Internal-Gravity-Wave Interactions in the Presence of Localized Chemical Heating in the Atmosphere

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Abstract

The dynamical processes in the atmosphere and atmospheric chemistry are coupled and have an impact on each other. The heating that results from chemical constituents affects internal gravity waves. Internal gravity waves, on the other hand, influence the distribution of a chemical in the atmosphere. These effects of gravity waves and chemical heating are the focus of this thesis.

We investigate analytical solutions of different forms of the chemical transport equation. We also describe numerical methods and show numerical results for the chemical transport equation. We study the effect of gravity waves on the chemical distribution analytically and numerically. The numerical results showing the effect of gravity waves on the distribution of the chemical are consistent with the analytical observations. The wave-induced mean flow resulting from nonlinear gravity wave interactions leads to modification of the distribution of the chemical.

We consider a configuration where gravity-wave equations are coupled with the chemical transport equation. We carry out linear and weakly-nonlinear analytical investigations to find the effect of the chemical heating on the gravity waves. We also carry out numerical investigations for the coupled equations and show numerical results. It is found that heating due to the chemical has a significant effect on the gravity waves, especially when the chemical is centred at the critical level. These numerical results are in general agreement with the analytical observations we obtain.

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Chapter 1

Introduction

1.1 Internal gravity waves and chemical species in the atmosphere

Surrounding our planet Earth, the atmosphere is considered thin relative to the radius of the Earth. Away from the Earth's surface, the density and pressure of the atmosphere, represented by air, decrease approximately exponentially with height, whereas the temperature decreases within some layers and increases within others. This variation of temperature leads to the classification of the atmosphere into four main layers separated by three boundaries. The layer starting from Earth's surface up to about 10 km is represented by the troposphere layer, bounded by the tropopause. On the top of the tropopause is the middle atmosphere, consisting of stratosphere and mesosphere layers separated by the stratopause boundary at about 50 km. The mesosphere is the higher layer of the middle atmosphere, and on the top of that is the thermosphere layer above the mesopause boundary at about 85 km [Marshall and Plumb (2008)].

The decay of the density of the atmosphere away from the Earth's surface

means that the atmosphere is approximately stably stratified. The buoyancy-restoring force resulting from the stratification, coupled with the gravitational force, leads to the generation of waves, which are called *internal gravity waves*. Internal gravity waves often propagate upward or downward in the atmosphere, and they may break down, leading to a turbulent flow.

Internal gravity waves have an influence on the weather and climate. Such influence should be considered especially in the case of simulating wind speed and temperature in the atmosphere. When the mean flow is equal to the phase speed of the wave, we then have the so-called *critical level*, which corresponds to a singularity in the linearized equations for internal gravity waves [Nappo (2002); Marshall and Plumb (2008)]. Clear-air turbulence, which is a non-obvious turbulent movement of air, may result from internal wave breaking. The speed of the wind in the atmosphere can be perturbed as a result of interactions between wave modes and between waves and the mean flow, especially in the vicinity of the critical level [Sutherland (2010)].

In the theoretical formulation considered here, we represent the gravity waves by a discrete or continuous spectrum of Fourier modes in space; e.g. a sum or integral over k of waves of the form

$$Ae^{ikx} + A^*e^{-ikx},$$

where x is a horizontal variable and the wave amplitude A depends on the wavenumber k , as well as on the other spatial variables and time. The amplitude A is complex, and A^* is its complex conjugate. The nonlinear terms in gravity-wave equations involve products of the Fourier modes. This means that, as the waves propagate, Fourier modes with wavenumbers $\pm 2k, \pm 3k, \dots$ develop in addition to wavenumbers $k + (-k) = 0$. These are proportional to $e^0, e^{\pm 2kix}, e^{\pm 3kix}$ and so

on. The zero wavenumber component corresponds to a change in the mean flow, and this change is referred to as the wave-induced mean flow.

