Vortex pairing and mixing in stratified shear flows

by

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Abstract

Kelvin-Helmholtz (KH) instabilities are an important source of mixing in oceans, lakes and the atmosphere. The process of vortex pairing can increase the amount of mixing. First, the effects of initial conditions on vortex pairing and mixing are studied by running Direct Numerical Simulations with a variety of initial perturbations. It is shown that when the subharmonic component of the perturbation is out of phase relative to the KH mode, vortex pairing is delayed or even eliminated. The amount of mixing in the simulations where the subharmonic mode is out of phase is approximately half of that in the simulations where the subharmonic mode is in phase. The time of pairing is also found to be sensitive to the phase of the subharmonic mode. A slight change of the phase can change time of pairing significantly when the subharmonic mode is close to being out of phase. Second, the effects of Prandtl number on KH instabilities, vortex pairing and mixing are studied. It is found that KH instabilities and vortex pairing are suppressed at higher Prandtl numbers, which tends to reduce the amount of mixing. This effect is counteracted by enhanced three-dimensional motions in higher Prandtl number flows. However, the general trend is for mixing and mixing efficiency to decrease as Prandtl number is increased.
Lay Abstract

Climate and ocean circulation models rely on parameterization of turbulence. Understanding small scale turbulent events in the atmosphere, oceans and lakes helps optimize the parameterization. The Kelvin-Helmholtz instability, a common instability causing small scale turbulence in nature, is studied using numerical simulations. The objective is to investigate mixing of scalars, e.g. temperature and salinity, occurring in Kelvin-Helmholtz instabilities under different circumstances. The effect of initial conditions is studied by running simulations with a variety of initial perturbations. Then the effect of molecular properties of the scalar, for example whether the scalar is temperature or salinity, on mixing is investigated.
Preface

A version of chapter 2 has been submitted for publication. The authors are myself, E. W. Tedford, M Rahmani, and G. A. Lawrence. I developed the ideas under the guidance of E. W. Tedford, M Rahmani, and G. A. Lawrence. I was responsible for preparing the manuscript and E. W. Tedford, M Rahmani, and G. A. Lawrence revised the manuscript.
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Chapter 1

Introduction

1.1 Motivation

Numerical modeling of environmental flows has been a valuable tool to understand complex flows in nature, for example atmospheric boundary flows over buildings or internal seiches in lakes. Subgrid-scale parameterizations are used in these models to describe small scale dynamic process that cannot be resolved due to computational constrains. Many closure schemes have been proposed to parametrize small scale turbulence, however the results given by different schemes can have non-negligible differences especially for inland water bodies or near-shore regions (Ivey et al., 2008). A better understanding of the small scale turbulence events in the atmosphere and ocean is therefore helpful to improve the accuracy of numerical models.

In the atmosphere, ocean, and lakes, fluids are stratified due to temperature or salinity. Shear may exist in these stratified fluids due to wind, inflows, or topography. When shear exists, shear instabilities may arise, causing the transition to turbulence and enhancing transport of scalars. There are three primary instabilities in stratified free shear flows, namely Kelvin-Helmholtz (KH) instabilities, Holmboe instabilities, Taylor-Caulfield instabilities. The velocity and density profiles determine which type of instabilities occurs. KH instabilities are the most widely known among these three instabilities. For this reason, this thesis is focused on KH instabilities, characterized by the roll-up of the density interface (Thorpe, 1971) and streamlines of cat’s eye shape (Drazin & Reid, 2004). After KH instabilities reach maximum amplitude, secondary instabilities grow causing the transition to turbulence. Most mixing occurs during this turbulent stage due to highly three-dimensional small scale motions (Caulfield & Peltier, 2000). However, flow in the pre-turbulent stage can affect mixing and mixing efficiency. When vortex pairing exists, it increases the Reynolds number by merging KH billows and increasing the length scale of large scale motion (Moser & Rogers, 1993). Three-dimensionality which causes more mixing (Rahmani et al., 2014) is increased as a result. If turbulence is in the transition regime, mixing efficiency is also increased (Shih et al., 2005). Therefore, we consider KH instabilities when vortex pairing exists.
1.2 Theoretical background

Much theoretical work on KH instabilities focuses on the linear stability theory which determines whether an infinitesimal perturbation of specific wavenumber is stable by solving an equation for the perturbation. Linear modal theory introduces normal mode perturbation that assumes growth rate is a constant to simplify the problems. Modal theory predicts the most unstable mode successfully for many hydrodynamic problems. However, the modal theory only considers part of the possible perturbations and therefore non-modal stability theory has been developed to find new unstable modes or understand non-modal growth (e.g. Arratia et al., 2013; Kaminski et al., 2014; Guha & Lawrence, 2014).

1.2.1 Linear modal stability theory

Linear modal stability theory for inviscid and non-diffusive stratified shear flows was established by Taylor (1931) and Goldstein (1931) independently. The resulting governing equation is called the Taylor-Goldstein (TG) equation. Miles (1961) and Howard (1961) proved the gradient Richardson number

\[ Ri = \frac{N^2}{(\partial U/\partial z)^2}, \]

where \( N \) is the Brunt-Väisälä frequency, is less than 0.25 somewhere is a necessary condition for instabilities to occur. In this section, we derive the viscous-diffusive TG equations, from which TG equation can be obtained by neglecting diffusivity and viscosity.

If we assume the fluid is incompressible and subject to the Bousinesq approximation, the governing equations for the total field variables \( u, p, \) and \( \rho \) are

\[ \begin{align*}
\nabla \cdot u &= 0, \quad (1.1) \\
\frac{\partial u}{\partial t} + (u \cdot \nabla)u &= -\frac{1}{\rho_0} \nabla p - g \frac{\rho}{\rho_0} \hat{k} + \nu \nabla^2 u, \quad (1.2) \\
\frac{\partial \rho}{\partial t} + (u \cdot \nabla) \rho &= \kappa \nabla^2 \rho, \quad (1.3)
\end{align*} \]

where \( \hat{k} \) is unit vertical vector, \( \rho_0 \) is a reference density, \( \nu \) is viscosity, and \( \kappa \) is diffusivity.

Consider a horizontal parallel flow \( U(z,t) \) and an undisturbed stratification \( \bar{p}(z,t) \) as the background flow. This flow is in equilibrium with the hydrostatic pressure \( \bar{p}(z) \). Substituting \( U, \bar{\rho}, \) and \( \bar{p} \) into equation (1.1), (1.2), and (1.3), we obtain the governing equations for \( U(z,t), \bar{\rho}(z,t), \) and \( \bar{p}(z,t) \), i.e.,

\[ \begin{align*}
\frac{\partial U}{\partial t} &= \nu \frac{\partial^2 U}{\partial z^2}, \quad (1.4) \\
0 &= -\frac{1}{\rho_0} \frac{\partial \bar{p}}{\partial z} - g \frac{\bar{p}}{\rho_0}. \quad (1.5)
\end{align*} \]
1.2. Theoretical background

\[ \frac{\partial \bar{\rho}}{\partial t} = \kappa \frac{\partial^2 \bar{\rho}}{\partial z^2}. \]  

(1.6)

Therefore, background shear \( U(z, t) \) and density \( \bar{\rho}(z, t) \) are diffusing independently. Background pressure \( \bar{p}(z, t) \) can be calculated by integrating equation (1.5) vertically. Squires’ theorem demonstrates that two-dimensional perturbation is more unstable than three-dimensional perturbation for shear instabilities in homogeneous shear flows. Koppel (1964) derived the governing equations for three-dimensional small perturbations in viscous and diffusive fluids and proved that two-dimensional perturbations are sufficient to consider the stability of stratified shear flows. Hence we consider the stability of a two-dimensional perturbation. The perturbed velocity, density, and pressure fields are

\[ u = U(z, t) + u'(x, z, t), \quad p = \bar{p}(z, t) + p'(x, z, t), \quad \rho = \bar{\rho}(z, t) + \rho'(x, z, t), \]  

(1.7)

where \( u', p', \) and \( \rho' \) are perturbations. The equations for perturbations \( u', p', \) and \( \rho' \) are obtained by substituting equation (1.7) into equation (1.1), (1.2), and (1.3) and subtracting the equation (1.4), (1.5), and (1.6) for background flow. Dropping non-linear terms, we obtain the equations for infinitesimal perturbations, i.e.,

\[ \frac{\partial u'}{\partial x} + \frac{\partial w'}{\partial z} = 0, \]  

(1.8)

\[ \frac{\partial u'}{\partial t} + w' \frac{dU}{dz} + U \frac{\partial u'}{\partial x} = -\frac{1}{\rho_0} \frac{\partial p'}{\partial x} + \nu \nabla^2 u', \]  

(1.9)

\[ \frac{\partial w'}{\partial t} + U \frac{\partial w'}{\partial x} = -\frac{1}{\rho_0} \frac{\partial \rho'}{\partial z} - g \frac{\rho'}{\rho_0} + \nu \nabla^2 w', \]  

(1.10)

\[ \frac{\partial \rho'}{\partial t} + U \frac{\partial \rho'}{\partial x} + w' \frac{d\bar{\rho}}{dz} = \kappa \nabla^2 \rho'. \]  

(1.11)

Introducing stream function \( \psi' \) defined by

\[ u' = \frac{\partial \psi'}{\partial z} \quad \text{and} \quad w' = -\frac{\partial \psi'}{\partial x}, \]  

(1.12)

equation (1.9), (1.10), and (1.11) become

\[ \frac{\partial^2 \psi'}{\partial t \partial z} - \frac{\partial \psi'}{\partial x} \frac{\partial U}{\partial x} + U \frac{\partial^2 \psi'}{\partial x \partial z} = -\frac{1}{\rho_0} \frac{\partial p'}{\partial x} + \nu \nabla^2 \frac{\partial \psi'}{\partial z}, \]  

(1.13)

\[ -\frac{\partial^2 \psi'}{\partial t \partial x} - U \frac{\partial^2 \psi'}{\partial x^2} = -\frac{1}{\rho_0} \frac{\partial \rho'}{\partial z} - g \frac{\rho'}{\rho_0} - \nu \nabla^2 \frac{\partial \psi'}{\partial z}, \]  

(1.14)

\[ \frac{\partial \rho'}{\partial t} + U \frac{\partial \rho'}{\partial x} - \frac{\partial \psi'}{\partial x} \frac{\partial \bar{\rho}}{\partial z} = \kappa \nabla^2 \rho'. \]  

(1.15)
1.2. Theoretical background

If we assume normal mode solutions of the following form,
\[ \psi' = \hat{\phi}(z)e^{i\alpha(x-ct)}, \quad \rho' = \hat{\rho}(z)e^{i\alpha(x-ct)}, \quad \text{and} \quad p' = \hat{p}(z)e^{i\alpha(x-ct)}, \quad (1.16) \]
where \( \alpha \) is the wavenumber and is real because the flow is unbounded in \( x \) direction. \( c \) can be complex and we denote it by \( c_r + ic_i \). The real part of \( c, c_r \), is phase speed, while the product of its imaginary part \( c_i \) with \( \alpha, \alpha c_i \), is growth rate. If \( c_i \) is negative, the perturbation is stable and decreases exponentially. However, if \( c_i \) is positive, the perturbation is unstable and grows exponentially. Substituting in normal mode solutions, equation (1.13), (1.14), and (1.15) become
\[ (U - c)\frac{d^2}{dz^2} - \frac{\rho_0}{\rho_1} - \partial^2 U \frac{\partial}{\partial z^2} \hat{\phi} = \frac{g}{\rho_0} \hat{\rho} + \frac{\nu}{i\alpha}(\frac{d^2}{dz^2} - \alpha^2)\hat{\rho}, \quad (1.17) \]
\[ \alpha^2(U - c)\hat{\phi} = \frac{g}{\rho_0} \hat{\rho} + \frac{\nu}{i\alpha}(\frac{d^2}{dz^2} - \alpha^2)\hat{\rho}, \quad (1.18) \]
\[ (U - c)\hat{\rho} + \frac{\rho_0}{g} N^2 \hat{\phi} = \frac{\kappa}{i\alpha}(\frac{d^2}{dz^2} - \alpha^2)\hat{\rho}. \quad (1.19) \]
Eliminating pressure \( \hat{p} \) in equation (1.17), we obtain the equation for \( \hat{\phi} \), i.e.,
\[ (U - c)(\frac{d^2}{dz^2} - \alpha^2)\hat{\phi} - \partial^2 U \frac{\partial}{\partial z^2} \hat{\phi} = \frac{g}{\rho_0} \hat{\rho} + \frac{\nu}{i\alpha}(\frac{d^2}{dz^2} - \alpha^2)\hat{\rho}. \quad (1.20) \]

Equation (1.20) and equation (1.19) are viscous diffusive TG equations. They determine the growth rate of each wavenumber mode. Note that the growth rate is in fact not a constant as the shear layer and background density profile are diffusing. During a short time, we can assume viscous diffusive TG equations are correct for a constant \( c \) since diffusion occurs slowly. Also, these two equations cannot be reduced into one equation for \( \hat{\phi} \) due to diffusivity.

