the dissipation as its length scale is much larger than that of the dissipation scale. So while SI may act to indirectly drive energy downscale, it is generally understood that energy dissipation is a result of the associated secondary instabilities (Kimura, 2024).

If we consider the linear theory provided in Chapter 2, we can predict the maximum growth rate in the inviscid case from the wave number angle k/m . However, turbulence set through ν_t , damps the smaller modes, such that the inviscid case is associated with the largest possible modes, as their growth rates are the largest (Fig. 2.1). From linear theory, we expect the theoretical horizontal wavelength k of the fastest growing mode to be $\lambda = 100m$. However, the results indicate the presence of much smaller wavelengths with higher modes, contrary to linear expectations. Our linear stability analysis shows

that only a high viscosity matters, setting the growth of the largest possible wavelength. However, in the case of Figure 5.5(d), where we set a very high viscosity, the wavelength that develops is still smaller than the largest possible wavelength. It is only with a very high resolution (Fig. 5.5(c)) do we find that the wavelength tends towards that found from linear theory in Chapter 2. Figures 5.4(a), 5.5(a) and show k with $\lambda < 10m$ further emphasising the need for higher resolution. This much smaller m has consequences for the associated secondary KHI, since KHI develop much earlier at higher values of m . That is, we see that smaller waves grow in a similar fashion to the larger waves. However, the smaller waves have a much larger vertical mode, meaning they become unstable with respect to KHI far quicker. While these first rounds of SI create their own turbulence, the small modes are not efficient enough to generate significant GSP and TKE, leaving the system still unstable to SI Fig. 5.5 (a) . The efficiency of the larger modes are made evident in the comparison to the optimal growth case (5.5 (b)). We see that the in 'RI04_high' run, 1-2 rounds of SI occur before the wavelength is similar to that of the 'optimal growth'.

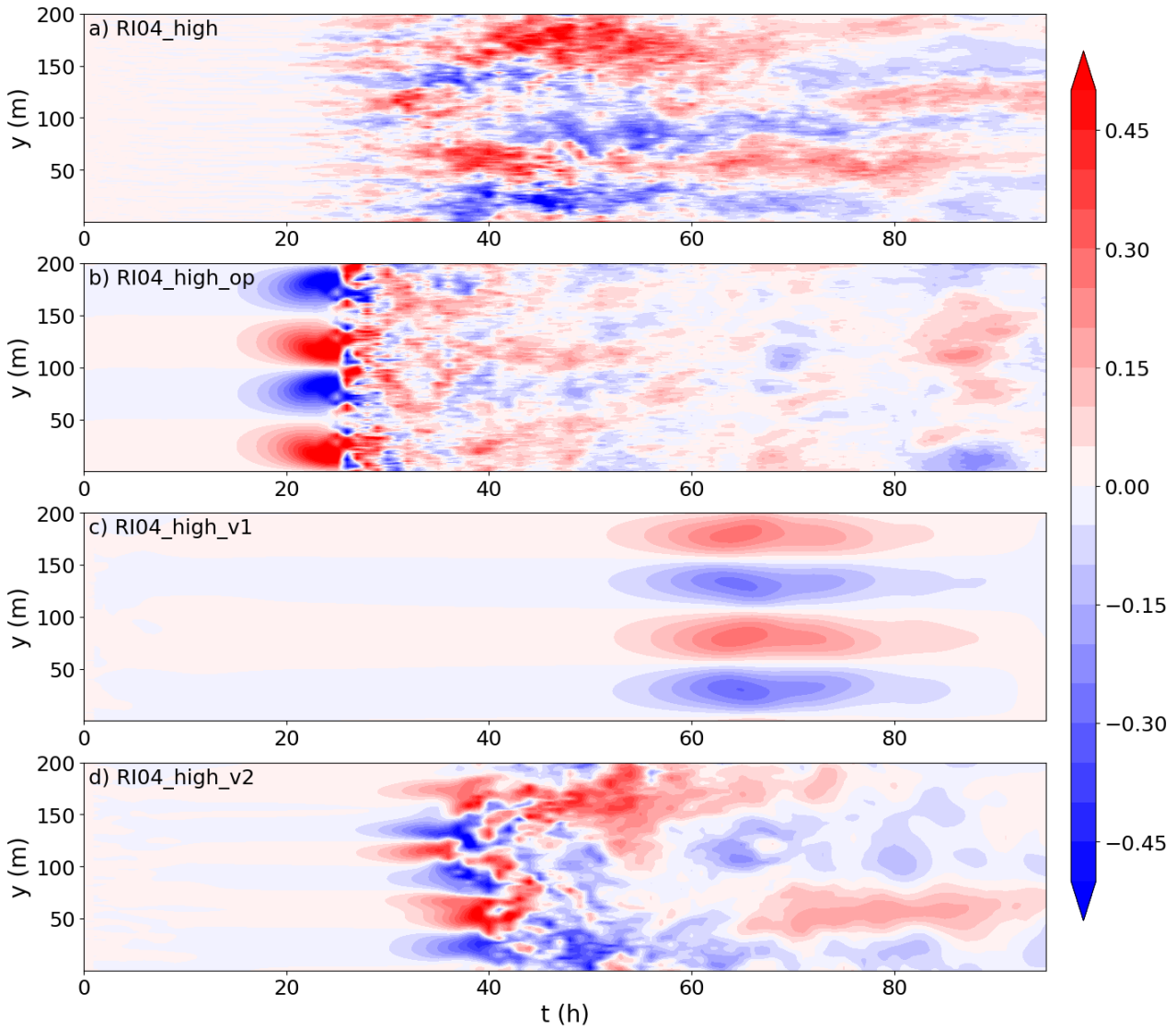


FIGURE 5.5: Time evolution of cross-frontal velocities (cms^{-1}). Shown are snapshots from a meridional section at $x = 30m$ for four different experiments.

As a prequel to Chapter 6, which deals with forcing, the runs ‘RI04_high_v1’, and ‘RI04_high_v2’ use a fixed viscosity of $1.e^{-3}m^2s^{-1}$ and $1.e^{-4}m^2s^{-1}$ respectfully. The fixed viscosity allows for the comparison to forced SI, where SI can be sustained due to surface buoyancy loss or down front winds (discussed in detail in Section 6.1). We see that while ‘RI04_high_v2’ becomes unstable its wavelength is smaller than the maximum possible wavelength as predicted by linear theory. Finally for ‘RI04_high_v1’, a fixed viscosity of $1.e^{-3}m^2s^{-1}$, we obtain the theoretically predicted wavelength, but the viscosity is so strong that KHI do not develop.

5.2.3 Restratification mechanism

If we now consider mean quantities, an overbar denotes the horizontal average, so that we can split velocities into a mean part and a perturbation, e.g. $v = \bar{v} + v'$. Note, that we consider cyclic boundary conditions in the horizontal, so that $\bar{w} = 0$ and $\partial_{x,y}(\bar{u}, \bar{v}, \bar{b}) = 0$. Equation (3.1) then becomes

$$\frac{\partial \bar{u}}{\partial t} - f\bar{v} = -\frac{\partial \overline{u'w'}}{\partial z} + \frac{\partial \overline{\nu_t \partial_z U}}{\partial z} \quad (5.1)$$

$$\frac{\partial \bar{v}}{\partial t} - f\bar{u} = -\frac{\partial \overline{v'w'}}{\partial z} + \frac{\partial \overline{\nu_t \partial_z v}}{\partial z} \quad (5.2)$$

And equation (3.2) becomes

$$\frac{\partial \bar{b}}{\partial t} + \bar{v}M^2 = -\frac{\partial \overline{b'w'}}{\partial z} + \frac{\partial \overline{\kappa \partial_z (b + b_b)}}{\partial z} \quad (5.3)$$

From here we can take the vertical derivative of equation (5.3)

$$\frac{\partial \overline{N^2}}{\partial t} + \partial_z(\bar{v}M^2) = -\frac{\partial^2 \overline{b'w'}}{\partial z^2} + \frac{\partial^2 \overline{\kappa \partial_z (b + b_b)}}{\partial z^2} \quad (5.4)$$

which gives a description of how N^2 evolves over time.

Turbulent fluxes, particularly $-\partial \overline{v'w'}/\partial z$ which sets $\bar{v}$, are most pronounced in the middle of the ML (Fig. 5.3). The divergence in the Reynolds stresses changes sign here, leading to a negative cross-front velocity at the surface and a positive cross-front velocity at the bottom of the domain (Fig. 5.6a) from $t=20h$ to $t=55h$. It is this secondary circulation, which restratifies the water column gradient. Such a cross-frontal secondary circulation is sometimes referred to as turbulent thermal wind (Gula et al., 2014).