The atmosphere contains major chemical constituents such as nitrogen N_2 , oxygen O_2 , argon Ar and water vapour H_2O , as well as tracer gases that are present in the atmosphere in smaller concentrations, such as carbon dioxide CO_2 , methane CH_4 and ozone O_3 . Although these trace gases are not present in high concentrations in the atmosphere, they play an important role in atmospheric reactivity and hence can affect the temperature of the Earth's surface. In general, chemical concentrations in the atmosphere are influenced by four kinds of activities: chemistry, emissions, deposition and transport. Such influence can be represented mathematically by the continuity equation [Marshall and Plumb (2008); Jacob (1999)].

Solar radiation is the principal source of energy for the Earth system. Solar radiation (photolysis) in the atmosphere leads to the creation of chemical species known as radicals. These radicals are involved in some chemical reactions in the atmosphere. Therefore, the incoming energy from solar radiation is essential in chemical processes in the atmosphere. Solar radiation is absorbed by many chemicals in the atmosphere, and chemical reactions involving this absorption are called photochemical reactions. Ozone is considered to be the major absorber of solar radiation in the stratosphere. The major absorber of solar radiation in the troposphere is water vapour. Thus ozone and water vapour are considered very important in studying the energy budget of the middle atmosphere [Brasseur and Solomon (1984), Brasseur and Jacob (2017), Hartmann (1994)].

The spatial distribution of ozone and other chemicals in the middle atmosphere is affected by transport, especially in the upper troposphere and lower stratosphere. Chemistry of the atmosphere is coupled with dynamics, and our

understanding of this coupling has been advanced by satellite and aircraft observations of chemical species, measurements and data simulations and numerical modelling. Understanding the distribution of ozone is important because depletion of ozone affects the amount of solar radiation that reaches the earth and ozone is an important greenhouse gas [Shepherd (2007)].

The stratosphere is dynamically stable, but waves propagating up from the troposphere transfer momentum and energy. Planetary-scale and synoptic-scale Rossby waves contribute to two-ways transport in the stratosphere. The breaking of Planetary-scale and synoptic-scale Rossby waves in the stratosphere leads to horizontal mixing. Gravity waves also propagate from the troposphere, and the importance of gravity wave effects increases with altitude because gravity wave amplitude increases exponentially with altitude. Vertical mixing arises mainly from gravity-wave breaking. The tropical part of upper troposphere lower stratosphere UTLS is the tropical tropopause layer TTL. The vertical profile of ozone in the TTL increases gradually with altitude whereas water vapour generally decreases [Shepherd (2007)].

Chemistry climate models (CCMs) and chemistry transport models (CTMs) are examples of models that include chemistry and dynamics. The uncertainty in gravity-wave drag, which is not well resolved, is considered to be an issue in CCMs. Artificial vertical diffusion is needed to overcome the insufficiently accurate numerical resolution. CTMs are driven by winds from meteorological analyses, so issues related to dynamics can be resolved; however, CTMs still have numerical problems. Additional problems are also introduced by errors from the data assimilation, which can affect the models over long time intervals [Shepherd (2007)].

Overall, the mesosphere is not well understood, especially the lower region,

compared with the stratosphere and with the upper region mesosphere-lower thermosphere MLT. Moving from the stratosphere to the lower mesosphere, the dynamics become more complicated, and there are more gravity waves relative to other larger-scale waves, more vertical mixing from vertically propagating gravity waves which are represented by shorter timescales and smaller spatial scales [Shepherd (2007)]. These issues underline the importance of studying gravity wave interactions with chemical species.

The interaction of internal gravity waves and chemical constituents in the atmosphere results in an impact on each other. Chemical processes, such as photochemical heating of chemical constituents in the atmosphere, lead to damping or enhancement of gravity waves [Zhu and Holton (1986); Xu (1999)]. Gravity waves, on the other hand, have an impact on chemical concentrations in the atmosphere. One such effect is inducing the wind speed as a result of wave-wave interaction of internal gravity waves. This affects the speed of transport of chemical constituents in the atmosphere.