If we assume the fluid is inviscid and non-diffusive, equation (1.20) and (1.19) could be reduced to one equation for \( \hat{\phi} \) only, i.e.,
\[ (U - c)(\frac{d^2}{dz^2} - \alpha^2)\hat{\phi} - \partial^2 U \frac{\partial}{\partial z^2} \hat{\phi} - \frac{N^2}{U - c} \hat{\phi} = 0. \quad (1.21) \]
This is the original TG equation.

We non-dimensionalize velocity by a velocity scale \( q \), density by \( \rho_1 \), and length by \( l \), then the viscous diffusive TG equations become
\[ (U^* - c^*)(\frac{d^2}{dz^*2} - \alpha^*2)\hat{\phi}^* - \partial^2 U^* \frac{\partial}{\partial z^*2} \hat{\phi}^* = J\hat{\rho}^* + \frac{1}{Re i\alpha^*}(\frac{d^2}{dz^*2} - \alpha^*2)^2 \hat{\phi}^*, \quad (1.22) \]
1.2. Theoretical background

\[(U^* - c^*) \hat{\rho}^* + \frac{\rho_0^*}{g^*} N^* \alpha^* \hat{\varphi}^* = \frac{1}{RePr} \frac{1}{i \alpha^*} \left( \frac{d^2}{dz^*} - \alpha^2 \right) \hat{\rho}^*, \quad (1.23)\]

where variables with * are dimensionless variables, \(Re = ql/\nu\), \(Pr = \nu/\kappa\), and \(J = \rho_1 gl/\rho_0 q^2\). \(J\) is the bulk Richardson number and measures the importance of stratification to the shear.

The growth rate and phase speed of each mode can be predicted by the TG equations once background velocity and density profiles are known. For this thesis, hyperbolic tangent velocity and density profiles are used as the initial background flow as in Hazel (1972), i.e.,

\[U = \frac{\Delta U}{2} \tanh \left( \frac{2z}{h_0} \right) \quad \text{and} \quad \tilde{\rho} = -\frac{\Delta \rho}{2} \tanh \left( \frac{2z}{\delta_0} \right), \quad (1.24)\]

where \(h_0\) is the thickness of the shear and \(\delta_0\) is the thickness of the density stratification. In this thesis, we only consider the case where \(\delta_0 = h_0\). We use \(\Delta U\), \(\Delta \rho\), and \(h_0\) as velocity, density, and length scales to non-dimensionalize field variables, therefore

\[Re = \frac{\Delta U h_0}{\nu} \quad \text{and} \quad J = \frac{\Delta \rho g h_0}{\rho_0 \Delta U^2}. \quad (1.25)\]

We fix Reynolds number \(Re\) at 1200, bulk Richardson number \(J\) at 0.07, and vary \(Pr\) varying from 1 to 64. This combination of parameters allows KH instabilities and vortex pairing. The growth rate as a function of wavenumber is almost independent of \(Pr\) and it is shown in figure 1.1 for \(Re = 1200\), \(Pr = 1\), and \(J = 0.07\). When \(\alpha h_0/2\) is between 0 and 1, the perturbation is unstable. The most unstable mode occurs at \(\alpha h_0/2 = 0.435\) with growth rate 0.14. The phase speed for this wavenumber is zero and therefore the most unstable mode is stationary.

Although linear modal stability theory gives the correct prediction of the most unstable mode’s wavenumber, it only considers the perturbations where time \(t\) and vertical coordinate \(z\) can be separated. In general the stability problem is an initial value problem and cannot be reduced to an eigenvalue problem. Also, the growth rate is a function of time. Whether the most unstable mode predicted by modal theory is the most unstable one for all possible perturbations needs to be answered by non-modal stability theory.

1.2.2 Linear non-modal stability theory

The drawbacks of linear modal stability theory are it only considers a special class of perturbation and does not explain the physical mechanism of instabilities. Farrell & Ioannou (1996) and Schmid & Henningson (2012) established a generalized stability theory for non-modal perturbations. Constantinoul & Ioannou (2011) applied the theory to show there is potential for large transient growth even if the background flow is stable for normal mode
1.3 Nonlinear evolution of KH instabilities

Linear theory is successful when perturbation is small. However, it soon breaks up when non-linear effects become non-negligible. To study the non-linear evolution of KH instabilities, researchers have carried out laboratory experiments (e.g. Thorpe, 1971; Winant & Browand, 1974; Koop & Brownad, 1979; Ho & Huang, 1982) and numerical simulations (e.g. Corcos & Sherman, 1976; Moser & Rogers, 1993; Caulfield & Peltier, 2000; Smyth...
et al., 2001; Mashayek & Peltier, 2012; Salehiour & Peltier, 2015b) in both homogeneous and stratified shear flows. In this section, we give a brief introduction to the non-linear evolution of KH instabilities in stratified fluids.

Figure 1.2: Snapshots of density field at non-dimensional time (a) $t^* = 75$, (b) $t^* = 107$, (c) $t^* = 200$, (d) $t^* = 400$ for a simulation with $Re = 1200$, $Pr = 16$, and $J = 0.07$.

KH instabilities typically evolve through four stages. During the first stage, the primary instability, i.e. KH instability, grows and saturates. It has been shown that this stage is almost two-dimensional (Caulfield & Peltier, 2000). The kinetic energy of the perturbation quickly increases as mean kinetic energy transfers energy to it through shear production. The potential energy of the system also increases through buoyancy flux. The density field during this stage is shown in figure 1.2 (a).

During the second stage, secondary instabilities grow and lead to the transition to turbulence. Different secondary instabilities may appear or dominate depending on Reynolds number $Re$, Prandtl number $Pr$, or bulk Richardson number $J$. Most secondary instabilities are three-dimensional, e.g. the convective core instability (e.g. Caulfield & Peltier, 2000; Klaassen & Peltier, 1985) and braid instabilities (Mashayek & Peltier, 2012). The convective core instability occurs for the parameters chosen in this thesis. Besides three-dimensional secondary instabilities, there is a widely known two-dimensional secondary instability, i.e. vortex pairing. Whether vortex pairing occurs depends on the competition between this
secondary instability and three-dimensional secondary instabilities. Vortex pairing has been observed in both experiments (see Thorpe, 1971; Winant & Browand, 1974; Koop & Brownad, 1979; Ho & Huang, 1982) and three-dimensional simulations (see Moser & Rogers, 1993; Smyth & Moum, 2000; Smyth et al., 2001; Rahmani et al., 2014). Figure 1.2 (b) shows the density field of a simulation during this stage when vortex pairing occurs. If three-dimensional secondary instabilities have a higher growth rate than vortex pairing and destroy the KH billows, vortex pairing does not occur. However, if vortex pairing grows much quicker than other three-dimensional secondary instabilities, two KH billows merge and Reynolds number is increased due to the increasing length scale of the large scale motion (Moser & Rogers, 1993). During this stage, three-dimensionality becomes observable.

During the third stage, the flow becomes highly turbulent and KH billows no longer exist. A snapshot of the density field during this stage is shown in figure 1.2 (c). Most of mixing occurs during this stage (Caulfield & Peltier, 2000; Rahmani et al., 2014) because small scale motions are prevalent in the middle of the shear layer. As a result, potential energy increases significantly. However, turbulence cannot be sustained and gradually decays. When the turbulence intensity, measured by buoyancy Reynolds number $Re_b$, becomes small, the active turbulent stage ends.

During the fourth stage, three-dimensional motions are weak and the flow gradually returns to a laminar state (see figure 1.2 (d)). Potential energy and mean kinetic energy become approximately constant. Both the thickness of velocity and density profiles are higher compared to the initial state. Also, the flow becomes more stable than the initial state.

### 1.4 Mixing efficiency

The quantification of turbulent diffusivity, $\kappa_\rho$, plays an important role in turbulent modeling of stratified flows. Osborn (1980) derived a formula relating turbulent diffusivity to dissipation rate of turbulent kinetic energy by assuming homogeneous and stationary turbulence, i.e.,

$$\kappa_\rho = \Gamma \frac{\varepsilon'}{N^2}, \quad \Gamma = \frac{R_f}{1 - R_f} \tag{1.26}$$

where $R_f$ is flux Richardson number (a measure of mixing efficiency) and defined as the ratio of buoyancy flux $b$ to shear production $P$ (Kundu & Cohen, 2008). $\Gamma$ is the flux coefficient and is usually assumed to be 0.2 in physical oceanography. However, turbulence in nature is always inhomogeneous and non-stationary (Ivey et al., 2008). Also, studies have found that $R_f$ depends on stratification (Rehmann & Koseff, 2004), turbulence intensity (Gargett, 1988; Caulfield & Peltier, 2000; Barry et al., 2001; Salehiour & Peltier, 2015b;
1.5. Objectives

Salehiour et al., 2016), and Prandtl number (Barry et al., 2001; Smyth et al., 2001; Rahmani et al., 2016; Salehiour & Peltier, 2015b).

Shih et al. (2005) extended the the definition of flux Richardson number to non-stationary turbulence by defining $R_f$ as,

$$R_f = \frac{b}{b + \varepsilon'},$$

(1.27)

and found the relation between flux coefficient $\Gamma$ and buoyancy Reynolds number $Re_b$ in uniformly stratified homogeneous turbulent flows. However as Smyth & Moum (2000) pointed out, mixing efficiency in uniformly stratified turbulence is different from that in non-uniformly stratified turbulence and Venaille et al. (2017) verified mixing efficiency does rely on the stratification profile. Also, the definition in Osborn (1980) and Shih et al. (2005) does not distinguish the irreversible mixing from the reversible mixing which can be returned to kinetic energy (Winters et al., 1995). To avoid this problem, Salehiour & Peltier (2015a) defined turbulent diffusivity using the irreversible flux defined in Winters et al. (1996) and background density profile. By doing this, Salehiour & Peltier (2015b) connects turbulent diffusivity to irreversible mixing efficiency commonly used in numerical studies. Moreover, Salehiour et al. (2016) created a contour plot of the irreversible mixing efficiency as a function of buoyancy Reynolds number and stratification. However, the difficulty of this new diffusivity is that it is not easy to compute. Also, the effect of Prandtl number has not been included.