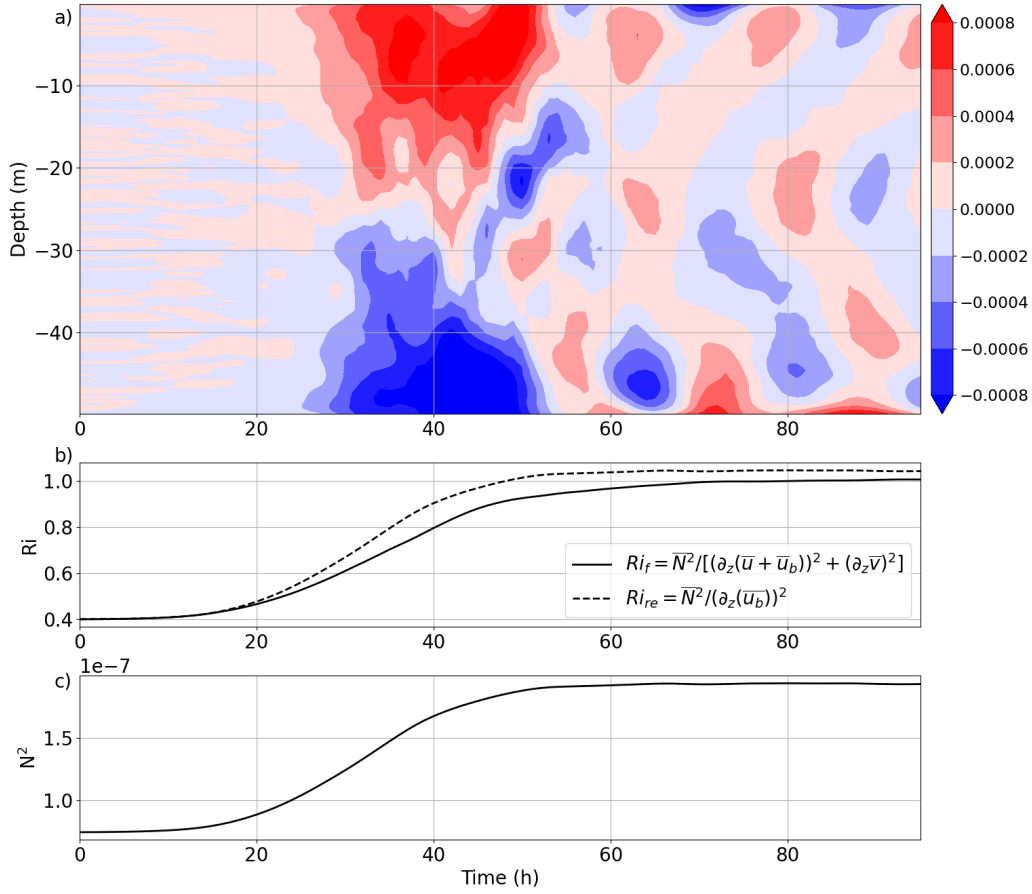


FIGURE 5.6: (a) Hovmöller of cross-frontal velocity ($\bar{v}$) over time ($m s^{-1}$). (b) Time evolution of Ri_f (full) defined as: $\bar{N}^2/[(\partial_z(\bar{u} + \bar{u}_b))^2 + (\partial_z\bar{v})^2]$ and the reduced Richardson number (Ri_{re}) defined as: $\bar{N}^2/(\partial_z(\bar{u}_b))^2$ (c) Evolution of N^2 over time. All plots are calculated from experiment RI04_high, where $Ri = 0.4$.

We find that both Ri_f , calculated using the full velocity shear, and Ri_{re} , calculated using the only the background velocity shear, increase and tend towards 1 over time (Fig. 5.6b). This indicates an evolution towards more stable conditions. It is also evident that both graphs have comparable trends. This suggests that the increase in Ri_b is mainly driven by N^2 whose evolution can be described by Eq. (5.4) and trend is comparable to those of Ri_b and Ri_{re} (Fig. 5.6c). The overall restratification is rather linear compared to the ‘RI04_high_op’(Fig. 5.3). The dominant term in the restratification process is $\partial_z(\bar{v}M^2)$ and is associated with the secondary mean circulation.

5.3 Discussion

To investigate the role SI plays in the restratification of the ocean column once destabilizing surface forcing ceases, we conducted a series of experiments using an idealized 3-D mixed layer ocean front modelled within the ‘Eady’ framework. The front was initially in thermal wind balance, with uniform buoyancy gradients. By setting $Ri_0 < 1$, we observed the growth and the eventual saturation of SI, whose growth rates aligned well with the linear predictions. The constant background horizontal buoyancy gradients resulted in an increase in Ri_b over time. Importantly, we found that small-scale KHIs can disrupt SI growth, potentially stabilizing the system depending on the resulting Ri_b values. In such cases where $Ri_b < 1$, SI redeveloped over longer timescales. All experiments showed a relatively fast restratification to a state stable against SI. This restratification results from a complex interplay of dynamics, with particular emphasis on the divergence of cross-frontal Reynolds stresses.

Comparisons between experiments with and without an attached stratified interior below the surface mixed layer show that PV fluxes from the base of the mixed layer and upper boundary are roughly equal, and that the PV fluxes from the interior are of minor importance. Additionally, we show that the alternating vertical momentum fluxes associated with SI lead to frontogenesis and the formation of sharp fronts at the mixed layer boundaries. These non-geostrophic fronts are hot-spots for vertical PV fluxes and mark the initial appearance of secondary KHI.

We found that when initialised with turbulence, specifically a white noise perturbation, SI-induced restratification initially differed in its early stages of development from the more theoretical initialisation of the optimal growth experiment. In the turbulent growth experiments, SI developed at much smaller wavelengths with higher vertical modes, which was consequential for the associated secondary KHI that developed much earlier and at higher m . In the ‘optimal growth’ run, we find undisturbed growth of SI modes initially, which leads to a high GSP. While the energy is transferred from the background flow into the SI modes, the energy is not used for mixing until KHI develops. At that point, the energy from the SI modes is transferred to 3-D turbulence and can be utilized for mixing. In the white noise case, KHI removed energy from the SI modes, providing a more continuous transfer from balanced motion to SI modes, to KHI modes, to diapycnal mixing. It should be noted that most of the cited literature employs a white noise approach.

In assessing the role of PV fluxes in SI stability, it is clear that PV fluxes from the ocean’s interior are not the dominant factor in the restratification process. Despite the presence of high PV water at depth, advective flux mechanisms driving these fluxes are robust against variations in underlying PV conditions and thus retain their symmetry and magnitude.

Positive PV fluxes from the boundaries were necessary due to impermeability. Sharp ageostrophic fronts, driven by SI-induced frontogenesis at the boundaries, are hotspots for these PV fluxes. The dynamics involved in these processes are complex, particularly concerning the transfer of energy, which contrary to the literature, was seen to be primarily governed by turbulent fluxes and influenced by GSP. The role of $\overline{b'w'}$ in the transfer appears to be less discernible from the data and remains unclear. The overall restratification showed a linear trend when compared to linear theory. A key mechanism identified for the restratification is an SI-driven divergence in the turbulent momentum fluxes or Reynolds stresses, in particular $(\frac{\partial \overline{v'w'}}{\partial z})$. This drives a cross-frontal secondary circulation, which restratifies the water column gradient. The mechanism is also referred to as turbulent thermal wind balance but is driven by SI here.

In chapter 6, we take a closer look at how forcing of SI, driven by down-front winds in a more realistic scenario, might modify these results.

Chapter 6

Storm Forced SI

Until this point in the thesis we have focussed either the linear theory of SI, or idealised spin-down simulations of a frontal zone using the Eady model. Both of which have been useful to study the dynamics associated with SI under controlled conditions. In an effort to draw parallels to the real ocean, the move to understand forced SI comes naturally.

The weakening of vertical stratification (N^2) in the presence of lateral buoyancy gradients can cause fq to become negative. As we have seen, SI growth then generally works to quickly return PV to a marginally stable state ($PV \approx 0$). However, with continued destabilizing surface forcing toward anticyclonic PV, what is generally known as forced symmetric instability (FSI) can continue to occur Taylor and Ferrari, 2009; Thomas and Taylor, 2010.