In this thesis, some mathematical models to study these interactions will be presented and analyzed using asymptotic methods and numerical solutions. In the next section, some previous work is described.

1.2 Previous work and motivation for the study

One of the first studies to compute the heating rates due to the absorption of solar radiation in the mesosphere was by Murgatroyd and Goody (1958). It was observed that the radiation almost approaches equilibrium except at the poles. Leovy (1964) studied the radiative equilibrium of the mesosphere as well as upper stratosphere, where two methods were used to calculate the equilibrium temperatures. A parameterization of the absorption of solar radiation was introduced by

Lacis and Hansen (1974). The method is based on multiple-scattering computations and is used in some global atmospheric circulation models. Park and London (1974) calculated the distributions of the heating rates due to the absorption of solar radiation by ozone and oxygen, and they observed that most of heating in the middle atmosphere is due the absorption of solar radiation by ozone. The radiative heating rates of water vapour and ozone, as well as the thermal cooling rates of carbon dioxide, were computed for the global atmosphere by Dopplack (1972) and Dopplack (1979). An analytical computation of heating due to ozone was introduced by Lindzen and Will (1973), which was then parametrized by Strobel (1978). Luther (1976) presented similar analytical approach to calculate the heating due to the absorption of solar radiation by nitrogen dioxide. Gille and Lyjak (1986) computed solar heating due to water vapour, ozone and other chemicals in the middle atmosphere by considering more accurate data taken from the Limb Infrared Monitor of the Stratosphere (LIMS).

In addition to computing the heating due to solar radiation, Garcia and Solomon (1983), Brasseur and Offermann (1986) and Mlynczak and Solomon (1991) considered the heating resulting from exothermic reactions which release chemical heating in the middle atmosphere. Mlynczak and Solomon (1991) and Mlynczak and Solomon (1993) investigated the heating efficiencies associated with the absorption of solar radiation by studying the energy released from solar heating.

There are many studies that discuss the interactions of gravity waves with chemical constituents in the atmosphere. The interaction of linear internal gravity waves with sodium species in the mesopause region of the atmosphere was investigated by Hickey and Plane (1995). They showed that gravity wave interaction leads to sodium fluctuations at specific altitudes around the sodium layer. Xu (1999) studied the effects of photochemical heating on the linear inertia-gravity

waves in the middle atmosphere under three cases: cooling process only, heating and cooling, or adiabatic process. It was found that the diabatic effect produced by photochemical processes affects gravity waves in different forms in the layers of the middle atmosphere. The effect that nonlinear photochemical reactions influenced by linear inertia gravity waves has on the chemical distribution of some species is discussed by Xu et al. (2000). Such effect was compared with background diffusion effect as well as the impact of chemical transport induced by gravity waves, and it was found that, in the vicinity of mesopause, the impact on chemical distribution associated with nonlinear photochemical reactions is much greater than other effects. Xu et al. (2003) investigated the impact of nonbreaking nonlinear gravity waves on the distribution of chemical species in the middle atmosphere. They constructed a model that coupled the nonlinear gravity equations and photochemistry of some chemical species, and they concluded that nonbreaking gravity waves influence the mean distribution of chemicals, especially at nighttime.

Most of the aforementioned studies have focused on the coupling between chemistry and dynamics of gravity waves through the temperature of chemical species. As mentioned before, gravity-wave interactions with the mean flow lead to a wave-induced mean flow. The effect of the wave-induced mean flow on the chemical species was not given much attention, perhaps because the gravity-wave equations were taken to be linear in most previous investigations. Although Xu et al. (2003) considered a nonlinear gravity-wave system, the investigation of the wave-induced mean flow and its impact on chemical species was not included. The investigation of this impact will be our main focus, where we study the full nonlinear system of internal gravity waves coupled with a nonlinear continuity equation for the chemical concentration and examine how the wave-induced mean flow can affect the distribution of chemical species in the atmosphere.