1.5 Objectives

The objective of this thesis is to investigate the effects of initial conditions and Prandtl number on vortex pairing and mixing in KH instabilities. $Re = 1200$ and $J = 0.07$ are chosen to allow vortex pairing and the length of the computation domain is two wavelengths of the KH instabilities. Chapter 2 focuses on the effect of initial condition on vortex pairing and mixing. Random perturbations are used to simulate unforced KH instabilities. Vortex pairing and mixing initialized by the same structure and amplitude random perturbations with different phase of the subharmonic mode are compared. A few additional simulations are initialized by eigenfunctions to viscous diffusive TG equations as a comparison with random perturbed simulations. Chapter 3 investigates the effect of Prandtl number on vortex pairing and mixing properties.
Chapter 2

Sensitivity of vortex pairing and mixing to initial conditions

2.1 Introduction

Fluids are often stratified in nature due to temperature or salinity, or both. The existence of shear may give rise to instabilities in these otherwise stably stratified flows. Kelvin-Helmholtz (KH) instabilities, also called Rayleigh instabilities in homogeneous fluids, are one of the most widely known shear instabilities. KH instabilities have been studied extensively in both homogeneous and stratified fluids using laboratory experiments (e.g. Thorpe, 1973; Browand & Winant, 1973; Winant & Browand, 1974), field observations (Seim & Gregg, 1994; Moum & Farmer, 2003; Geyer et al., 2010), and numerical simulations (e.g. Patnaik et al., 1976; Klaassen & Peltier, 1985; Caulfield & Peltier, 2000; Mashayek & Peltier, 2012, 2013; Rahmani et al., 2014). They are characterized by stationary two-dimensional periodic elliptic vortices called KH billows, which are connected by thin tilted braids of high strain rate (Corcos & Sherman, 1976).

When KH instabilities reach maximum amplitude (saturate), they are susceptible to several secondary instabilities, e.g. vortex pairing (Browand & Winant, 1973; Winant & Browand, 1974; Koop & Browand, 1979; Ho & Huang, 1982), convective core instability due to the overturn of fluid caused by the roll-up (e.g. Klaassen & Peltier, 1985; Caulfield & Peltier, 2000), and instabilities that are located in braid regions and extract energy from the mean shear or strain (see Mashayek & Peltier, 2012). Which secondary instabilities exist or dominate depends on non-dimensional parameters governing the flows, i.e. Reynolds number, Richardson number, and Prandtl number. In low to intermediate Reynolds number flows, vortex pairing is a dominant two-dimensional secondary instability. It can increase the vertical scale of motion and thickness of the shear layer (Corcos & Sherman, 1984; Smyth & Peltier, 1993). As a result, the effective Reynolds number is also increased. Since the amount of mixing and mixing efficiency are higher for higher Reynolds numbers in the mixing transition regime (Rahmani et al., 2014), vortex pairing is an efficient way to enhance mixing and mixing efficiency. The dominant three-dimensional secondary instability in this Reynolds number regime is the convective core instability (Klaassen & Peltier, 1985;
2.1. Introduction

Caulfield & Peltier (2000). Caulfield & Peltier (2000) show that the growth rate of the convective core instability mainly comes from the mean shear, while the two-dimensional KH instability acts as a catalyst in the sense that it provides the flow on which the secondary instability grows. This competition of vortex pairing and three-dimensional secondary instabilities determines whether vortex pairing occurs or not. The competition is dependent on the initial non-dimensional parameters, and also on the details of the initial perturbations (Caulfield & Peltier, 2000; Metcalfe et al., 1987), e.g. the amplitudes of KH, the subharmonic components, and three-dimensional motions.

Some researchers have studied the dependence of secondary instabilities on initial conditions in shear layers without density stratification, for example Patnaik et al. (1976), Ho & Huang (1982), Ho & Huerre (1984), and Metcalfe et al. (1987). Patnaik et al. (1976) show that shredding replaces pairing when the KH and the subharmonic modes are completely out of phase. One vortex is strengthened and the other is weakened in that case. However, shredding is seldom observed in experiments due to the existence of ambient noise other than pure eigenfunctions of the Orr-Sommerfeld equation. Ho & Huang (1982) study the spreading rate of a spatially varied shear layer under different forcing. They show that perturbing the flow with different frequencies can change the the number of vortices merging together and the spreading rate of the shear layer. They also show that the subharmonic mode of the most unstable mode is necessary for pairing, otherwise pairing is significantly delayed. Metcalfe et al. (1987) study the effect of the most unstable mode, the subharmonic mode, and one three-dimensional mode in initial perturbations on primary and secondary instabilities of homogeneous shear flows using numerical simulations. Their results show that vortex pairing can suppress the modal growth rate of a three-dimensional mode when the subharmonic mode reaches finite amplitude and the three-dimensional mode is small. However, one should be careful that this may be only valid for flows initialized by eigenfunctions of certain amplitude.

Numerical investigations of shear instabilities in stratified flows have also found that vortex pairing depends on initial conditions, e.g. Klaassen & Peltier (1989) and Smyth & Peltier (1993). Klaassen & Peltier (1989) obtain the amplitude ratios of the first three harmonics (with wavenumber $\frac{1}{2} \alpha_{kh}$, $\alpha_{kh}$, and $\frac{3}{2} \alpha_{kh}$ where $\alpha_{kh}$ is the wavenumber of the most unstable mode predicted by the Taylor-Goldstein equation) in a two-wavelength domain from a numerical simulation perturbed by white noise. They employ these three modes to study the impact of the phase of the subharmonic and third harmonic mode on vortex pairing for two-dimensional flows. Their results demonstrate that pairing is delayed and the growth rate of the subharmonic mode is decreased if the subharmonic and the third modes are out of phase relative to KH instabilities. However, the time of vortex pairing may be sensitive to the $\frac{3}{2} \alpha_{kh}$ mode if the subharmonic mode is out of phase. Smyth &
2.1. Introduction

Peltier (1993) show similar results in two-dimensional simulations.

The effects of initial perturbations on vortex pairing and mixing in stratified shear flows warrants further investigation. In the present study, we investigate how vortex pairing is influenced by the phase difference of the subharmonic component relative to KH component and extend the study of pairing to three-dimensional flows, by carrying out eight numerical simulations with a variety of initial perturbations. We also investigate whether initial non-modal growth of these two modes, or the existence of other modes in the initial perturbations, affects vortex pairing and mixing properties.

There are four types of perturbations commonly used to excite primary and secondary instabilities in numerical simulations of stratified shear flows. The first type is pure two-dimensional eigenfunctions (e.g. Patnaik et al., 1976; Klaassen & Peltier, 1989). This type is usually used for two-dimensional simulations. The second type of perturbation is a combination of the eigenfunction of the most unstable mode and a smaller amplitude random noise to excite secondary instabilities (e.g. Smyth & Peltier, 1993; Caulfield & Peltier, 2000; Mashayek & Peltier, 2012; Rahmani et al., 2014; Salehiour & Peltier, 2015; Rahmani et al., 2016). An implicit assumption of this type of perturbation is that the KH mode dominates initially and three-dimensional perturbations grow linearly while KH instabilities saturate.

The third type of perturbations is a combination of sinusoidal waves of wavenumbers $\alpha_{kh}$ and $\frac{1}{2}\alpha_{kh}$ with vertical exponential decay, and random noise (e.g. Smyth & Moum, 2000; Smyth & Winters, 2003; Alexakis, 2009). The fourth type is pure random noise (e.g. Carpenter et al., 2010; Mashayek & Peltier, 2013). The present study was motivated by the observation that two sets of small random perturbations, that are generated by the same random number generator with different seeds, can trigger very different flows, i.e. vortex pairing occurs in one simulation but not in the other simulation. To verify the conjecture that if the subharmonic mode is out of phase relative to KH mode vortex pairing may not occur, we conduct numerical simulations where the background flow is perturbed by the same pure random number perturbations with differing phase of the subharmonic mode. We also compare flows perturbed by pure random perturbations with flows perturbed by eigenfunctions.

The numerical methods and diagnostic tools are described in section 2.2. A simplified pairing mechanism is described in section 2.3. Section 2.4 describes the process of vortex pairing and the growth rate of the subharmonic mode in two-dimensional simulations. In section 2.5, three-dimensional results are compared with two-dimensional results and mixing is compared in different simulations.
2.1. Introduction

Figure 2.1: Vorticity snapshots of two-dimensional simulations $R02D$ (left panel, phase of the subharmonic mode is $\theta_{sub}^M \approx 0$) and $R\pi/2 2D$ (right panel, phase of the subharmonic mode is $\theta_{sub}^M \approx -\pi/2$). The snapshots labeling with 3D are vorticity field of simulations $R03D$ (left) and $R\pi/2 3D$ (right) at $y = \frac{L_y}{2}$. Pairing is delayed in two-dimensional simulation $R\pi/2 2D$ but completely eliminated in the three-dimensional simulation $R\pi/2 3D$. Black circles are fluid particles located at vortex centers at $t = 30$. 
2.2 Methodology

2.2.1 Mathematical model

Hyperbolic tangent functions are used for the background velocity and density profiles, as first introduced by Hazel (1972),

\[
\dot{\rho} = -\frac{\Delta \rho}{2} \tanh \left( \frac{2z}{\delta_0} \right) \quad \text{and} \quad U = \frac{\Delta U}{2} \tanh \left( \frac{2z}{h_0} \right),
\]

where \( \delta_0 \) is the thickness of the density interface and \( h_0 \) is the thickness of the velocity interface. Four non-dimensional parameters characterize the flows, i.e. bulk Richardson number \( J \), Reynolds number \( Re \), Prandtl number \( Pr \), and the scale ratio \( R \) which are defined as

\[
J = \frac{\Delta \rho g h_0}{\rho_0 (\Delta U)^2}, \quad Re = \frac{\Delta U h_0}{\nu}, \quad Pr = \frac{\nu}{\kappa}, \quad R = \frac{h_0}{\delta_0}.
\]

In this study, \( J = 0.07 \), \( Re = 1200 \), \( Pr = 16 \), \( R = 1 \). The flow is susceptible to Kelvin-Helmholtz instabilities for this combination of \( J \) and \( R \) (see Smyth & Winters, 2003, for a review of instability types).

We assume the fluid is incompressible and apply the Boussinessq approximation, so the governing equations for the system are

\[
\nabla \cdot \mathbf{u} = 0,
\]

\[
\frac{D\mathbf{u}}{Dt} = -\frac{1}{\rho_0} \nabla p - \frac{\rho}{\rho_0} g \hat{k} + \nu \nabla^2 \mathbf{u},
\]

\[
\frac{D\rho}{Dt} = \kappa \nabla^2 \rho,
\]

where \( \kappa \) is molecular diffusivity, \( \nu \) is kinetic viscosity, \( \rho_0 \) is a reference density, and \( \hat{k} \) is the unit vertical vector.

2.2.2 Direct Numerical Simulations

The governing equation (2.3), (2.4), and (2.5) are solved by a pseudo-spectral code developed by Winters et al. (2004) and later improved by Smyth et al. (2005). The code employs the third order Adams-Bashforth time stepping scheme. Boundary conditions are horizontally periodic and vertically free slip and no flux for our simulations.

The resolution of DNS is typically determined by the Kolmogrov scale, \( L_k = (\nu^3/\varepsilon')^{1/4} \), in homogeneous fluids where \( \varepsilon' \) is viscous dissipation rate of turbulent kinetic energy. Moin & Mahesh (1998) suggest that the grid spacing in DNS should be \( O(L_k) \). In stratified flows with \( Pr > 1 \), the smallest scale that needs to be resolved is the Batchelor scale (Batchelor,
2.2. Methodology

Rey  Pr  J  Lx/h0  Ly/h0  Lz/h0  Nx  Ny  Nz
1200  16  0.07  14.43  7.22  15  320  160  320

Table 2.1: Numerical parameters for all the simulations. The number of grid points is for the velocity field and is half that of the density field.