Evidence of SI in the ocean has been found by Ramachandran et al., 2018 in fronts in the Bay of Bengal, by Peng et al., 2020 in a submesoscale filament in the Benguela upwelling region and by Bosse et al., 2021 around a deep convection area in the north-western Mediterranean Sea. This suggests that SI does not require strong classical fronts such the Gulf Stream, and might be ubiquitous in the open ocean. Dong et al., 2021 pin the likely hood of SI occurring in the ocean to surface buoyancy flux (B_0) that is positive, $EBF > 0$, $PV < 0$ and $(H - h)/H \geq 0.05$ where H is the bottom of the SI layer given by the depth where PV becomes positive (Bachman et al., 2017), and h is the thermocline (Fig. 6.1). Note that although less well understood, SI can still occur when EBF and B_0 are of opposite signs with these conditions commonly found in the real world.

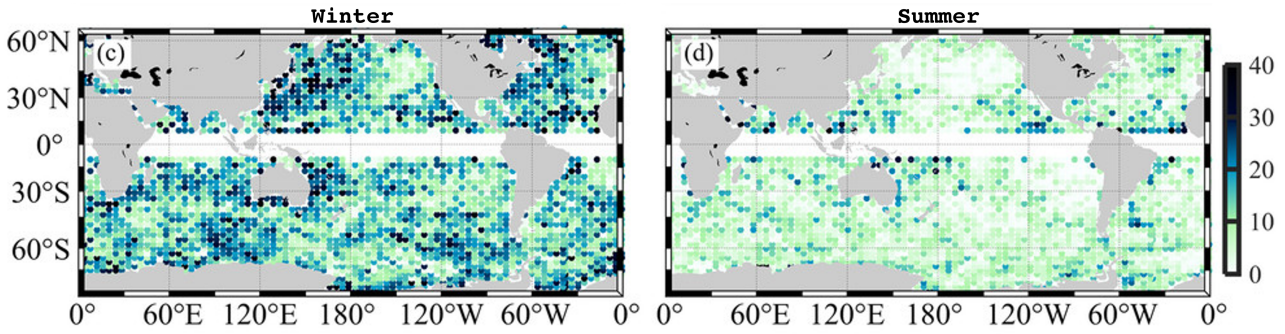


FIGURE 6.1: The relative likelihood (%) of SI. Results in (left) winter (February in the Northern Hemisphere and August in the Southern Hemisphere) and (right) summer (August in the Northern Hemisphere and February in the Southern Hemisphere). Figure adapted from (Dong et al., 2021).

Understanding the dynamics of oceanic and atmospheric processes at fine scales is crucial for improving our predictions of weather and climate patterns. In recent years, the study of submesoscale processes, particularly fronts and instabilities, has garnered significant attention due to their pivotal role in energy transfer and mixing in these systems. As previously mentioned it is the scale of the given instabilities that inhibits their resolution in climate models. In this section we try to connect our idealised Eady type setup to a more realistic setting. We present a unique simulation of a double submesoscale front with turbulence resolved down to 2.5 meters. The level of detail here allows for the resolution of KHI, SI and regular shear instabilities.

6.1 Atmospheric forcing and forced SI dynamics

Since the criterion for SI depends on the sign of the PV, and since PV is materially conserved, the ability for SI to develop in the flow is closely tied to boundary forcing. That is, we need forcing that is capable of changing the bulk PV. At the surface, diabatic and frictional processes can lower the potential vorticity of the surface layer, leaving the system prone to SI formation. Thomas and Lee, 2005 showed that

$$f\hat{k} \cdot \left(\nabla_h b \times \mathbf{F} - \omega_a \frac{Db}{Dt} \right) > 0. \quad (6.1)$$

can be related to the surface forcing via an effective buoyancy flux, namely that PV is destroyed if

$$\mathcal{F}_{SI} = \underbrace{\left(\frac{\boldsymbol{\tau}_w \times \hat{\mathbf{k}}}{\rho_0 f} \right) \cdot \nabla_h b \Big|_{z=0}}_{\text{EBF}} + B_0 > 0. \quad (6.2)$$

where: - $\boldsymbol{\tau}_w = (\tau_x, \tau_y)$ is the wind stress vector and $\nabla_h b \Big|_{z=0}$ is the horizontal surface buoyancy gradient. $(\boldsymbol{\tau}_w \times \hat{\mathbf{k}})/\rho_0 f$ is referred to as the Ekman transport and B_0 is the surface buoyancy flux or forcing.

This surface buoyancy flux, which is driven by atmospheric cooling (i.e. the surface of the ocean loses heat to the atmosphere), reduces the PV and results in denser fluid on top of lighter fluid. This can induce convective mixing (Fig. 6.2b). When sufficiently large enough to overcome the stabilizing influences of vertical stratification and rotation, it can also precondition a flow to SI (Thomas and Lee, 2005). Atmospheric buoyancy loss is not the only mechanism to destroy PV. A second way that this can occur is when winds blow down-front, in the direction of the frontal jet. This incites an across-frontal circulation (ψ_w in fig. 6.2a) driven by the Ekman transport which heaves dense fluid over lighter fluid. The ability for the Ekman flow to destabilize the water column when the wind-stress is down front is sometimes referred to as Ekman buoyancy flux (Thomas and Lee, 2005; Thomas and Taylor, 2010). In conjunction with buoyancy forcing (6.2), its destabilization can either be enhanced or suppressed.

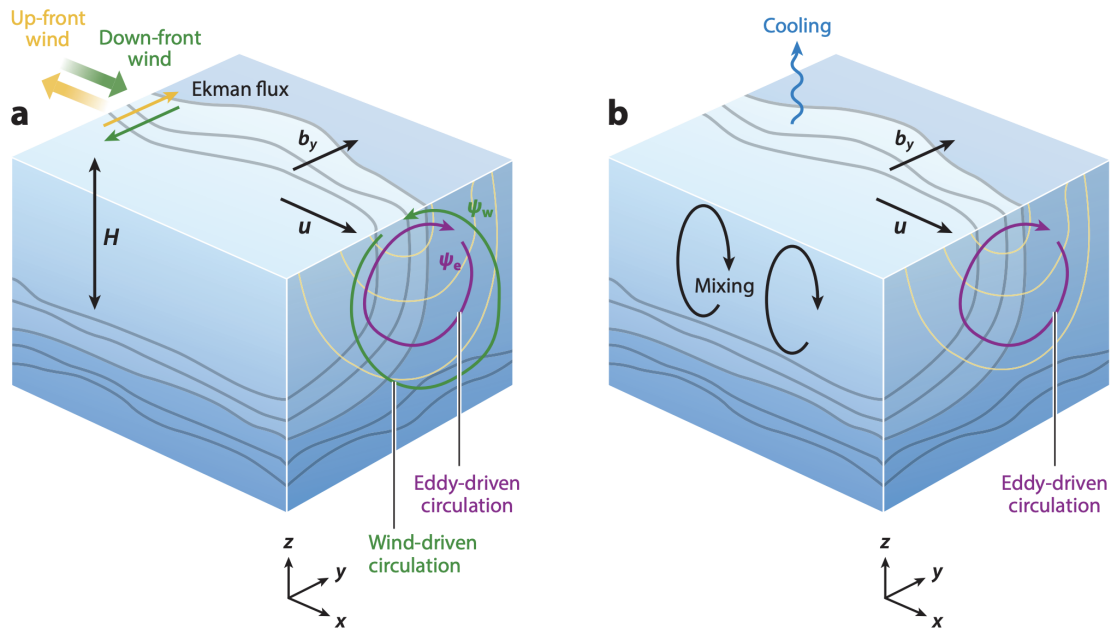


FIGURE 6.2: A schematic illustrates how surface forcing influences a frontal zone. Mixed-layer eddies produce an overturning streamfunction, ψ_e , that works to flatten the isopycnals and increase stratification within the mixed layer. (a) When the wind stress has a component directed down the front, it generates an Ekman transport from the denser to the less dense region. This wind-driven overturning circulation, ψ_w (indicated in green for down-front winds), counteracts the stratifying effect of the mixed-layer eddies. In contrast, if the wind is oriented up-front, it moves less dense water over more dense water, causing ψ_w (not illustrated for up-front winds) to align with ψ_e and aid in restratifying the mixed layer. (b) Surface cooling generates a vertical buoyancy flux that opposes the buoyancy flux associated with eddies. If the cooling is sufficiently intense, it can inhibit the ability of mixed-layer eddies to increase stratification. The along-front velocity u , the mixed-layer depth H , and the cross-front buoyancy gradient b_y are marked in the schematic. Figure taken from Mahadevan, 2016.