We consider a model that consists of the equations for internal gravity waves, which are influenced by chemical heating, coupled with a continuity equation that describes the transport of the chemical and includes terms that represent chemical reaction and diffusion processes. Internal gravity-wave equations are derived by applying the Boussinesq approximation to the fundamental equations of fluid dynamics. The Boussinesq approximation is used to model a configuration in which density variations are considered only in terms involving buoyancy forces in the equations of fluid dynamics. This approximation is commonly used in fluid applications and was used to derive equations for gravity waves by Bretherton (1966), Booker and Bretherton (1967), Campbell and Maslowe (2003) and Kundu et al. (2012).

The continuity equation in the model, representing the chemical in the atmosphere, has a source term corresponding to the reaction processes. We study this equation analytically as well as numerically before considering the full model where the continuity equation is coupled with the gravity-wave equations. The source term in the continuity equation depends on the particular chemical. In reality, there are many different chemicals present in each region of the atmosphere, and some of these react with each other. Fitzgibbon et al. (2005) presents a coupled set of equations for 20 chemicals, which are coupled to each other by their nonlinear source terms. Here we consider configurations with just one chemical present, where the source term is either linear or nonlinear based on form given in Brasseur and Solomon (1984). We consider models for water vapour (H_2O), ozone (O_3) and chlorine monoxide (ClO). We specify the initial distribution of these chemicals following Gille and Lyjak (1986), where they show initial profiles for the chemicals based on data taken from LIMS.

The analytical investigations of the continuity equation representing the chem-

ical in the atmosphere include the case where the advection speed of the chemical is perturbed. This perturbation corresponds to gravity-wave-induced mean flow. We find that the concentration of the chemical is affected by the perturbed mean flow and this modification in the chemical mixing ratio is qualitatively determined by the behaviour of the perturbed mean flow.

From numerical computation of the effect of gravity wave equation on the advection speed of the chemical, we find that the wave-induced mean flow has a considerable effect on the distribution of the chemical concentration. This effect mainly appears in the vicinity of the critical level, where the wave-induced mean flow is maximum. The effect of the gravity waves causes perturbations in the chemical concentration, which are eventually seen to follow the qualitative behaviour of the gravity-wave-velocity perturbations. This is consistent with our analytical observation obtained by asymptotic solutions of the perturbed chemical equation. This effect of gravity waves on the chemical mixing ratio is also in agreement with the results obtained by Garcia and Solomon (1983) and Xu et al. (2003).

We carry out analytical linear and nonlinear investigations on the equations of gravity waves affected by the chemical heating. Linear approximations of the streamfunction of the gravity waves with constant background mean flow as well as mean flow with vertical shear are obtained. We find that gravity waves are greatly influenced by the presence of the chemical heating.

We then obtain numerical solutions of the full model, where the gravity waves affect the chemical, while gravity waves are affected by the heating rate of the chemical under investigation. In these numerical simulations, we consider transport equations for water vapour, ozone and chlorine monoxide which are based on the equations given by Brasseur and Solomon (1984). In addition to observations seen from the effect of gravity waves on the advection speed of the chemical, we

find that gravity waves are greatly affected, especially around the zero component of the wavenumber of Fourier representations of functions. These numerical results are consistent with the approximations obtained by the analytical investigations. Leovy (1966), Zhu and Holton (1986) and more recently Xu (1999) pointed out that interaction of chemical constituents with gravity waves lead to fluctuations in gravity waves. We find that these observations are in agreement with our analytical as well as numerical results on the effect of the chemical on gravity waves.