1959), \( L_B = L_k / \sqrt{Pr} \). In our simulations, \( \Delta z/L_B \) is always less than 4.0 and \( \Delta z/L_K \) is always less than 2.0 (\( \Delta z \) of the density field is half of the velocity field.). The dissipation rate \( \epsilon' \) used to calculate \( L_K \) is averaged within the initial shear layer \(-h_0/2 < z < h_0/2\) where turbulence is the most energetic. The domain length \( L_x \) is set to two wavelengths of the most unstable mode to allow vortex pairing. The spanwise width of the domain \( L_y \) for the three-dimensional simulations is one wavelength of the primary KH instability, which is at least six wavelengths of most unstable spanwise mode (for the most unstable spanwise wavenumber see Klaassen & Peltier, 1989). The height is \( 15h_0 \) which is sufficient to remove the effects of the horizontal boundaries. The numerical details are summarized in table 2.1.

We ran two sets of simulations to study the effect of initial perturbations on vortex pairing and mixing. One set is perturbed by random perturbations, three of them are two-dimensional and three of them are three-dimensional simulations. The other set is perturbed by eigenfunctions of KH and the subharmonic modes with the same amount of kinetic energy (defined in equation (2.13)) as in random perturbation simulations. The eigenfunction simulations are performed in two dimensions only. All simulations are listed in table 2.2.

For random perturbation simulations, inherently three dimensional random perturbations of \( u' \) and \( w' \) are added to the background flow to excite instabilities in three-dimensional simulations. They are given by the following equations,

\[
u' = cr_u(x, y, z) \frac{\Delta U}{2} \left( 1 - \left| \tanh \left( \frac{2z}{h_0} \right) \right| \right), \tag{2.6}
\]

\[
w' = cr_w(x, y, z) \frac{\Delta U}{2} \left( 1 - \left| \tanh \left( \frac{2z}{h_0} \right) \right| \right), \tag{2.7}
\]

where \( r_u \) and \( r_w \) are random numbers between -1 and 1, and \( c \) sets the maximum amplitude of perturbations. In the present study, \( c = 0.1 \), which is the same magnitude as in the simulations of Smyth & Winters (2003) and Carpenter et al. (2010), and small enough for perturbations to grow linearly initially. To study the effects of the phase of the subharmonic component, these simulations are initialized by the same perturbations except that the phase of the subharmonic mode is changed. The initial conditions in two-dimensional simulations
2.2. Methodology

are spanwise averaged values of those in corresponding three-dimensional simulations.

The phase of each wavenumber component is defined in terms of two-dimensional vertical velocity $w_{2d}$, i.e.,

$$A \sin \left( k \frac{2\pi}{L_x} x + \theta_k \right) = \Re \left\{ e^{ikax} \hat{w}_{2d,k} \left( z = \frac{L_z}{2} \right) \right\}, \quad (2.8)$$

where $A$ is a real number, $\hat{w}_{2d,k}$ is the $k$th Fourier component of $w_{2d}$. Note that $k = 2$ corresponds to the KH component and $k = 1$ corresponds to the subharmonic component, i.e., a wavelength equal to the domain length, $L_x$. Initially each Fourier component experiences non-modal growth and the phase of every component defined in equation (2.8) changes. When the subharmonic component becomes approximately modal, i.e., identical to the eigenfunction of the Taylor-Goldstein equation (this occurs around $t = 24$ for three random perturbation simulations), the phase becomes almost constant for some time until non-linear effects become important. We define $\theta_{\text{sub}}$ as the phase of the subharmonic component relative to the KH component and $\theta_{\text{sub}}^M$ as the phase of the subharmonic component when it becomes modal. We use three different phases in the random perturbation simulations. They are designated $R$ followed by the approximate modal phase $\theta_{\text{sub}}^M$, and 2D or 3D depending on the number of dimensions used in the simulation. For example, $\theta_{\text{sub}}^M$ is approximately $0$, $-\frac{\pi}{4}$, and $-\frac{\pi}{2}$ respectively in three-dimensional simulations $R03D$, $R\frac{\pi}{4}3D$, and $R\frac{\pi}{2}3D$ (exact phase values are listed in table 2.2).

Simulations perturbed by eigenfunctions are named by the same rule, but the first letter is $E$, indicating that they are perturbed by eigenfunctions. For these eigenfunction perturbed simulations, the phase of the subharmonic mode does not change initially and $\theta_{\text{sub}}^M$ is the initial value. $\theta_{\text{sub}}^M = -\frac{\pi}{2}$ for $E\frac{\pi}{2}2D$ and $\theta_{\text{sub}}^M = 0$ for $E02D$.

2.2.3 Diagnostic tools

Hereafter, all results are presented in non-dimensional form. Specifically, velocity is non-dimensionalized by $\Delta U$, density is non-dimensionalized by $\Delta \rho$, length by $h_0$, time by $h_0/\Delta U$, and pressure by $\rho_0(\Delta U)^2$. Following Caulfield & Peltier (2000), the velocity is decomposed into three parts, i.e.,

$$\bar{u} = \langle u \rangle_{xy}, \quad u_{2d} = \langle u \rangle_y - \langle u \rangle_{xy}, \quad u_{3d} = u - \bar{u} - u_{2d}. \quad (2.9a-c)$$

Given these definitions, the total kinetic energy $K$ is defined as

$$K = \frac{\langle u \cdot u \rangle_{xyz}}{2}, \quad (2.10)$$
2.2. Methodology

Random perturbations

<table>
<thead>
<tr>
<th>Run</th>
<th>$R02D$</th>
<th>$R\frac{\pi}{4}2D$</th>
<th>$R\frac{\pi}{2}2D$</th>
<th>$R03D$</th>
<th>$R\frac{\pi}{4}3D$</th>
<th>$R\frac{\pi}{2}3D$</th>
<th>$E02D$</th>
<th>$E\frac{\pi}{2}2D$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t_M$</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$\theta_{sub}/\pi$</td>
<td>0.04</td>
<td>-0.21</td>
<td>-0.46</td>
<td>0.05</td>
<td>-0.21</td>
<td>-0.48</td>
<td>0</td>
<td>0.5</td>
</tr>
<tr>
<td>$t_{kh}$</td>
<td>80</td>
<td>82</td>
<td>85</td>
<td>80</td>
<td>81</td>
<td>84</td>
<td>81</td>
<td>87</td>
</tr>
<tr>
<td>$t_{sub}$</td>
<td>106</td>
<td>110</td>
<td>146</td>
<td>107</td>
<td>113</td>
<td>129</td>
<td>104</td>
<td>249</td>
</tr>
<tr>
<td>$t_p$</td>
<td>108</td>
<td>112</td>
<td>148</td>
<td>109</td>
<td>113</td>
<td>-</td>
<td>107</td>
<td>249</td>
</tr>
<tr>
<td>$t_{3d}$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>143</td>
<td>146</td>
<td>123</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$t_f$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>221</td>
<td>214</td>
<td>187</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$M(t = 400)/K_0$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.072</td>
<td>0.068</td>
<td>0.036</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$E_c(t = t_f)$</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.229</td>
<td>0.223</td>
<td>0.198</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 2.2: The simulations beginning with $E$ are perturbed by eigenfunctions, while those beginning with $R$ are perturbed by the same random perturbations except different phases of the subharmonic mode. The kinetic energy of KH and the subharmonic modes in eigenfunction simulations are the same as in random perturbation simulations. $t_{kh}$, $t_{sub}$, and $t_p$ are defined in section 2.4. $t_{3d}$, $t_f$ and $E_c$ are defined in section 2.5.

and can be partitioned into three parts $\overline{K}$, $K_{2d}$, $K_{3d}$, i.e.,

$$K = \overline{K} + K_{2d} + K_{3d},$$

(2.11)

where

$$\overline{K} = \frac{\left\langle \mathbf{u} \cdot \mathbf{u} \right\rangle}{2}, \quad K_{2d} = \frac{\left\langle \mathbf{u}_{2d} \cdot \mathbf{u}_{2d} \right\rangle_{xz}}{2}, \quad K_{3d} = \frac{\left\langle \mathbf{u}_{3d} \cdot \mathbf{u}_{3d} \right\rangle_{xyz}}{2},$$

(2.12a–c)

and the subscripts indicate averaging over that direction.

Fourier transforms are applied to $u_{2d}$ and $w_{2d}$ in order to identify the contribution of each wavenumber component to the total $K_{2d}$, so that the kinetic energy of the $k$th component is

$$K_{2d,k} = \left\langle |\hat{u}_{2d,k}|^2 + |\hat{w}_{2d,k}|^2 \right\rangle_{xz}, \quad k \geq 1$$

(2.13)

where $\hat{u}_{2d,k}$ and $\hat{w}_{2d,k}$ are the Fourier components of $u_{2d}$ and $w_{2d}$ of wavenumber $2\pi k/L_x$. Hence,

$$K_{2d} = \sum_{k=1}^{N_x} K_{2d,k}.$$  (2.14)

Note that $k = 1$ corresponds to the subharmonic component and we denote it as $K_{sub}$.  


2.3 Pairing mechanism

Before discussing results, we first illustrate the vortex pairing mechanism in figure 2.2 using the vertical velocity of the KH instability (blue) and subharmonic mode (red). This figure shows two cases with the phase equal to 0 and $-\frac{\pi}{2}$. The circles represent core centers associated with KH instabilities and the squares are potential vortex cores associated with the subharmonic mode. The arrows show the direction of the mean flow. In figure 2.2 (a), the phase of the subharmonic mode $\theta_{\text{sub}} = 0$ and its associated core center is at the centre of two KH billows. The subharmonic mode displaces the left KH billow upward and the right KH billow downward. The two KH billows are then advected toward each other by the mean flow, cross each other, and merge into one larger billow. This is the optimal phase for pairing. In figure 2 (b), the phase of the subharmonic mode is $\theta_{\text{sub}} = -\frac{\pi}{2}$ and two KH core centers are at the nodes of the subharmonic mode. The phase of the subharmonic mode needs to shift towards 0 or $\pi$ to impose a vertical velocity at the two KH core centers for vortex pairing to occur. As a result, pairing is delayed until this shift occurs.

$k = 2$ corresponds to KH instability and we denote it as $K_{kh}$. These two components of the kinetic energy characterize the kinetic energy of the primary and subharmonic components.
2.4 Two-dimensional results

2.4.1 Degree of modality

In the randomly perturbed simulations, initially the subharmonic component experiences non-modal growth. We use the Hermitian angle (Scharnhorst, 2001) between the subharmonic component \( \hat{w}_{2d, sub} \) and the initial eigenfunction of the subharmonic mode \( \hat{w}_{eig, sub} \) to measure the degree of modality, i.e.,

\[
r(t) = \frac{\left| \sum_{k=1}^{Nz} \hat{w}_{2d, sub}^* \hat{w}_{eig, sub} \right|}{\sqrt{\sum_k |\hat{w}_{2d, sub}|^2 \sum_k |\hat{w}_{eig, sub}|^2}} \tag{2.15}
\]

where * denotes the complex conjugate and || denotes the amplitude of a complex number. This Hermitian angle \( r(t) \) is the ratio between the length of the orthogonal projection of the subharmonic component onto the eigenfunction to the length of itself. It is always between 0 and 1, and \( r = 1 \) only when the subharmonic component of the random perturbation is identical to the eigenfunction.

Figure 2.3 shows the evolution of \( r \) for the three random perturbation simulations \( R02D, R_{\pi/4}2D, \) and \( R_{\pi/2}2D \). Initially, \( r \) is close to zero because the subharmonic component of the initial random perturbations is significantly different from the eigenfunction. However, as the subharmonic component evolves to the eigenfunction, \( r \) increases to 1. We define the time required for the subharmonic component to become modal, \( t_M \), as the time when \( r \) first exceeds 0.99, which is when \( t = 24 \) for these three simulations. Note that before \( t = 24 \), the three simulations are evolving linearly and therefore appear identical in figure 2.3.