Taylor and Ferrari, 2010 illustrated how strong atmospheric forcing on a persistent front can produce a distinctive two-layer structure within the SML. This structure is characterized by an upper convective layer where turbulence is driven by buoyancy loss, and a deeper layer where turbulence results from forced SI. Recent high-resolution turbulence microstructure observations conducted across a submesoscale filament in the Benguela upwelling region confirm the existence of these separate turbulent layers (Peng et al., 2020).

6.2 Model setup and configurations

The model run conducted in this chapter is a double-front setup presenting a distinct dynamical environment where submesoscale turbulence, frontal interactions, and wind-driven processes evolve in a fundamentally different manner compared to the more commonly studied scenarios of a single-front setup.

In the double-front regime, a vertical extent H of the ML depth is set to $50m$, and an attached stratified interior of $N^2 = 1 \times 10^{-6}s^{-2}$ beneath it, as graphically represented in figure 6.3. We set up two fronts with opposing geostrophic velocities, one down-wind and one up-wind. Notice the increase in the horizontal domain length compared to the previous chapters. For efficiency, we have slightly reduced the resolution to $\delta = 2.5m$ in the horizontal and $\delta = 1m$ in the vertical. Our time step increases to $dt = 1s$ as well. A wind stress is applied which varies in time, and the coriolis parameter is set such that $f = 7.29e^{-5}s^{-1}$. The set of equations which define the model remain much the same as in 3.1 and 3.2 except now there is no background velocity such that $\mathbf{U} = \mathbf{u}$, and no background buoyancy.

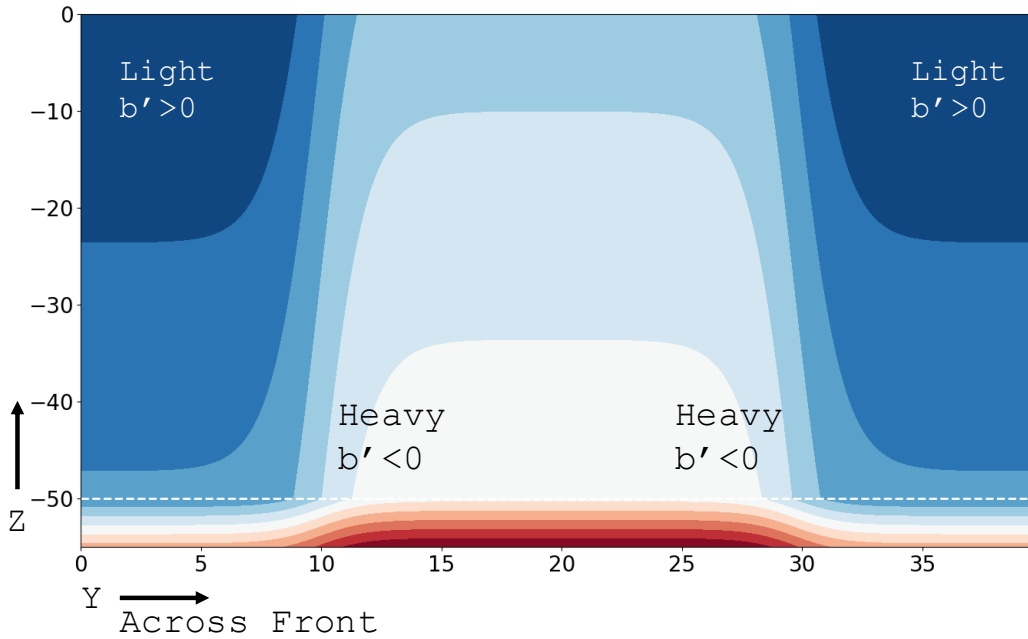


FIGURE 6.3: A double frontal region highlighting the across front density variation b_b ($m.s^{-2}$). The across front stratification is balanced by thermal wind shear in $\bar{u}_b$ ($m.s^{-2}$) which varies only in the vertical, while the buoyancy is once more a linear function of y and z . The full depth (168m) has been limited for graphical purposes. The white dashed line represents the mixed layer depth, which is set at 50m. Note the extent of the across front direction which is set in [km], while the vertical remains in [m].

The flow now features vertical relative vorticity (ζ) such that the stability criterion for SI (1.21) now becomes $f q = f(f + \zeta)N^2 - M^4$ (Bachman and Taylor, 2014). Since the geostrophic velocity only has a component in the x-direction, the stability criterion can be written as:

$$q = \left(f - \frac{\partial u_g}{\partial y} \right) \left(\frac{N^2}{f} \right) - \left(\frac{M^4}{f} \right) \quad (6.3)$$

However, as discussed in Chapter 1.4.4, $f q < 0$ is a necessary but not sufficient condition for SI development. In the case of forced SI for example, if surface cooling (B_0) reduces N^2 such that $f q < 0$, without lateral buoyancy gradients, regular GI would develop rather than SI. Figure 6.4 gives various regimes of instability as a function of the following angle $\psi_{Ri_b} = \tan^{-1} \left(\frac{|\nabla_h b|^2}{f^2 N^2} \right)$ with instability occurring when $\psi_{Ri_b} < \psi_c = \tan^{-1} \left(-\frac{\zeta_g}{f} \right)$ (Thomas et al., 2013). It is useful for determining not only when instability occurs, but also in providing insight into which of the instabilities will dominate. For example, for unstable stratification ($N^2 < 0$) and $-180^\circ < \psi_{Ri_b} < -135^\circ$, gravitational instability will occur.

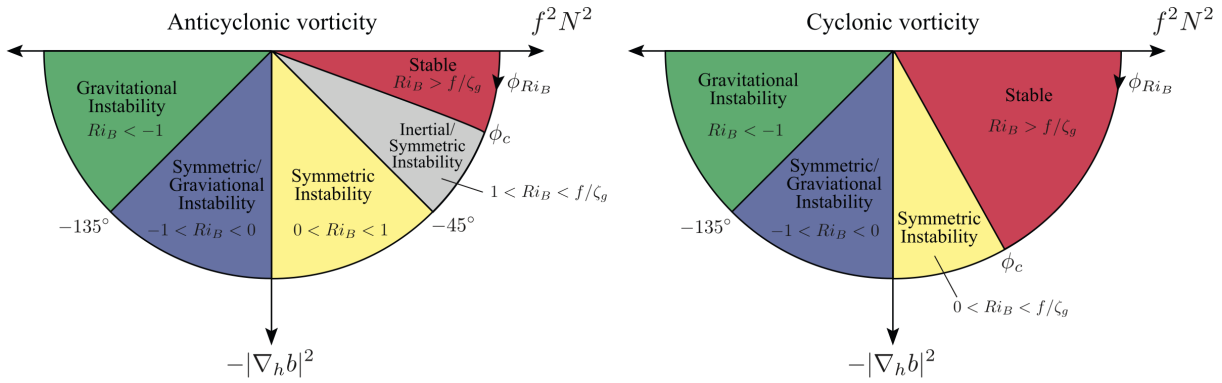


FIGURE 6.4: Regimes of gravitational instability (GI), inertial instability and symmetric instability (SI) that arise when $f q < 0$ and the vertical relative vorticity (ζ) is either anticyclonic (left) and cyclonic (right).

Although the linear stability analysis performed by Thomas et al., 2013 was done around a simple basic state with uniform velocity and buoyancy gradients, the use of the Thomas angle allowed them to successfully identify various dynamical regimes when applied pointwise to LESs of the Gulf Stream front.

6.3 Results

In this chapter we approximated the geostrophic velocity from thermal wind balance as $u_g = -M^2/f$ with a smoothing applied to b , in db/dy , applied via running mean in the

meridional direction with a window size of 80 m.

6.3.1 Frontal evolution under wind forcing

The winds applied to force the numerical simulations in this section are configured such they are down-front, advecting denser water from the heavier side of the front over lighter waters. This across-front advection of density reduces vertical stratification, ultimately initiating convection.