1.3 Overview of the thesis

Chapter 2 is devoted to the derivation of the fundamental equations. We start the chapter by introducing Boussinesq equations for stratified fluid flow. These equations are derived by applying the Boussinesq approximation to the fundamental equations of fluid dynamics, the continuity, momentum and energy equations. The derivation of the fundamental equations of fluid dynamics is given in Appendix A. The derivation of the equations for internal gravity waves under the Boussinesq approximation is discussed in Appendix B. Section 2.2 introduces the equation representing the concentration of a chemical in the atmosphere. The nondimensionalization of the equations for gravity waves, as well as the chemical equation, is given in Section 2.3. Section 2.4 contains the derivation of gravity waves perturbation. Section 2.5 describes the configuration of the model we consider in this thesis.

The analytical and numerical solutions of different forms of the chemical transport equation are investigated in Chapter 3. The discussion starts with analytical solutions for the linear advection diffusion equation with a linear damping term and then describes a special case where there is an exact travelling-wave solu-

tions for a nonlinear advection diffusion equation with a nonlinear reaction term and constant advection speed. In Section 3.2.2, we then consider the case where constant advection speed in the nonlinear equation is perturbed by a spatially dependent function and use asymptotic analysis to approximate solutions for the nonlinear equation. Section 3.3 is devoted to the description of the numerical method involving finite differences to compute travelling-wave solutions as well as numerical results.

Chapter 4 provides some analysis of a configuration where the gravity wave equations include a forcing term due to chemical heating. A linear steady-state analysis is given in Section 4.1. Section 4.2 is devoted to the weakly-nonlinear analysis where the mean flow of streamfunction as well as the mean density equations are derived. The description of a numerical method to solve gravity-wave equations as well as numerical results are shown in Section 4.3.

Chapter 5 concerns the effect of internal gravity waves on the chemical transport equation. In this chapter, it is assumed that the effect of the heating due to the chemical is small enough that it can be neglected in the gravity-wave equations. The discussion starts with a description of a numerical method to solve the chemical equation, where the initial chemical distribution is spatially localized in the form of Gaussian profile in both spatial directions. With this profile, we use a spectral method instead of finite differences, as shown in Section 5.2. First, in Section 5.2, we solve the chemical equation for a case with no gravity-wave perturbations present. Then, in Section 5.3, we proceed to solve the problem where gravity-wave perturbations affect the mean flow and the wave-induced mean flow affects the distribution of the chemical.

In Chapter 6, we consider the configuration where the gravity-wave equations and the chemical-transport equation are coupled. In this chapter, the gravity

waves affect the distribution of the chemical, and the chemical has an impact on gravity waves. The configuration where gravity-wave equations are coupled with a transport equation for ozone is presented in Section 6.1, where we consider a steady-state as well as a time-dependent ozone. The steady-state case corresponds to the situation where the chemical has an effect on gravity waves, whereas gravity waves do not affect the chemical. Section 6.2 discusses the configuration where gravity-wave equations are coupled with a transport equation for water vapour. The configuration where gravity-wave equations are coupled with Fisher's equation is given in Section 6.3. Also Section 6.3 contains a discussion of the gravity-wave equations coupled with chlorine monoxide.

The conclusions of the thesis are given in Chapter 7. The derivation of the basic fluid equations is given in Appendix A. Appendix B is devoted to applying the Boussinesq approximation on the fluid equations obtained in Appendix A, which include the effect of chemical heating. Appendix C illustrates the WKB method used to give asymptotic solutions in Chapter 3. Appendix D discusses the linearized gravity-wave equations without chemical effect.

1.4 Original contributions of the thesis

In this section we list the original contributions of the thesis. These include the following:

Chemical transport equation with perturbed advection:

In Section 3.2.2, we consider Fisher's equation with perturbed advection which corresponds to the situation where gravity-wave perturbation is affecting the mean flow. In this case, there is no exact solution in closed form. Instead, we use a perturbation method to study the behaviour of the travelling-wave solution.