2.4.2 Phase evolution

The phases for the five two-dimensional simulations perturbed by either random perturbations or the eigenfunctions are plotted in figure 2.4 (a). Initially, in the eigenfunction perturbation simulations, the phase does not change. In the three random perturbation simulations, before \( t = 25 \), the phases change because of non-modal growth. Since the subharmonic component is growing linearly, the phase differences between any two of the three random perturbation simulations are constant. The phase is not meaningful during this time as the subharmonic component has not become modal and the phase is the phase at the vertical center \( (z = \frac{L_z}{2}) \) of the domain (see equation 2.8). The phase before \( t_M \) is therefore shown as thin lines. Between \( t = 25 \) and \( t = 50 \), the phases stay almost constant. During this period, the phases are approximately \( 0, -\frac{\pi}{4}, -\frac{\pi}{2} \) for \( R02D, R_{\pi/4}2D, \) and \( R_{\pi/2}2D \)
2.4. Two-dimensional results

Figure 2.3: Evolution of $r$ for random perturbation simulations $R02D$, $R_{\pi/4}^\pi 2D$, and $R_{\pi/2}^\pi 2D$.

(see table 2.2). After $t = 50$, the phases of the subharmonic mode in simulations $R_{\pi/4}^\pi 2D$ and $R_{\pi/2}^\pi 2D$ shift toward 0 (figure 2.4 (a)). For the eigenfunction simulation $E_{\pi/2}^\pi 2D$, the phase begins to shift after $t = 200$ and is not shown in this figure.

2.4.3 Lagrangian trajectories

The Lagrangian trajectories of two fluid particles located at the density inflection points at $t = 30$ for $R02D$, $R_{\pi/4}^\pi 2D$, and $R_{\pi/2}^\pi 2D$ are tracked as representatives of KH billow centres. Time $t = 30$ is the earliest time that the vortex centres are identifiable. The trajectories of two fluid particles initially located at $Lx/4, 3Lx/4$ are also tracked for the two eigenfunction simulations, $E02D$ and $E_{\pi/2}^\pi 2D$. The Lagrangian trajectories show good agreement with the paths of inflection points on the $\rho_0$ isopycnal until the two KH billows get close to each other. Figure 2.1 shows the evolution of the vorticity field with the two fluid particles shown as black circles. These two fluid particles approximately represent the vortex centres until small scale motions prevail, e.g. at $t = 146$ for simulation $R02D$.

Figure 2.4 (b) shows the horizontal coordinates of the two fluid particles. Initially the horizontal distance between the two fluid particles for the eigenfunction simulations is almost constant since the KH instabilities are stationary. After approximately $t = 75$, the two fluid particles quickly converge for the optimal phase simulation $E02D$. When the horizontal distance becomes zero, one fluid particle (billow) is on top of the other. This time is defined as the time of pairing, $t_p$, and listed in table 2.2 (for three-dimensional simulations, $t_p$ is obtained by averaging two sets of trajectories each composed of 21 fluid particles spread over the spanwise direction). The two vortices become closer and merge in simulation $E_{\pi/2}^\pi 2D$, but only at $t = 249$ (see table 2.2) because the phase needs to shift.
Figure 2.4: (a) Evolution of the phase of the subharmonic mode. The phase before $t_M$ is shown as thin lines. The phase shift toward 0 in simulation $E\frac{\pi}{2}2D$ begins after $t = 150$ and is not shown in this figure. (b) $x$ coordinates of two fluid particles located at two vortex centers at $t = 30$ for random perturbation simulations or located at $L_x/4$ and $3L_x/4$ initially for eigenfunction perturbation simulations. Pairing occurs at $t = 249$ for simulation $E\frac{\pi}{2}2D$ and is not shown in this figure (see table 2.2). (c) Growth rate of the subharmonic mode. The vertical dashed line indicates the saturation time of KH instabilities in simulation $R\frac{\pi}{4}2D$. 

2.4. Two-dimensional results
toward the optimal value and pairing is delayed. Unlike the results of the eigenfunction simulations, in the random perturbation simulations there is an oscillation of the fluid particles. For these three simulations, the distance between two fluid particles is always the smallest for $R02D$ and largest for $R\pi2D$. Also, pairing occurs first in $R02D$ and last in $R\pi2D$, so $t^R02D_p < t^R\pi2D_p < t^R\pi2D$. Relating figure 2.4 (b) with the phase evolution in figure 2.4 (a), we find that two fluid particles begin to move together when the phase approximately stops changing. Therefore, pairing occurs earliest if the subharmonic is in phase and latest if it is out of phase. $t^R\pi2D_p$ is just slightly larger than $t^R02D_p$, which suggests that if the subharmonic mode is not close to being out of phase, the difference caused by the phase is small. Also, the time of pairing for simulation $R02D$ is close to $E02D$, but pairing happens much earlier for simulation $R\pi2D$ than $E\pi2D$. Hence, the existence of the other components in initial perturbations does not affect the time of pairing if the phase is optimal. However, if the subharmonic mode is close to $\pm\pi2$, the time of pairing is sensitive to initial perturbations, e.g. the existence of the other components or whether the subharmonic component is exactly the eigenfunction.

### 2.4.4 Growth rate

In this section, we discuss temporal changes in the kinetic energy of the subharmonic component. Figure 2.4 (c) shows the growth rate for three random perturbation simulations and two eigenfunction simulations. $t_{kh}$ is defined as the time when $K_{kh}$ (the 2D kinetic energy of the KH mode) reaches its first maximum, also called saturation time. This occurs at approximately $t = 81$ with slight variations for all simulations (see table 2.2). The vertical dashed line in this figure indicates $t_{kh}$ for $R\pi2D$.

Initially, the growth rates of the subharmonic mode for the two eigenfunction simulations ($E02D$ and $E\pi2D$) are the same and decline as the shear layer diffuses. The estimated growth rate using the viscous diffusive Taylor-Goldstein equation and the mean flow has the same decreasing trend as the growth rates based on $K_{2d,sub}$ (the 2D kinetic energy of the subharmonic mode). For the random perturbation simulations ($R02D$, $R\pi2D$, and $R\pi2D$), the growth rate during the non-modal stage of growth can be either smaller or larger than the modal growth rate as shown by Guha & Lawrence (2014). For all five simulations, the growth rate is independent of the phase in the initial linear stage of growth, i.e. before around $t = 45$.

After around $t = 45$, non-linear effects and the phase become important. After $t = 45$ and before $t_{kh}$, the growth rates in the late pairing simulations ($E\pi2D$ and $R\pi2D$) significantly drop compared to the other simulations, which is consistent with the simulations of Klaassen & Peltier (1989). The growth rate in the $R\pi2D$ simulation stays closer to the earlier pairing simulations $R02D$ and $E02D$. Therefore the subharmonic mode is only sup-
pressed if the phase is close to $\pm \frac{\pi}{2}$. The growth rates in simulations $R02D$ and $E02D$ are almost the same and the growth rates in simulations $R\frac{\pi}{2}2D$ and $E\frac{\pi}{2}2D$ are almost the same. This suggests that if the phase and amplitude of the subharmonic and KH are the same for an eigenfunction perturbation and a random perturbation, the growth of the subharmonic mode is the same before saturation of KH instabilities. In other words, the existence of the other components in initial perturbations and initial non-modal growth have negligible effects on the growth rate during this non-linear growth stage.

At saturation of KH, in $R02D$, $R\frac{\pi}{4}2D$, and $E02D$, the phase is close to optimal. The growth rates then quickly decrease to zero. In these three simulations, the first zero crossing of the growth rate is close to $t_p$ and denotes the saturation of the subharmonic mode, i.e. the global maximum of $K_{\text{sub}}$.

In $R\frac{\pi}{2}2D$, after $t_{kh}$ the growth rate begins to increase. This coincides with the phase shift toward the optimal value (see figure 2.4 (a)). In this simulation, the saturation of the subharmonic mode occurs much later at $t = 146$. In $E\frac{\pi}{2}2D$, the phase remains at $-\frac{\pi}{2}$ and the growth rate continues to decrease. Unlike the other simulations, the growth rate crosses zero before saturation of the subharmonic mode (at $t = 249$). Comparison between simulations $R02D$, $R\frac{\pi}{4}2D$, and $E02D$ shows that the growth rate is almost the same even until pairing as long as the phase is not close to $-\frac{\pi}{2}$. However, comparison between simulations $R\frac{\pi}{2}2D$ and $E\frac{\pi}{2}2D$ shows that the growth rate is sensitive to the exact form of the subharmonic itself or the existence of the other components in initial conditions.

In table 2.2, the saturation times of KH and the subharmonic mode and time of pairing ($t_{kh}$, $t_{\text{sub}}$, and $t_p$) are summarized. Pairing occurs first in simulation $E02D$, second in $R02D$, third in $R\frac{\pi}{4}2D$, fourth in $R\frac{\pi}{2}2D$, and last in $E\frac{\pi}{2}2D$. In all simulations $t_{\text{sub}}$ is close to the time of pairing, $t_p$. Ho & Huang (1982) obtain a similar result qualitatively in their experiments.

### 2.4.5 Visualization of vertical velocity of the subharmonic component

We show the evolution of normalized vertical velocity of the subharmonic component, i.e. $\Re\{e^{i\alpha_{kh}x^2/2\hat{w}_{2d,sub}/(\|\hat{w}_{2d,sub}\|^2)}\}$ at five discrete times in simulations $R02D$ and $R\frac{\pi}{2}2D$ in figure 2.5 to examine its structure change. At $t = 10$, the velocity component still shows some randomness because it has not become modal as indicated in the low value of $r$ in figure 2.3. The structure is the same for two simulations except a phase difference, as the flow is evolving linearly. At $t = 25$, the velocity component looks regular and is almost identical to the eigenfunction (not shown in this figure). Again, it is consistent with the fact that $r$ is more than 0.99. The asymmetry in the velocity component comes from the initial randomness. At $t = 75$ (before $t_{kh}$), the structure does not change much and still stays close to the structure at $t = 25$ in simulation $R02D$. In simulation $R\frac{\pi}{2}2D$, however,
2.4. Two-dimensional results

Figure 2.5: The normalized vertical velocity of the subharmonic component, i.e. $\Re\{e^{i\alpha_k x/2} \hat{w}_{2d,sub}/(|\hat{w}_{2d,sub}|_z)\}$ in two-dimensional simulation $R02D$ (left panel) and simulation $R_{\pi/2}2D$ (right panel).
the velocity component clearly changes its structure and this change is caused by non-linear interaction between different modes. This is also shown by the fact that $r$ hardly changes in simulation $R02D$, but drops in simulation $R\frac{\pi}{2}2D$. Smyth & Peltier (1993) show that the growth rate of the subharmonic component mainly comes from the mean flow even in the nonlinear growth stage before saturation of KH instabilities. Hence, the structure change of the subharmonic velocity component in late pairing simulation $R\frac{\pi}{2}2D$ accounts for the decrease in growth rate shown in figure 2.4 (c), given that the mean flow is almost the same before $t_{kh}$ for two simulations. At $t = 100$, two KH billows start to pair in simulation $R02D$ (see figure 2.4 (b)). The corresponding velocity component becomes slightly deviated from the eigenfunction. This deviation is more significant for $t = 125$. In simulation $R\frac{\pi}{2}2D$, at $t = 100$ the velocity component is significantly different from that at $t = 25$ and so is true for $r$. Correspondingly, the growth rate is still low. At $t = 125$, the structure becomes similar to the eigenfunction again, more accurately the structure at $t = 80$ in simulation $R02D$. This explains the high growth rate at this time shown in figure 2.4 (c).