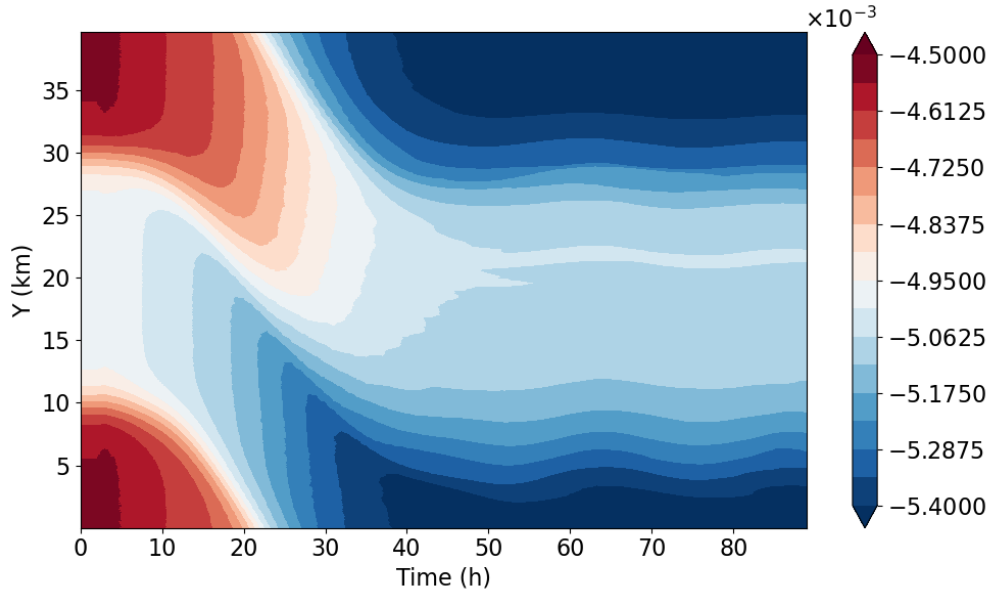


FIGURE 6.5: Time evolution of buoyancy at $z = -10\text{m}$ showing the advection of the double frontal zone under 48 hour long wind forced conditions ($m.s^2$).

We can view the effect of the wind forcing on the positional displacement of the front from the Hövmoller plot of buoyancy given in figure 6.5. Over the initial 48 hours there is a clear lateral shift in the position of the frontal interface. We find a general domain wide decline in buoyancy, which is due to the storm induced mixing. Cooler less buoyant water from the interior is mixed into the upper ML, lowering the overall buoyancy.

The wind forcing implemented is horizontally homogeneous, with a time evolution given in figure 6.6a. Since $\tau_y = 0$, the wind stress is confined to the x -component, expressed as $\tau_w = (\tau_x, 0)$. τ_x varies with time and is constrained to a minimum value of 0.002.

We can find the effect of the wind on the stability of the front by considering the EBF from Eq. 6.2. The cross product $\tau_w \times \hat{k}$ rotates τ_x into the cross frontal-direction such that:

$$\frac{\boldsymbol{\tau}_w \times \hat{\mathbf{k}}}{\rho_0 f} = \left(0, \frac{\tau_x}{\rho_0 f}\right) \quad (6.4)$$

the surface horizontal buoyancy gradient, which can be expressed as:

$$\nabla_h b = \left(\frac{\partial b}{\partial x}, \frac{\partial b}{\partial y}\right) \quad (6.5)$$

Given that $\tau_y = 0$, the x -component of $\nabla_h b$ does not contribute to the EBF. Therefore, the EBF is simply given by:

$$\text{EBF} = \frac{\tau_x}{\rho_0 f} \frac{\partial b}{\partial y} \Big|_{z=0} \quad (6.6)$$

We know that FSI can occur if $EBF + B_0 > 0$ (Bachman et al., 2017), since there is no surface buoyancy flux, we find that FSI can occur everywhere where the EBF in Fig. 6.6 (b) is positive. The trajectory of the EBF over time is much like the advection of the front (6.5), and its extent is confined to at most $\approx 5km$ wide.

From this we find that the total EBF over the period of the forcing is given as:

$$EBF_t = \int_0^{48} \frac{\tau_x}{\rho_0 f} \frac{\partial b}{\partial y} \Big|_{z=0} dt \quad (6.7)$$

Calculating only the positive EBF, we find that $EBF_t = 7852\text{m}^3.s^{-4}$.

Understanding the setup of the double front is critical to understanding the dynamics of its evolution when subjected to wind forcing. Initially (Fig. 6.3), both fronts are stable to instability, with lighter water overlaying heavier water. However owing to the wind forcing in the positive x -direction, the fronts are exposed to opposing geostrophic velocities, one down-wind and one up-wind. Thus the Ekman transport fluxes water northwards resulting in noticeable changes in the stratification and mixed layer depth of the system (Fig. 6.7).

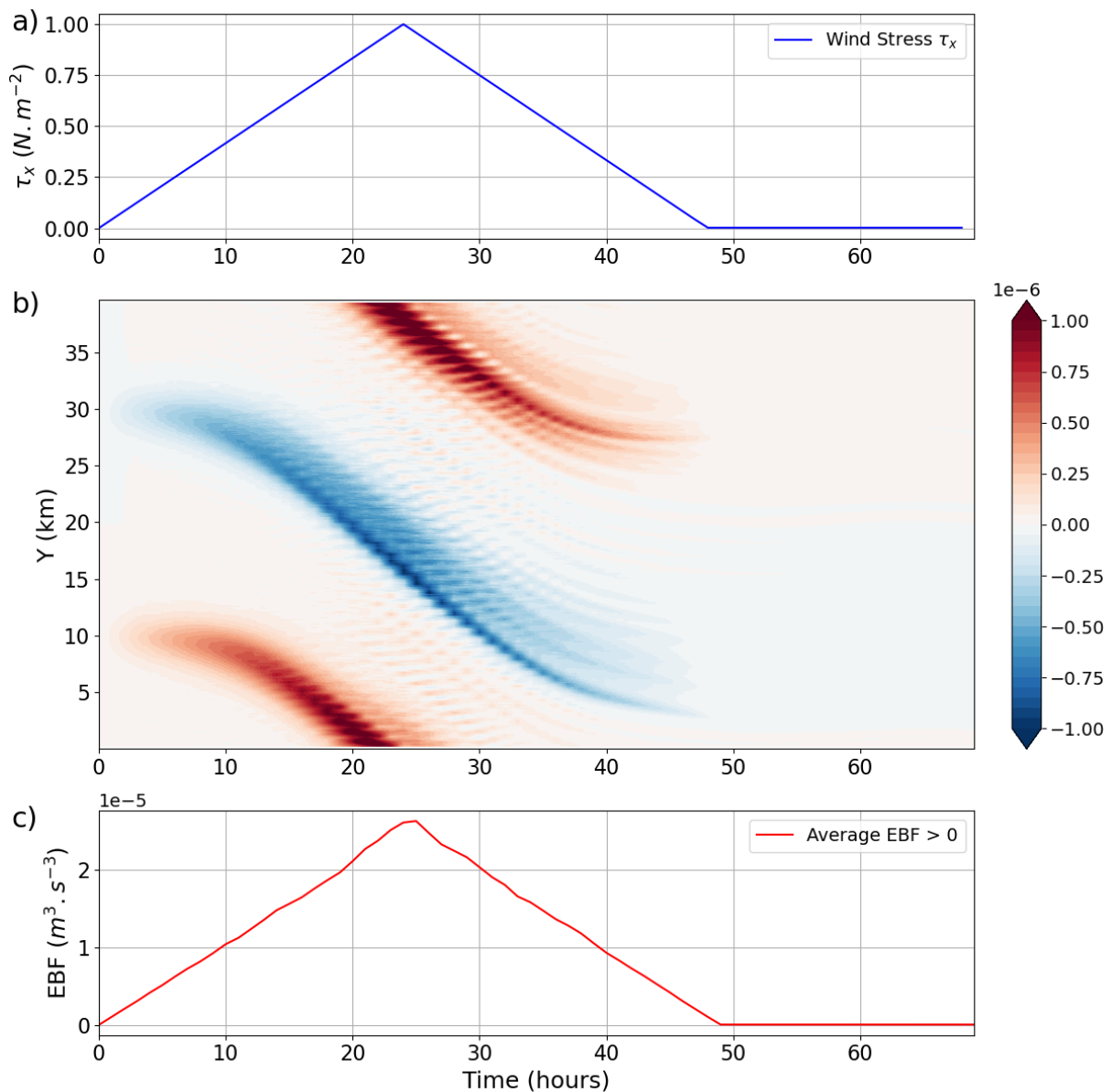


FIGURE 6.6: (a) Wind forcing profile τ_x at the surface over the first 48 hours of the model ($N \cdot m^{-2}$). (b) Progression of the buoyancy structure of the double frontal region over time ($m^2 \cdot s^2$). Owing to the surface forcing over the initial 48h, the two fronts are advected southwards. (c) The evolution of the positive Ekman buoyancy flux (EBF) at the surface over time ($m^3 \cdot s^{-3}$)

In the northern most front, the EBF results in a net transport of colder water over warmer water, leading to a steeping of the isopycnals in the ML, and a deepening of the MLD to about 65m. While the left front exhibits a net transport of water in the same direction, in contrast, warmer water is advected over colder water. We see a slight flattening of the isopycnals and minor stabilization of the water column and shallowing of the MLD to around 45m.