The solution corresponding to the leading order can be found exactly. The first-order solution is approximated asymptotically by the WKB approximation. We find that the first-order solution is proportional to the qualitative behaviour of the perturbation of the mean flow. We also observe that the first-order solution decays to zero at both boundary where the rate of decay is different from one side to the other. This found to be consistent with numerical solutions obtained in Section 3.3.

Gravity waves affected by localized chemical heating:

In Section 4.1 we study the linearized form of gravity-wave equations affected by chemical heating. We consider a steady-state amplitude of gravity waves that affected by a steady-state chemical. We derive an equation that looks like the Taylor–Goldstein equation but with a forcing term. We carry out analytical investigations considering several configurations and eventually find approximations for the streamfunction that represent gravity waves affected by a localized chemical heating.

Nonlinear time-dependent equations affected by time-dependent chemical heating is considered in Section 4.2. We carry out weakly-nonlinear analysis and derive equations for the wave-induced mean flow and wave-induced mean density. These equations can be used to compute gravity-wave drag. The equations we obtain for the wave-induced mean flow and wave-induced mean density include the effect of the localized chemical heating. Thus, these equations can be used in a parameterization scheme to account for the effect of gravity waves affected by chemical heating.

Gravity waves effect on the chemical distribution:

In Section 5.3, we numerically investigate the effect of gravity-wave perturbations on the chemical distribution. We show that gravity-wave perturbations lead to an impact on the mean flow which then affects the chemical distribution. We observe that the nonlinearity of gravity waves as well as the presence of the critical level lead to a significant effect on the the chemical distribution.

Gravity waves coupled with localized chemical heating:

In Chapter 6, we consider gravity waves coupled with chemical heating. We explore several chemicals where we obtain their initial profiles based on observational studies. We consider steady-state chemical as well as time-dependent chemicals. We carry out numerical investigations of several coupled models corresponding to the different chemicals. We compare between these different cases and also compare with the corresponding analytical observations obtained from the weakly-nonlinear analysis obtained in Section 4.2.

Chapter 2

Fundamental Equations

2.1 Boussinesq equations for stratified fluid flow

In the field of fluid applications, waves are usually classified as surface waves and internal waves. Surface waves propagate along the surface of the fluid or along an interface between two fluids, whereas internal waves propagate within the fluid. In the atmosphere, the combined effects of the gravitational force and the buoyancy force (which results from the vertical stratification of the density) give rise to fluctuations in the fluid flow. These fluctuations are considered to be internal waves because they occur within the atmosphere and are referred to as internal gravity waves or simply as gravity waves.

From this point and throughout the thesis, the equations will be in terms of the two dimensions in space x and z , where x represents the horizontal coordinate and z represents the vertical coordinate. Physically, the horizontal coordinate x represents the south-to-north direction, whereas the vertical coordinate z represents the altitude in the atmosphere.

The heating released from a chemical due to the effects of solar radiation or other chemical processes leads to a change in the energy of the atmosphere in

a localized region. The structure of gravity waves propagating in this region is then affected. In Appendix A, we derive equations for the conservation of mass, momentum and energy in a fluid flow. These lead to equations for the gravity-wave fluctuations. In a situation where there is heat release from a chemical, we include the effect of heating due to a chemical in the energy equation for the gravity waves. In Appendix A, this effect of heating is included in (A.27) and represented by $Q_{chemical}$. Here we give a formula for $Q_{chemical}$. As in Appendix A, we consider a fluid with density ρ within some control volume V . Let J represent the rate of heat added to the control volume per unit mass as a result of the chemical heat release. Since ρdV measures the mass within an elemental volume dV , the rate of heat added to such mass is then $(\rho J dV)$. It follows that the rate of heating due to a chemical over the whole control volume is

$$Q_{chemical} = \iiint_V \rho J dV.$$

Thus, the total rate of heating in the control volume, A_1 , given in (A.27), has the form

$$A_1 = \iiint_V \rho J dV - \iint_S \mathbf{q} \cdot d\mathbf{S} + Q_{visc}, \quad (2.1)$$