2.5 Three-dimensional results

2.5.1 Kinetic energy

Kinetic energy of the subharmonic component in two- and three-dimensional random perturbation simulations are compared in figure 2.6 to illustrate the effects of three-dimensional motions on vortex pairing. The peak energy of the subharmonic mode is reduced in all three-dimensional simulations. The kinetic energy of the subharmonic mode, $K_{sub}$, is least affected by three-dimensional motions in the optimal phase simulation, i.e. 0 phase. This is because vortex pairing happens before the three-dimensional motions develop. The saturation time of the subharmonic mode for $R03D$ is almost identical to the $R02D$ simulation (see figure 2.6 (a) and table 2.2). The comparison between $R\frac{\pi}{2}2D$ and $R\frac{\pi}{2}3D$ is similar (see figure 2.6 (b)). Thus when the phase is close to the optimal value, vortex pairing is delayed slightly in three-dimensional simulations.

Vortex pairing does not occur in the three-dimensional simulation $R\frac{\pi}{2}3D$, which is shown in the significant difference between the two lines in figure 2.6 (c). The peak in the three-dimensional kinetic energy in $R\frac{\pi}{2}3D$ is much smaller and occurs earlier (see table 2.2) than the peak in the three-dimensional kinetic energy in $R03D$ and $R\frac{\pi}{2}3D$. During the extra time needed in $R\frac{\pi}{2}3D$ for the phase shift from $-\frac{\pi}{2}$ to $\sim 0$, the three-dimensional motions grow and suppress vortex pairing before it can occur.
2.5. Three-dimensional results

Figure 2.6: Kinetic energy of the subharmonic mode $K_{sub}$ and three-dimensional kinetic energy $K_{3d}$ in two-dimensional and three-dimensional simulations.

2.5.2 Mixing

We follow the framework in Winters et al. (1995) to compare the mixing between simulations. The potential energy is then defined as,

$$ P = g\langle \rho z \rangle_V. \quad (2.16) $$

Potential energy $P$ is partitioned into background potential energy $P_b$ and available potential energy $P_a$ defined as

$$ P_b = g\langle \rho z_b \rangle_V, \quad P_a = P - P_b, \quad (2.17a, b) $$

where $z_b$ is the location of fluid parcels after being re-arranged into a statically stable state (see Winters et al., 1995; Caulfield & Peltier, 2000). Available potential energy characterizes the energy that can be exchanged between potential energy and kinetic energy, while the increase in background potential energy quantifies irreversible mixing in a closed system.

The amount of mixing caused by fluid’s motion is

$$ M = \Delta P_b - \phi t = \int \phi_M dt, \quad (2.18) $$

where $\phi_M$ is the rate of mixing and $\phi_i$ is the mixing caused by molecular diffusion without fluid motion, i.e.,

$$ \phi_i = \frac{-\kappa g (\bar{\rho}_{top} - \bar{\rho}_{bottom})}{L_z}. \quad (2.19) $$
Figure 2.7: (a) The increase in total potential energy $\Delta P$ divided by initial kinetic energy $K_0$, (b) the increase in mixing $M$ divided by initial kinetic energy $K_0$.

Cumulative mixing efficiency (Caulfield & Peltier, 2000) is used as a measure of overall mixing properties in this study. It is defined as

$$E_c = \frac{\int_{t_3d}^{t_f} \phi_M dt}{\int_{t_3d}^{t_f} \phi_M dt + \int_{t_3d}^{t_f} \epsilon dt}, \quad (2.20)$$

where $t_f$ is defined as the time when buoyancy Reynolds number $Re_b = \epsilon'/\nu \langle N^2 \rangle_z$ first drops below 20 after $t_{3d}$. This period is chosen as studies indicate that turbulence is active as long as $Re_b > 20$ (Smyth & Moum, 2000).

Figure 2.7 (a) shows the increase in the total potential energy, $\Delta P$, with time. The first peak in $R03D$ and $R^{\pi/3}3D$ represents vortex pairing and the first peak in $R^{\pi/2}3D$ represents saturation of KH. Time variation of $\Delta P$ is the same for the three simulations before $t = 80$, indicating that the KH instability is independent of the subharmonic mode. The peak due to vortex pairing does not exist for $R^{\pi/2}3D$ since pairing never occurs. Overall, the increase in total potential energy with vortex pairing is much higher than without vortex pairing because vortex pairing efficiently increases the vertical scale of fluid’s motion. The increase in total potential energy in $R^{\pi/2}3D$ is slightly lower than $R03D$.

Figure 2.7 (b) shows the amount of mixing divided by initial kinetic energy for three-dimensional simulations, $M/K_0$. For all simulations, the amount of mixing is negligible before saturation of KH instabilities as the flow is well-organized and mixing is only slightly greater than the mixing due to molecular diffusion. After about $t = 130$, the amount of mixing significantly increases as small scale motions reach sufficient amplitude. As turbulence subsides, the amount of mixing gradually approaches a constant. The difference in
mixing among the three simulations becomes noticeable after about $t = 150$. The amount of mixing in simulation $R03D$ with vortex pairing is higher than simulation $R\pi \times 3D$ without pairing, since vortex pairing increases the amount of stirring. At $t = 400$ the amount of mixing $M/K_0$ in simulation $R03D$ (0.072) is double that of simulation $R\pi \times 3D$ (0.036). Therefore the density interface after re-laminarization is sharper in $R\pi \times 3D$. Mixing in simulation $R\pi \times 3D$ stays close to and is slightly lower than simulation $R02D$. Hence, the amount of mixing is significantly reduced if the subharmonic mode is out of phase and vortex pairing does not occur. If the phase of subharmonic mode relative to KH mode is not close to $\pm \frac{\pi}{2}$, the effect of phase on mixing is small.

Finally the cumulative mixing efficiency defined in equation (2.20) as a measure of mixing efficiency during the active turbulence stage is compared in table 2.2 among the three different initial conditions to obtain the range of mixing efficiency. We find the maximum and minimum cumulative mixing efficiency are 0.229 (with pairing) and 0.198 (without pairing). Eigenfunction simulations with the same phase and amount of three-dimensional motions give the same mixing efficiency. The cumulative mixing efficiency for turbulence caused by shear instabilities is around 0.2 as indicated in many numerical studies (Peltier & Caulfield, 2003). Therefore the strong and weak pairing simulations set the bounds for cumulative mixing efficiency for flows with the same initial non-dimensional parameters and the same amount of perturbation energy.

2.6 Discussion

We find that vortex pairing is sensitive to initial conditions when the phase of the subharmonic mode is close to $\pm \frac{\pi}{2}$. For simplicity in this discussion, we use $t_{sub}$ to characterize the time of pairing. In general, $t_{sub}$ is a function of all modes in initial conditions, not only the subharmonic mode.

We consider the sensitivity of $t_{sub}$ to the phase of the subharmonic mode by running two-dimensional simulations perturbed by KH and the subharmonic mode eigenfunctions. Note that $t_{sub}$ is minimal in simulations with $\theta_{sub}^M = k\pi$, and is maximal when $\theta_{sub}^M = (k + \frac{1}{2})\pi$ where $k$ is an integer. Also, $t_{sub}$ is an even function of $\theta_{sub}^M$ and symmetric about $\theta_{sub}^M = (k + \frac{1}{2})\pi$. We calculate $t_{sub}$ for 12 discrete phases in the range of $-\frac{\pi}{2}$ to 0 and plot the results and the symmetric part between 0 and $\frac{\pi}{2}$ in figure 2.8. The figure shows that the time of pairing is not sensitive to the phase when the phase is close to 0. However, the time of pairing varies significantly near $\theta_{sub}^M = \pm \frac{\pi}{2}$, which indicates that $t_{sub}$ is sensitive to the phase when the phase is close to $\pm \frac{\pi}{2}$. Also, slight deviation from the eigenfunction of the subharmonic mode in initial conditions can also change the time of pairing. Hence, the delay of vortex pairing is sensitive to the functional form of the subharmonic component,
2.7 Conclusions

Two-dimensional and three-dimensional DNSs were performed to investigate the effect of initial conditions on vortex pairing and mixing that are subject to KH instabilities. We focused on the impact of phase of the subharmonic mode on vortex pairing and mixing. In two-dimensional simulations, vortex pairing is delayed if there is a phase difference between KH and the subharmonic mode. This delay is small when the subharmonic mode is slightly out of phase. However, when the phase difference becomes close to $\pm \frac{\pi}{2}$, the delay increases significantly and is also sensitive to the other details of the initial conditions. Comparison between eigenfunction simulations and random perturbation simulations shows that the response of the flow is similar provided the phase difference is small and not close to $\pm \frac{\pi}{2}$. If the subharmonic mode is close to being out of phase, small deviations from the eigenfunctions of the KH and subharmonic mode will alter the time of pairing.

In three-dimensional simulations, vortex pairing is always suppressed by three-dimensional
motions and the suppression is greater when the phase difference is larger. Three-dimensional motions can even grow to sufficient amplitude and eliminate pairing when the phase difference is sufficiently large. Weaker pairing leads to less mixing and a reduced mixing efficiency. The decrease in mixing and mixing efficiency is greater as the subharmonic mode becomes close to being out of phase, similar to the behavior of the delay of pairing.
Chapter 3

The effect of Prandtl number on KH instabilities

3.1 Introduction

KH instabilities are an important mechanism for mixing in statically stable stratified fluids, e.g., in both the atmosphere and ocean. In the atmosphere, the air is stratified due to temperature and the Prandtl number \( Pr \) is about 0.7. In the ocean, the Prandtl number is about 7 if the stratifying agent is heat and is about 700 if the stratifying agent is salt. In this chapter, the main objective is to understand the dependence of mixing on Prandtl numbers.

There have been many studies in KH instabilities, but most numerical studies have focused on flows with Prandtl number close to 1 (e.g. Caulfield & Peltier, 2000; Mashayek & Peltier, 2013) as high Prandtl number flows require a high resolution for the density field. In experimental studies, the stratifying agent is usually salt and Prandtl number is about 700 (e.g. Thorpe, 1973; Winant & Browand, 1974). However, high resolution measurements were lacking in these experimental studies. Moreover, the dependence of mixing on Prandtl number in KH instabilities in stratified flows is complicated. Klaassen & Peltier (1985), Mashayek & Peltier (2013), Salehiour & Peltier (2015b), and Rahmani et al. (2016) have shown that turbulence intensity is stronger at higher Prandtl number and therefore the potential for mixing is higher. However, lower molecular diffusivity can decrease the amount of mixing that occurs. Therefore, the effect of Prandtl number on mixing is still not well understood and needs further investigation.

Some researchers have investigated the effect of Prandtl number on KH instabilities, secondary instabilities, and mixing properties, for example Klaassen & Peltier (1985), Smyth et al. (2001), Rahmani et al. (2016), Mashayek & Peltier (2012), Salehiour & Peltier (2015b). Klaassen & Peltier (1985) show that Prandtl number can suppress primary KH instabilities and increase the growth rate of the secondary convective core instabilities in intermediate Reynolds number stratified flows. Mashayek & Peltier (2012) and Salehiour & Peltier (2015b) studied the effect of Prandtl number on several secondary instabilities at high Reynolds number. Smyth et al. (2001) show that mixing efficiency for \( Pr = 7 \) is significantly
lower than that for $Pr = 1$ in a two wavelength domain, where vortex pairing occurs. Rahmani et al. (2016) show that while mixing and mixing efficiency are slightly increased in low Reynolds number flows because high Prandtl number enhances three-dimensional motions, mixing and mixing efficiency are reduced due to smaller diffusivity in intermediate Reynolds number flows. Salehiour & Peltier (2015b) studied the effect of Prandtl number in high Reynolds number flows for Prandtl number up to 16. They show that mixing efficiency is reduced in higher Prandtl number flows and the dependence is weaker than in low Reynolds number flows. In high Reynolds number flows, three-dimensional secondary instabilities prevent vortex pairing. However, in low to intermediate Reynolds number flows, vortex pairing can increase the vertical scale (Corcos & Sherman, 1984; Smyth & Peltier, 1993; Moser & Rogers, 1993) of the motions and the amount of mixing (Rahmani et al., 2014). In the present study, we investigate the dependence of vortex pairing, three-dimensional motions, and mixing on Prandtl number.