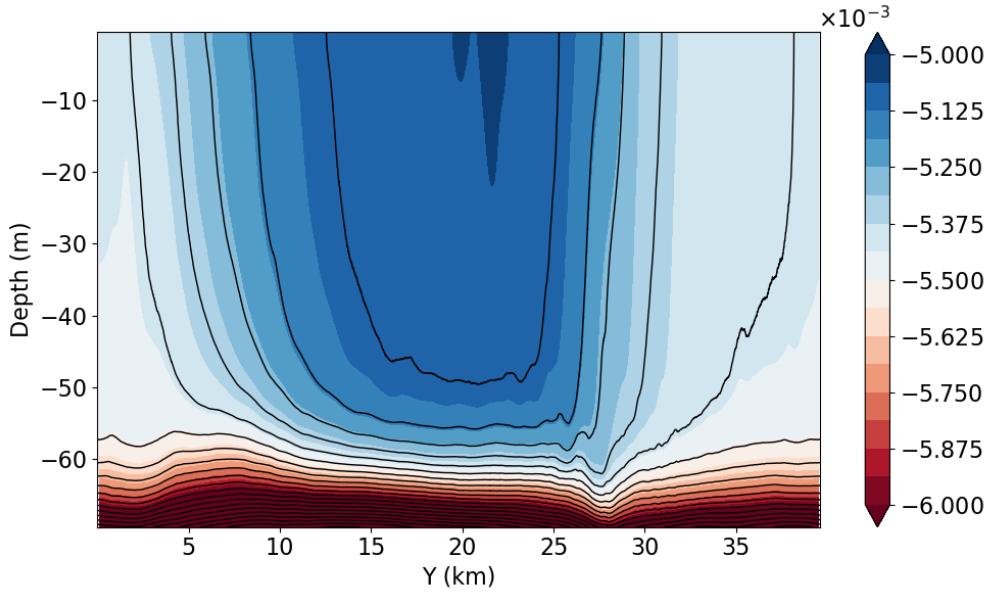


FIGURE 6.7: Average Buoyancy ($t = 49$ to $72h$) following the storm for the wind forced experiment ($m.s^2$). The contours (black) showing the zonally averaged isopycnals.

6.3.2 PV and stratification

To conclusively demonstrate whether or not SI is present in the domain, we start the analysis by measuring the PV of the system from 6.3. Regions of negative PV are most prominently clustered in the more northern front, between between 25km and 31km, and constrained to the upper 50m of the domain. There is a sharp increase in positive PV in the water column around 28km. This is associated with the initial frontal jet and where ζ would have changed sign. However the general picture of PV is expected, $f q < 0$, thus necessary conditions for SI development has been met. The story of PV in the region becomes more apparent if we analyse the domain average over time (Fig. 6.10).

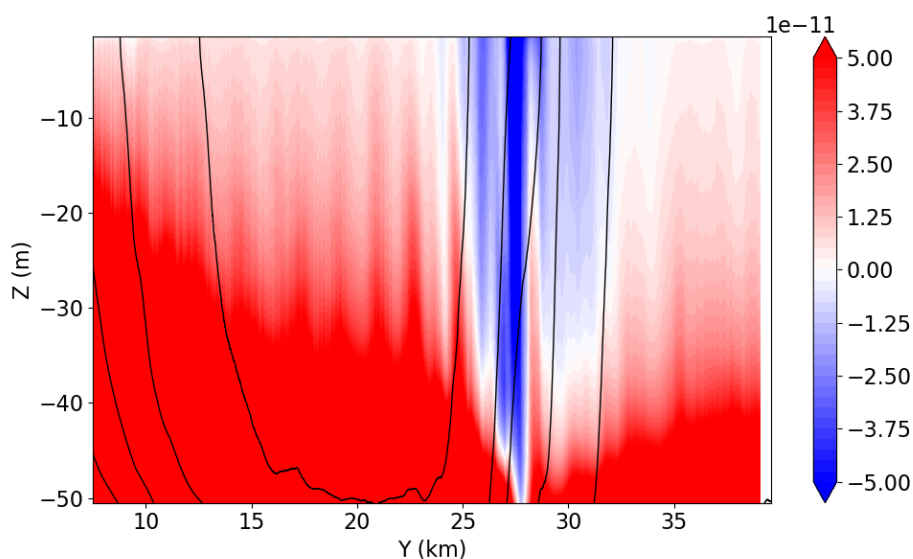


FIGURE 6.8: Potential vorticity (PV) q at $t = 48h$ for the wind forced double front experiment (s^{-3}). The overlay of contours (black) showing the zonally averaged isopycnals.

Figure 6.9, a Hovmöller of N^2 , provides insights into the stability of the stratification over time. Initially we see that the stratification is low in the southern front and much higher in the more northern front. During the storm the stratification is driven to lower levels throughout the domain. This is due to wind induced mixing or denser waters from below into the upper 10 to 30m. After the wind forcing has ceased ($t = 48h$), and the fronts have been advected to their final positions, we see the effect of the inertial oscillations on a wide extent of the more southerly front. The positive signature oscillates with inertial period approximately every 24 h. At this time, the northern front, has very low stratification, which is seen in the low PV signature of figure 6.8. As the run progresses we see a positive region of N^2 , concentrated in a small band, highlighting a very strong restratification in the area.

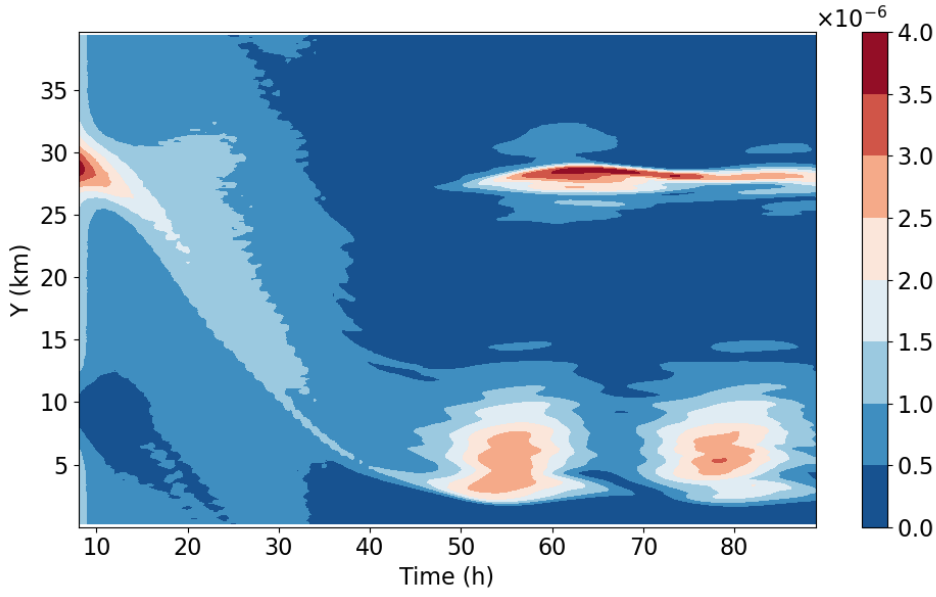


FIGURE 6.9: Evolution of the vertical buoyancy gradient (N^2) averaged over 10 to 30m for $t = 8$ to 90 h for the wind forced experiment highlighting changes in the stratification between the two fronts over time (s^{-2}).