where $\mathbf{q}$ represents the heat flux vector added to the control volume per unit area and Q_{visc} represents the rate of heat added to the flow within the control volume by the effect of viscosity. The continuity equation (A.3), momentum equations (A.22) and (A.24) and energy equation (A.31), which are derived in Appendix A, are given as

$$\frac{\partial}{\partial t} \rho(\mathbf{x}, t) + \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) = 0. \quad (2.2)$$

$$\rho \frac{D\mathcal{U}}{Dt} = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (2.3)$$

$$\rho \frac{D\mathcal{W}}{Dt} = \rho g_z - \frac{\partial p}{\partial z} + (\mathcal{F}_z)_{visc}. \quad (2.4)$$

$$\rho \frac{D}{Dt} \left(e + \frac{|\mathbf{u}|^2}{2} \right) = -\nabla \cdot \mathbf{q} - \nabla \cdot (p\mathbf{u}) + \rho(\mathbf{g} \cdot \mathbf{u}) + \rho J, \quad (2.5)$$

where t is the time, $\mathbf{x} = (x, z)$ is the position vector, $\mathbf{u}$ is the fluid-velocity vector, $\mathcal{U}$ is the horizontal component of the fluid velocity, $\mathcal{W}$ is the vertical component of the fluid velocity, g is the body force, p is the pressure force, $(\mathcal{F})_{visc}$ is the viscous force, the subscripts in g and $(\mathcal{F})_{visc}$ denote the x and z components, respectively, and e is the internal energy.

In Appendix B, we apply the Boussinesq approximation to the continuity, momentum and energy equations (2.2)–(2.5). The Boussinesq approximation is commonly used in fluid applications, and it is considered appropriate under certain conditions as discussed by Spiegel and Veronis (1960). Boussinesq (1903) proposed that the perturbation density is very small and thus can be ignored in the fluid equations except if it is combined with gravity. He also suggested that the change in density with respect to pressure is negligible compared to the change in density with respect to temperature. Under the Boussinesq approximation, the continuity equation (for the conservation of mass of the fluid) is approximated as $\nabla \cdot \mathbf{u} = 0$, and the energy conservation (2.5) can be written in terms of the fluid temperature and then further rewritten in terms of the fluid density ρ as described in Appendix B, where there is a linear relation between the temperature and density under the Boussinesq approximation. The effect of the chemical heating in equation (2.5) then appears as a nonhomogeneous term in the density equation.

Equations (2.3) and (2.4) can be combined by rewriting in terms of the streamfunction $\Psi(x, z, t)$. The streamfunction $\Psi(x, z, t)$ is defined in terms of the horizontal and vertical velocities as $\mathcal{U} = -\Psi_z$ and $\mathcal{W} = \Psi_x$, where the subscripts denote partial derivatives.

Applying the Boussinesq approximation to equations (2.2)–(2.5), as shown in Appendix B, we obtain the Boussinesq equations (B.39) and (B.40) for a stratified fluid flow,

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + \nu \nabla^2 (\nabla^2 \Psi), \quad (2.6)$$

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = \kappa \nabla^2 \rho - \alpha J, \quad (2.7)$$

where subscripts denote partial derivatives, $\nu = \frac{\mu}{\rho_0}$ is the kinematic viscosity coefficient, κ is the thermal diffusivity coefficient and $\alpha = \frac{\rho_0}{T_0 C_p}$ is the chemical heating coefficient.