The numerical methods and simulations are described in section 3.2. Section 3.3 discusses the effect of Prandtl number on primary KH and vortex pairing in two-dimensional flows to remove the effect of three-dimensional motions. Three-dimensional results are described and compared with two-dimensional results in section 3.4.

3.2 Methods

As in Chapter 2, we use hyperbolic tangent functions as background density and velocity profiles, i.e.,
\[
\bar{\rho} = -\frac{\Delta \rho}{2} \tanh\left(\frac{2z}{\delta_0}\right) \quad \text{and} \quad U = \frac{\Delta U}{2} \tanh\left(\frac{2z}{h_0}\right). \tag{3.1a, b}
\]
In all simulations, the initial density interface thickness, $\delta_0$, is set to be equal to the thickness of the velocity profile, $h_0$. We keep Reynolds number $Re$, bulk Richardson number $J$ unchanged and vary Prandtl number $Pr$ from 1 to 64 to examine the effect of Prandtl number. In this chapter, $Re = 1200$ and $J = 0.07$. For this combination of non-dimensional numbers, the background flow is susceptible to KH instabilities.

Since density variation is small, the Boussinessq approximation is assumed. The governing equations, the Navier-Stokes equations with the Boussinessq approximation, are solved by the numerical code developed by Winters et al. (2004) and later improved by Smyth et al. (2005). The grid spacing of density field is half of that of velocity field in the code. The code uses the third order Adams-Bashforth time stepping scheme. The boundary conditions are horizontally periodic and vertically free slip and no flux.

We run both two and three dimensional numerical simulations to investigate the effect of Prandtl number on the flows. Inherently three-dimensional random perturbations are added...
3.2. Methods

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Table 3.1: Numerical parameters for all the simulations. The number of grid points is for the density field and is double of the velocity field.

to the background flow to excite primary and secondary instabilities for three-dimensional simulations. The perturbations are added to velocity fields and are given by equation (2.6) and (2.7). The maximum amplitude of perturbations is 0.08ΔU, which is small enough to ensure the flow evolves linearly initially. The same perturbations are used for different Prandtl number simulations to remove the effect of initial conditions. The initial conditions in two-dimensional simulations are the spanwise averaged values in three-dimensional simulations.

The horizontal domain length \( L_x \) is two wavelengths of the most unstable mode predicted by Taylor-Goldstein equation to allow vortex pairing. The spanwise width for three dimensional simulations is one wavelength of the KH instability, which is at least six wavelengths of the most unstable spanwise mode (for the most unstable spanwise wavenumber see Klaassen & Peltier, 1985, 1989). The domain height is \( 15h_0 \), which is sufficient to make the flows unaffected by vertical boundaries. The smallest scale needed to be resolved in DNS for homogeneous turbulence is Kolmogrov scale, \( L_k = (\nu/\varepsilon')^{1/4} \), where \( \nu \) is the molecular viscosity and \( \varepsilon' \) is dissipation rate of turbulent kinetic energy. Moin & Mahesh (1998) suggest that grid spacing should be \( O(L_k) \) in DNS. The resolution for stratified flows with \( Pr > 1 \) is however determined by the Bachelor scale, \( L_B = L_k/\sqrt{Pr} \). In this chapter, dissipation rate \( \varepsilon' \) averaged within \( -h_0/2 < z < h_0/2 \) where turbulence is most energetic is used to calculate the Bachelor scale. For all simulations, \( \Delta z/L_B < 4.3 \). Grid numbers (for density field) and other numerical parameters are listed in table 3.1. All simulations are named \( P_x(nD) \) where \( P \) indicates the simulations are investigating Prandtl number effects, \( x \) is the value of the Prandtl number, and \( n \) indicates whether the simulation is 2D or 3D.
3.3 Two-dimensional results

In this section, we examine the effect of Prandtl number on KH instability and vortex pairing in two-dimensional simulations. The focus is the effect of Prandtl number on vortex pairing.

3.3.1 KH instability

We first compare KH instability in simulations with different Prandtl number. Figure 3.1 (a) shows the kinetic energy of the KH mode, $K_{kh}$. The first maximum of $K_{kh}$ corresponds to the saturation of KH instabilities and this time is defined as the saturation time of KH instabilities, $t_{kh}$. The saturation time of KH instabilities is almost the same for all simulations and shown as stars in the figure.

Figure 3.1 shows that, before $t = 50$, the amplitude of $K_{kh}$ is negligible for all the simulations. After $t = 50$, the difference between different Prandtl number simulations appears. KH instabilities are always weaker for higher Prandtl number flows before the first maximum. To measure the thickness of the mean velocity profile and mean density profile, two integral scales are introduced by Smyth & Moum (2000), i.e. $I_u$ and $I_\rho$:

$$I_u = \int_{-Lz/2}^{Lz/2} 1 - \left( \frac{2\bar{u}}{\Delta U} \right)^2 \, dz,$$

and

$$I_\rho = \int_{-Lz/2}^{Lz/2} 1 - \left( \frac{2\bar{\rho}}{\Delta \rho} \right)^2 \, dz. \tag{3.2}$$

Bulk Richardson number based on these two scales, $J(t) = \Delta \rho g I_u^2 / \rho_0 I_\rho$, is used to measure the strength of stratification. Figure 3.2 shows the evolution of $I_u$, $I_\rho$, and $J(t)$. Until
3.3. Two-dimensional results

Figure 3.2: The integral thickness of the mean velocity profile $l_u$ (a), thickness of the mean density profile $l_p$ (b), and bulk Richardson number $J(t)$ based on $l_u$ and $l_p$.

$t = 50$, the thickness of velocity profile is the same for all the simulations as KH mode is still very weak and molecular diffusion is the main process expanding the mean velocity profile. However, the thickness of density profile is higher in the $Pr = 1$ than the other $Pr$ cases due to higher molecular diffusivity. For the other $Pr$ cases, diffusion of the mean density is negligible. Hence, before $t = 50$, bulk Richardson number $J(t)$ is greater and the stratification is stronger in higher $Pr$ flows. Also, bulk Richardson number is much lower in $Pr = 1$ than the other cases. Therefore, the reduction in $K_{kh}$ is much larger from $Pr = 1$ to 9 than from $Pr = 9$ to 64. Figure 3.3 shows the density field at $t_{kh}$ for different Prandtl number flows. It shows that from $Pr = 1$ to 9 the height of KH billows significantly decreases, and from $Pr = 9$ to 64 the height decreases slightly.

3.3.2 Vortex pairing

Figure 3.1 (b) shows the kinetic energy of the subharmonic component $K_{sub}$. Before saturation of KH (shown as stars), $K_{sub}$ is approximately the same in all the simulations. Therefore, the growth of the subharmonic mode is almost independent of Prandtl number before the subharmonic mode becomes dominant.

After saturation of KH instabilities, the difference between different Prandtl number simulations becomes noticeable. From $Pr = 1$ to 64, the growth of the subharmonic component decreases and the first maximum is reduced. The first (also global) maximum is defined as the saturation of the subharmonic component and indicates the merging of two KH billows. The reduction is more significant from $Pr = 1$ to 9 than from $Pr = 9$ to 64. Therefore, high Prandtl number has a suppressing effect on vortex pairing and the suppressing effect is more significant from $Pr = 1$ to 9 than from $Pr = 9$ to 64. As explained in chapter 2, the mechanism of vortex pairing is that one KH vortex is displaced upward and the other downward. Figure 3.2 shows that at $t_{kh}$ (around $t = 92$), bulk Richardson number $J$ increases as $Pr$ increases because of slower diffusion of density. Hence, in high
3.3. Two-dimensional results

Prandtl number flows, KH vortices need to overcome stronger stratification to pair.

Figure 3.3: Density field at four instances for two-dimensional simulations. From left to right, \( Pr = 1, 9, 16, \) and 64. Row (a) shows density field at \( t = 92, \) around saturation time of KH instabilities for all cases. Row (b) shows the density field at \( t = 130, \) around saturation of subharmonic mode. Row (c) shows the density field at \( t = 150 \) when the merged billow has not been destroyed by small scale motions. Row (d) shows the density field at \( t = 170 \) when the merged billow has been destroyed.

The saturation time of the subharmonic mode is defined as \( t_{sub}. \) Saturation time of the subharmonic mode slightly increases from \( Pr = 1 \) to 64 as shown in figure 3.1 (b) and table 3.1. Hence, vortex pairing is slightly delayed in high Prandtl number flows. Figure 3.3 (b) shows the density field at \( t = 130 \) (around \( t_{sub} \)). In \( Pr = 1 \) simulation, the merged billow core is almost isopycnal due to diffusion. However, in higher Prandtl number flows, the structure of two KH billows are still identifiable due to lower diffusivity and the shape
3.4 Three-dimensional results

of the merged KH billows is less similar to an ellipse. The height of the merged billow decreases as Prandtl number increases, indicating that stirring, i.e. the increase of total potential energy, decreases as Prandtl number increases.

After two KH billows pair, $K_{sub}$ oscillates with a high amplitude in $Pr = 1$. This oscillation is caused by the nutation of merged billow (Guha & Lawrence, 2014). However, in the other flows, the amplitude of oscillation is very small because small scale motions develop and destroy the merged billow. Figure 3.3 (c) shows that at $t = 150$ there is still no small scale motions in $Pr = 1$ simulation and the merged billow is regular. As $Pr$ increases, small scale motions become more dominant. After one oscillation, $K_{sub}$ quickly drops and stops oscillating because the merged billow is destroyed in all simulations as shown in figure 3.3 (d).

![Figure 3.4](image)

Figure 3.4: Kinetic energy of the subharmonic component, $K_{sub}$ in two-dimensional simulations and corresponding three-dimensional simulations: (a) $Pr = 1$; (b) $Pr = 9$; (c) $Pr = 16$; (d) $Pr = 64$.

3.4 Three-dimensional results

In this section, we examine effects of Prandtl number on vortex pairing and mixing when three-dimensional motions exist. As Caulfield & Peltier (2000) and Rahmani et al. (2014)
have shown, before saturation of KH instabilities, three-dimensional motions can be neglected if initial perturbations are small enough. We first compare vortex pairing in the two-dimensional results with that in the three-dimensional results to illustrate the effect of three-dimensional motions. Then we investigate the effect of Prandtl number on three-dimensional motions. We finally examine how mixing properties are influenced by the molecular property, i.e., Prandtl number.

3.4.1 Vortex pairing

We compare the kinetic energy of the subharmonic component, $K_{sub}$, in two-dimensional simulations with that in three-dimensional simulations in figure 3.4. For all Prandtl number simulations, the maximum of $K_{sub}$ is reduced by three-dimensional motions. Nevertheless, the saturation time of the subharmonic component is not affected by three-dimensional motions in all simulations. Hence, three-dimensional motions can suppress pairing, but do not delay pairing. Also, the reduction of maximum $K_{sub}$ caused by three-dimensional motions does not show a clear trend with Prandtl number.