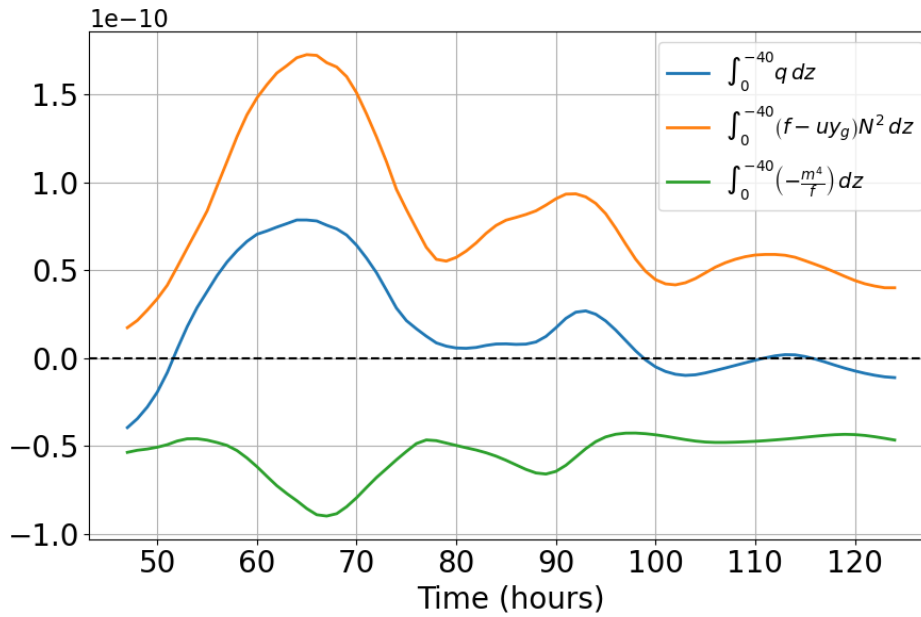


FIGURE 6.10: Time series of the horizontally averaged ($y = 26\text{km}$ to 31km) and vertically integrated ($z = 0 : -50\text{m}$) potential vorticity (q) for the wind forced double front experiment (ms^{-3}).

As the EBF heaves colder water over warmer water, the stratification decreases and the effects of the baroclinicity become more significant eventually overcoming the stabilizing influences of vertical stratification and rotation. At $t = 48$ we find $q < 0$, the frontal region

is primed with negative PV. The PV remains negative for the next 16 hours until $t = 52$. In this time conditions seem to be favourable for SI formation. Its evident how quickly the term $(f - uy_g) N^2$ drives q above 0, providing further insight into the positive band of N^2 in 6.9 in the region. Once the mean $q > 0$, and the system is stable to SI, we find that inertial oscillations still persist as seen in Fig. (6.10), where q oscillates with the inertial period.

6.3.3 Energetics

TKE allows us to quantify the intensity of the turbulence during the first 24h following the wind forcing. High TKE values indicate regions with a lot of mixing and turbulent motion. We see the highest values of TKE throughout the water column, constrained to the more northern front (Fig. 6.11). We also see positive TKE on the southern side of the more southerly front.

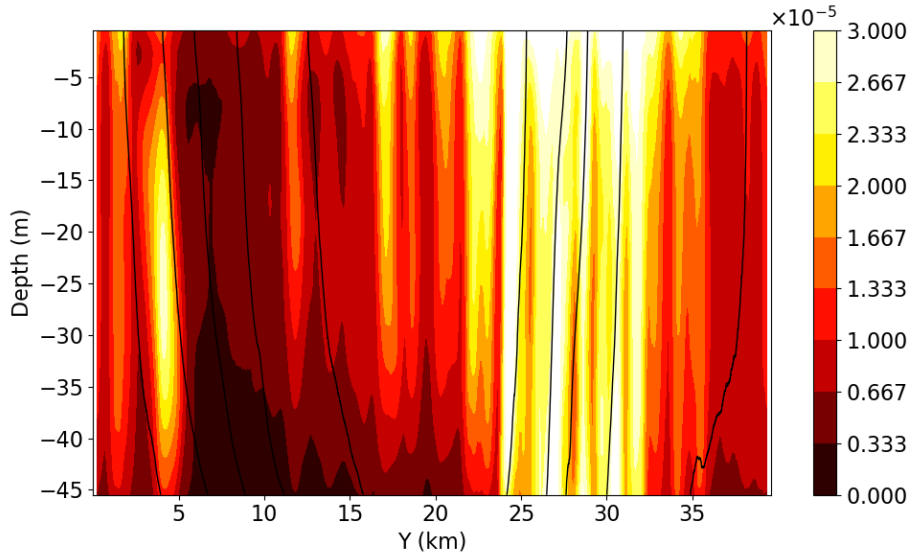


FIGURE 6.11: Horizontally averaged TKE for the wind forced experiment ($m^2.s^{-3}$) averaged over $t = 48$ to 72 h. The contours (black) showing the zonally averaged isopycnals.

Figure 6.12, gives time averaged snapshots of the GSP and AGP for the first 24h following the wind forcing. We see that positive GSP dominates the northern front driving changes in the TKE in this region. The inertial oscillations that take place following the storm are responsible for the large positive AGSP that we find in the southern flank of the southern front. This is a result of the stronger vertical shear associated with the Ekman flow in conjunction with the inertial oscillations. Here we find that the increased stratification prevents mixing of momentum in the vertical. Directly after the wind forcing

we find that cross frontal velocities converge here (not shown), leading to strong shear and AGSP. Conversely, 12 hours later during the second phase of the oscillation, we find strong divergence in the flow (not shown), thus there is a constant source of AGSP.

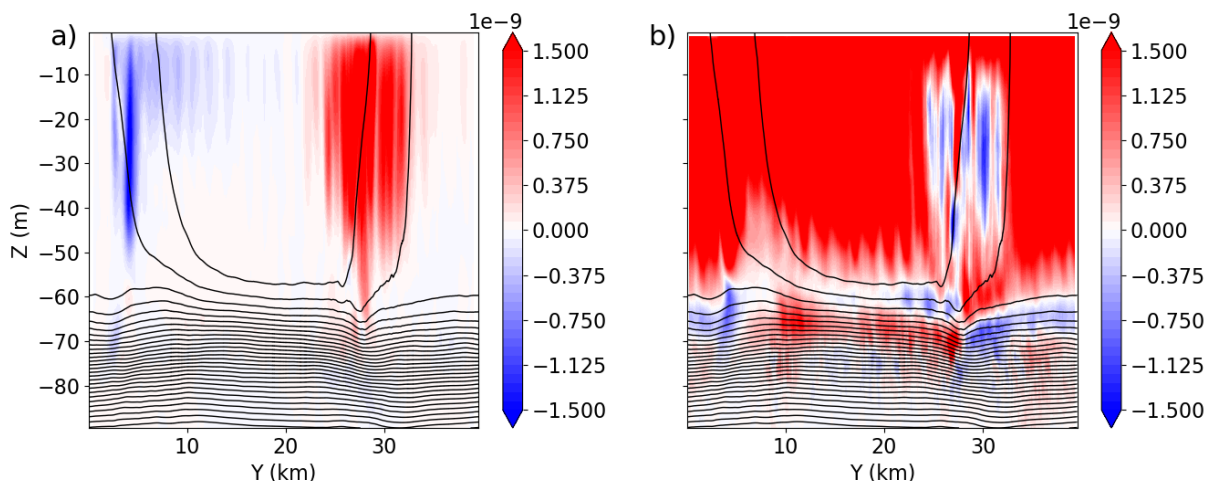


FIGURE 6.12: Horizontally averaged (a) geostrophic shear production (GSP) and (b) ageostrophic shear production (AGSP) for the wind forced experiment averaged over $t = 48$ to 72 h ($m^2 \cdot s^{-3}$).

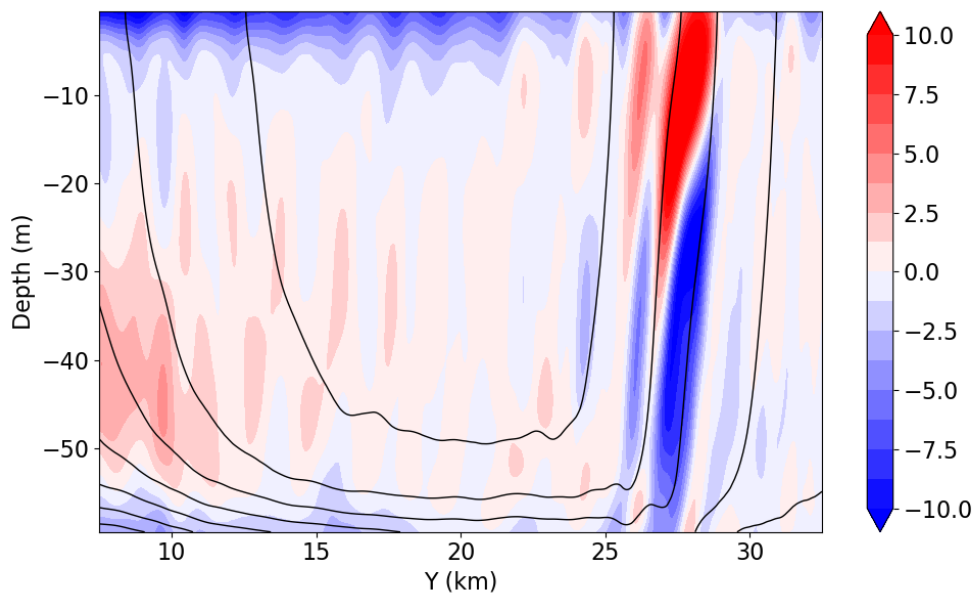


FIGURE 6.13: Cross-frontal velocity ($\bar{v}$) averaged over the time period $t = 49$ to 72 h ($cm \cdot s^{-1}$).

Much like in the idealised simulations, the Reynolds stresses, and in particular $-\frac{\partial \overline{v'w'}}{\partial z}$ which sets $\bar{v}$, are most pronounced in the middle of the ML and where ζ within the SI-unstable front changes sign. Again we find that the divergence in the Reynolds stresses change sign here, which leads to a negative cross-front velocity at the bottom and a positive cross-front velocity at the top of the domain (Fig. 6.13). This modified turbulent thermal wind drives an overturning that leads to the restratification of the water column, the process is evident in Fig. 6.7, where it is confined to the positive buoyancy band in the northern front, starting at around 48h.

6.3.4 Discussion

In the wind-forced simulation, the interaction between wind-induced Ekman transport and lateral buoyancy gradients was critical in shaping the dynamics of the system and subsequent release of energy stored in the geostrophic shear. The results underscore the nuanced response of the upper ocean to atmospheric forcing, highlighting significant differences in the evolution of the northern and southern fronts under identical wind stress conditions.

Despite being subjected to the same down-front wind forcing, the two fronts exhibit vastly different behaviours due to the orientation of their buoyancy gradients relative to the wind stress. In the northern front (initially southern), the Ekman buoyancy flux acts to advect denser water over lighter water, reducing the vertical stratification and consequently the PV. This destabilization primes the front for the development of SI. Consequently we find that the turbulent fluxes associated with $\frac{\partial \overline{v'w'}}{\partial z}$ drive a cross frontal velocity which acts to restratify the region.

Conversely, in the southern front (northern initially), the EBF transports lighter water over denser water, leading to a slight flattening of the isopycnals and a minor stabilization of the water column. The stratification in this region remains higher, with PV staying positive, preventing the onset of SI. However here, inertial oscillations have a more commanding role, than in the SI-unstable front, modulating the stratification, causing it to oscillate with the inertial period ($\approx 24h$). Thus we see the importance of diurnal variability in regulating turbulence, with associated large positive AGSP, driving the change in TKE in this region. In contrast, GSP is the dominant source of TKE in the SI-unstable front, the result being energy extraction from the buoyancy gradients down to turbulent motions.

Chapter 7

Conclusions

7.1 Overview

Contemporary theory and simulations highlight the importance instability formation in submesoscale fronts in the downward transport and eventual dissipation of energy in the ocean. In an effort to understand this we have presented a thorough investigation into the evolution of these fronts in the surface mixed layer (SML) that are susceptible to symmetric instability (SI). We started the study with an initial analysis of the linear theory of SI. Proceeding this, we used a Large Eddy Simulation (LES) in an idealised Eady model framework, to explore spin-down setups, comprised of both one-layer and the more complex two-layer frontal zones. The latter consisting of an attached thermocline with high potential vorticity (PV). We focussed on understanding the role of SI and its associated bulk potential vorticity increase in the equilibration and restratification of the front. We then compared our results to simulations of more realistic ocean conditions consisting of wind-driven forced SI, whereby destabilising surfacing forcing acts to remove PV from the front, sustaining SI and its bulk potential vorticity increase associated with an Ekman buoyancy flux (EBF).

7.2 Main summary

In this study, we began with an analysis into the linear theory associated with SI. The linear theory predicts that in the inviscid case, for a given front in thermal wind balance, the maximum growth rate σ associated with SI is dependent solely on the wave number vector (k/m). We found that only large eddy viscosity (ν_t) has a sensible impact on the growth rate of SI, effectively damping the smaller-scale modes. We find that the largest possible waves have the largest growth rate. Additionally we found that the emergence of secondary Kelvin-Helmholtz instabilities (KHI) plays a critical role in suppressing further

SI growth, and that this coupling of KHI with SI which is modified by (pre-)existing turbulence (ν_t) is more intricate than initially expected. Our findings from the linear theory have significant implications for the numerical simulations.

Following the linear theory, we presented a validation of our LES model, using PV and its associated fluxes as a diagnostic. PV is notoriously difficult to diagnose accurately, with associated errors in the context of this study, having consequences for incorrectly interpreting the stability of a system to various instabilities. The model validation found an almost perfect agreement, with no numerical errors or artificial fluxes. Furthermore we found a minimum resolution of $2m$ required to resolve the secondary KHI. In the pure spin down simulations, we demonstrated how classical SI cells, invariant to the along front direction, grow almost parallel to the slope of the isopycnals, and how the energetics and transport properties of these cells depend heavily on the initialised Richardson number (Ri_0). We found the role of an attached thermocline beneath the mixed layer (ML) to be of minor importance when added to the setup. Rather, the necessary pv fluxes associated with the restratification comes from non-conservative fluxes at the boundaries. These fluxes show a maximum in frontal regions, a result of the vertical boundaries associated with the finite SI region. A main driver of restratification was identified as the divergence of the Reynolds stresses which induces a cross-frontal overturning circulation. In particular the Reynolds stresses associated with the SI-modes were found to be particularly efficient in driving restratification.

We found that the life-cycle of SI is an interplay between growing SI-modes and associated secondary KHI, with KHI acting to dampen any further growth of the SI modes. This connection between growing SI modes and KHI strongly influences the efficiency of the restratification process. Since SI modes with large wavelengths have longer time to develop before the effects of KHI acted to dampen them. Consequently during their growth, it was the larger SI-induced Reynolds stresses which resulted in more geostrophic shear production (GSP). This mechanism was found to be the most efficient in leading the restratification process. Furthermore, for a fixed Ri_0 , the wavelength of the growing SI modes - and consequently their efficiency in restratification - is influenced by the level of resolved- and parameterised turbulence, which set by the eddy viscosity.

In the wind-forced simulation we expanded the across-front domain to the km scale, presenting a novel experiment in terms of the level of resolved turbulence for the given grid size. We analysed a double-front setup where the subtlety of the orientation of the across front gradient in relation to down front winds became evident. During the wind forcing event, the overall buoyancy of the system decreased as a result of mixing between the upper ML and the deeper denser waters. Given the orientation of the lateral gradients associated with each front, the wind induced Ekman buoyancy flux (EBF) either

advected water of opposite sign or water of the same into the upper region of the domain. In response to lighter water being advected on top of denser water we found a mild restratification in the one front. While denser water being advected above lighter water further steepened the isopycnals of the given front, ultimately driving the PV to negative values, and priming the domain locally for the development of SI. In this local region, we found large amounts of turbulent kinetic energy (TKE) which also coincided with regions of large GSP. Along with a positive EBF, and a change in sign of cross-frontal velocities in the water column we found SI to drive the restratification of the area. This became evident in the Hovmöller diagram of the vertical buoyancy gradient (N^2) where a region of positive N^2 confined to a thin band developed after $\approx 48h$. In the region stable to SI, the onset of inertial oscillations due to the increased stratification triggered TKE changes through associated ageostrophic shear production (AGSP). This also highlights the importance of diurnal variability in modulating turbulence. Although both fronts had low initial stratification, and both were subject to the same homogeneous wind forcing, the associated energy transfers differed significantly. This has significant consequences for the resolved turbulence in climate models.

Through a combination of theory and high-resolution simulations, this work highlights the importance of accurately capturing the effects at the submesoscale and in particular the role of SI in mixed layer energetics, all in an effort to develop energetically consistent climate models.

7.3 Outlook

It goes without saying that environmental systems are complex and multi-faceted and typically cannot be reduced to the sum of their parts. The complexity and variability of natural processes like oceanic turbulence, where multiple factors can be at play simultaneously across different spatial and temporal scales is testament to this. Analyses like this are meant to provide a small insight into the dynamics that underpin geophysical system that we live in. Naturally next steps would be to increase the complexity adding other physical effects, such as the interaction of SI with Langmuir circulations or waves. A comparison to observations to supplement our findings would also make sense.

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