3.4.2 Kinetic energy

We examine the three kinetic energy components, i.e. $\bar{K}$, $K_{2d}$, and $K_{3d}$, in all three-dimensional simulations with different Prandtl number in figure 3.5. For all simulations, before saturation of KH instabilities, three-dimensional motions are negligible. Two-dimensional motions are dominated by the KH mode. As shown in the two-dimensional results, KH instabilities are stronger in lower Prandtl number flows. Moreover, more energy is transferred to two-dimensional kinetic energy $K_{2d}$ from the mean kinetic energy $\bar{K}$ in lower Prandtl number flows. Also as explained in the two-dimensional results, the effects of Prandtl number on the flows during this stage are mainly caused by the differing diffusion rate of density field before KH instabilities reach finite amplitude. The three kinetic energy components are similar for flows of $Pr = 9$ to $Pr = 64$ as diffusion is negligible before KH instabilities reach finite amplitude.

After the saturation of KH instabilities and before vortex pairing, three-dimensional motions gradually become important, though two-dimensional motions are still stronger than three-dimensional motions. At the time of pairing, $K_{3d}$ is slightly higher for higher Pr number flows. This is consistent with Klaassen & Peltier (1985), who find that the growth rate of the dominant three-dimensional secondary instability is higher for higher Pr. However, two-dimensional kinetic energy $K_{2d}$ is higher in lower Pr flows. Hence, high Pr enhances three-dimensional motions, however KH instabilities and vortex pairing are suppressed by high Pr. Also, it should be noted that the mean kinetic energy is mainly
3.4. Three-dimensional results

Figure 3.5: The three kinetic energy components, (a) $\overline{K}$, (b) $K_{2d}$, and (c) $K_{3d}$, in three-dimensional simulations. Three key times, $t_{kh}$, $t_{sub}$, $t_{3d}$, are shown as stars, squares, and circles.
3.4 Three-dimensional results

lost due to vortex pairing rather than KH instabilities.

After the time of pairing, $t_{sub}$, for flows where $Pr$ is higher than 1, three-dimensional kinetic energy $K_{3d}$ continues to increase and reaches its maximum value. As $Pr$ increases, the maximum of $K_{3d}$ also increases. Note that maximum $K_{3d}$ is less than maximum of $K_{2d}$ for $Pr = 1$ flow and the other way around for higher $Pr$ flows. Therefore, three-dimensional motions are more dominant in higher $Pr$ flows. At $t_{3d}$, more mean kinetic energy is lost for higher $Pr$ flows because of stronger three-dimensional motions, though less mean kinetic energy is lost at the time of pairing for higher $Pr$ flows.

After three-dimensional kinetic energy reaches its maximum, turbulence decays and the flows re-laminarize. In the end, more kinetic energy is lost and velocity field is diffused more in higher $Pr$ flows. The kinetic energy is either lost to heat or transferred to potential energy as discussed in the next section.

3.4.3 Mixing

Figure 3.6 (a) shows the increase of potential energy normalized by initial kinetic energy and (b) shows the normalized background potential energy. Before saturation of KH instabilities, the amount of stirring, $\Delta P/K0$, decreases as $Pr$ increases, as the KH wave kinetic energy $K_{kh}$ does. The decreasing trend of stirring with $Pr$ can be explained by the lower height of KH billows in higher $Pr$ simulations as shown in figure 3.3 (a). During this stage, mixing is mainly caused by molecular diffusion as the flow is still well organized. In addition to lower amount of stirring in higher $Pr$ flows, lower molecular diffusivity decreases the amount of mixing further. The amount of mixing during this stage is negligible for all simulations.

After saturation of KH instabilities, potential energy continues to increase due to vortex pairing. The first maximum of potential energy occurs after time of pairing because the rotation of merged billow brings more heavy fluid particles upward as shown in figure 3.3 (b) and (c) and increases potential energy. The first maximum of potential energy is lower for higher $Pr$ flows since the size of the merged KH billow is smaller for higher $Pr$ flows. The amount of mixing occurred during this stage is dominant by molecular diffusion as three-dimensional motions are still small. Hence, less stirring and lower molecular diffusivity lead to less mixing in higher $Pr$ flows. Also, the amount of mixing is much lower for $Pr > 1$ than $Pr = 1$.

After the first maximum of potential energy, potential energy decreases and reaches a local minimum at $t_{3d}$. During this stage, two-dimensional kinetic energy $K_{2d}$ also decreases, but three-dimensional kinetic energy increases. Hence, the energy stored in available potential energy is transferred to three-dimensional kinetic energy $K_{3d}$ through buoyancy flux. During this stage, the merged KH billow is destroyed and small scale motions become prevalent. Also, mixing occurs at a higher rate due to turbulent mixing than the previous stage.
3.4. Three-dimensional results

The amount of mixing still decreases as $Pr$ increases.

After three-dimensional kinetic energy reach its maximum, part of kinetic energy is transferred to potential energy and potential energy increases again. After some oscillation, potential energy gradually reaches a constant as the flow returns to an approximate laminar state. The energy stored in available potential energy is transferred to background potential energy by mixing and background potential energy increases to total amount of potential energy. From $Pr = 1$ to $9$, the amount of mixing significantly decreases because vortex pairing is suppressed by higher $Pr$ and less stirring occurs in $Pr = 9$. Although three-dimensional motions are stronger in $Pr = 9$, the effect of weaker pairing on mixing is more significant. From $Pr = 9$ to $Pr = 16$, mixing slightly increases due to stronger three-dimensional motions, although pairing is weaker in the latter case. From $Pr = 16$ to $64$, mixing is almost the same.

![Figure 3.6](image)

Figure 3.6: (a) The increase of potential energy normalized by initial kinetic energy, $\Delta P/K_0$. (b) The increase of background potential energy normalized by initial kinetic energy, $\Delta P_b/K_0$. Three key times, $t_{kh}$, $t_{sub}$, $t_{3d}$ are shown as stars, squares, and circles.
3.4. Three-dimensional results

3.4.4 Mixing efficiency

In this section, we first compare the evolution of mixing efficiency in different $Pr$ flows in figure 3.7 (a). Following Caulfield & Peltier (2000), the instantaneous mixing $E_i$ is defined as

$$E_i = \frac{\phi_M}{\phi_M + \varepsilon}.$$  \hspace{1cm} (3.3)

Mixing efficiency $E_i$ is negligible before $t = 50$ as KH mode has not reached finite amplitude. After that, mixing efficiency begins to rise for all $Pr$ flows due to the rolling up of the density interface. During this stage, mixing efficiency $E_i$ decreases as $Pr$ increases, because molecular diffusion is the dominant mechanism of mixing. Even until around $t = 180$, this relation between $E_i$ and $Pr$ is valid. After that, the flow becomes fully turbulent and mixing efficiency is around 0.2 as observations and numerical simulations have shown. Mixing efficiency for $Pr = 1$ is larger than that for the other $Pr$. However, there is not a clear trend from $Pr = 9$ to 64. Therefore, we compare cumulative mixing efficiency $E_c$ during the active turbulent stage $t \in [t_{3d}, t_f]$ in figure 3.7 (b). From $Pr = 1$ to 9, cumulative mixing efficiency significantly decreases. Nevertheless, from $Pr = 9$ to $Pr = 16$, $E_c$ slightly increases. Although this non-monotonic trend is inconsistent with existed studies, for example Smyth & Moun (2000), Salehiour & Peltier (2015b), and Rahmani et al. (2016), it is still possible because mixing efficiency also depends on $Re_b$ and $Ri$. From $Pr = 9$ to 64, the change of mixing efficiency is much less than that from $Pr = 1$ to 9.

![Figure 3.7: (a) Instantaneous mixing efficiency $E_i$ and (b) cumulative mixing efficiency $E_c$ during the period $t \in [t_{3d}, t_f]$](image)

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3.5 Conclusion and discussion

We ran two-dimensional and three-dimensional simulations to examine the effect of Prandtl number on KH instabilities, vortex pairing, and mixing. Two-dimensional results show that KH instabilities and vortex pairing are suppressed in high Prandtl number flows and the suppression is more significant from $Pr = 1$ to 9 than from 9 to 64. The suppressing effect of higher Prandtl number on KH instabilities is mainly due to diffusion occurring before KH instabilities reach finite amplitude as Klaassen & Peltier (1985) propose. This effect does not appear in Salehiour & Peltier (2015b) and Rahmani et al. (2016) because the eigenfunction of KH mode is added to background flow in these two studies rather than a pure random perturbation.

As shown in the previous chapter, three-dimensional motions can suppress vortex pairing. Nevertheless, the suppressing effect of three-dimensional motions on vortex pairing does not show a clear trend with $Pr$. Since KH instabilities and vortex pairing are suppressed in higher Prandtl number flows, the amount of stirring and mixing caused by these two events are also lower in higher Prandtl number flows. However, three-dimensional motions increase monotonically and tend to increase mixing as $Pr$ increases. Because these two contradicting effects on mixing, mixing for $Pr = 1$ is much higher than the other $Pr$ flows where mixing is almost the same. It should be noted that three-dimensional motions are enhanced by higher $Pr$ is only valid in certain non-dimensional parameter space. Rahmani et al. (2016) find that three-dimensional motions are enhanced in low Reynolds number flows and Salehiour & Peltier (2015b) shows that in high Reynolds number flows three-dimensional motions do not vary monotonically as $Pr$ increases. In the present study, the growth rate of the convective core instability (also the dominant three-dimensional secondary instabilities), increases as $Pr$ increases (Klaassen & Peltier, 1985). For other initial non-dimensional parameters, the growth rate of other secondary instabilities might be lower for higher $Pr$ (see Mashayek & Peltier, 2012). Similar to mixing, cumulative mixing efficiency in $Pr = 1$ during the active turbulent stage is much higher than the other $Pr$ flows. Overall, cumulative mixing efficiency shows a decreasing trend with $Pr$. 


Chapter 4

Conclusions

Kelvin-Helmholtz instabilities in stratified flows have been studied by running Direct Numerical Simulations. The effects of initial conditions and Prandtl number on vortex pairing and mixing have been investigated. In chapter 2, we compare the numerical results with a variety of initial perturbations. Klaassen & Peltier (1985) and Smyth & Peltier (1993) show that vortex pairing is delayed if the subharmonic mode is out of phase relative to the KH mode. We find that the delay increases as the phase difference increases by running simulations with eigenfunctions of the KH and subharmonic modes. Moreover, the delay is sensitive to the phase and other details of the initial perturbations as the phase difference becomes close to $\pm \frac{\pi}{2}$. In three-dimensional simulations, vortex pairing is always suppressed by three-dimensional motions and the suppression is greater if the phase difference is larger. Vortex pairing may even be eliminated by three-dimensional motions if the subharmonic mode is out of phase. In the case with the subharmonic mode being out of phase, mixing is significantly reduced because of no pairing. The reduction of mixing also increases as the phase difference increases.

In chapter 3, we examine the effect of Prandtl number on vortex pairing and mixing. Two-dimensional simulation results show that KH instabilities are suppressed in higher Prandtl number flows due to less diffusion of the density field before KH mode reaches finite amplitude as proposed by Klaassen & Peltier (1985). The suppressing effects become weaker as Prandtl number increase from 9 to 64 than from 1 to 9. Comparison of three-dimensional and two-dimensional results shows that three-dimensional motions can suppress vortex pairing, but not delay pairing. The suppression of three-dimensional motions on vortex pairing does not show a clear trend with Prandtl number. However, three-dimensional motions are stronger in higher Prandtl number flows. This may be only valid for certain non-dimensional numbers as different secondary three-dimensional instabilities may vary differently with Prandtl number. Whether mixing is decreased or increased as Prandtl number increases depend on the two contradicting effects: weaken pairing; enhance three-dimensional motions. As Prandtl number increases from 1 to 9, vortex pairing is significantly weakened, which results in less stirring. Hence, mixing decreases as Prandtl number increases from 1 to 9. From $Pr = 9$ to 64, mixing is almost the same. We finally examine the effect of Prandtl number on mixing efficiency. Mixing efficiency in $Pr = 1$ is
much higher than that in the other $Pr$ flows. Overall, mixing efficiency shows a decreasing trend with $Pr$. 