2.2 Transport equation for chemical species

Equations (2.6) and (2.7) describe the evolution of the fluid flow and the effect of the chemical heating on the fluid properties. The chemical heating release depends on the concentration of the chemical in the region under consideration. The chemical concentration also varies in space and time. Thus, the full model should have an equation representing the chemical. In this section, we derive an equation that models the chemical in the atmosphere by applying the law of conservation of mass in a similar approach to what is shown in Appendix A. Let V be a fixed control volume, n be the number density of the chemical, which is defined as the number of molecules of the chemical present in a specified volume, and s be a local source term that represents the effect of chemical reactions. The rate of change in mass inside the control volume V equals the net mass that flows out of the control volume through the surface S due to the advection and diffusion of the chemical balanced by the net production of the chemical in the control volume due to the reaction (local source term s). This can be expressed

as

$$\frac{\partial}{\partial t} \iiint_V n dV = - \iint_S n \mathbf{U} \cdot \mathbf{dS} - \iint_S (-\mathcal{D} \nabla n) \cdot \mathbf{dS} + \iiint_V s dV, \quad (2.8)$$

where t is the time, $\mathbf{U}$ is the advection speed of the background wind and $\mathcal{D}$ denotes the diffusion rate. Applying the divergence theorem to the first and second terms in the right-hand side of (2.8), we obtain

$$\frac{\partial}{\partial t} \iiint_V n dV = - \iiint_V \nabla \cdot (n \mathbf{U}) dV + \mathcal{D} \iiint_V \nabla^2 n dV + \iiint_V s dV, \quad (2.9)$$

which is rearranged to give

$$\iiint_V \left[\frac{\partial}{\partial t} n + \nabla \cdot (n \mathbf{U}) - \mathcal{D} \nabla^2 n - s \right] dV = 0. \quad (2.10)$$

Assuming n and $\mathbf{U}$ are continuous functions everywhere in the volume V , equation (2.10) equals zero only if the integrand equals zero, so we get

$$\frac{\partial n}{\partial t} + \nabla \cdot (n \mathbf{U}) = \mathcal{D} \nabla^2 n + s. \quad (2.11)$$

A similar approach to derive equation (2.11) is shown by, for example, Fowler (2011) and Bird et al. (2002).

Equation (2.11) is a differential equation in time and space, which is used to model a chemical in the atmosphere in terms of its number density as shown for example by Fowler (2011), Bird et al. (2002) Brasseur and Solomon (1984), Brasseur and Jacob (2017) and Leovy (1966).

The mixing ratio is commonly used to represent chemicals in the atmosphere. Let C represent the mixing ratio of the chemical; it is a dimensionless variable

defined in terms of the number density by

$$C = \frac{n}{n_a}, \quad (2.12)$$

where n_a is the number density of air. For a two-dimensional configuration represented in terms of a horizontal variable x and vertical variable z , we consider fluid flow satisfying the Boussinesq approximation with continuity equation $\nabla \cdot \mathbf{u} = 0$, and equation (2.11) can be written in terms of mixing ratio C as (Brasseur and Jacob (2017))

$$C_t + U C_x + W C_z = \mathcal{D}(C_{xx} + C_{zz}) + S(C), \quad (2.13)$$

where the subscripts denote the partial derivatives with respect to time t and the spatial variables x and z , U and W are the horizontal and vertical components of the fluid velocity and $S(C)$ represents the local source term written in terms of the mixing ratio. The source term $S(C)$ in equation (2.13) corresponds to the reaction processes (production and loss) of the chemical in the atmosphere. This term can be linear, in the case of unimolecular (first-order processes), or it can be nonlinear in the case of bimolecular processes. It can also be a combination of both linear and nonlinear terms [Brasseur and Solomon (1984)]. Other previous work, e.g. Fitzgibbon et al. (2005), considered many chemicals where each chemical is modelled by an equation of the form (2.13) and some chemicals react with each other. In that case, the nonhomogeneous term $S(C)$ in each equation is a nonlinear term that models the chemical reactions. Throughout the thesis, we will consider situations where there is only one distinct chemical present with concentration given by (2.13) and with the source term S depending solely on the mixing ratio, C , of the chemical under investigation.

The total derivative of C following the motion of a fluid with velocity compo-

nents U and W is defined as

$$\frac{DC}{Dt} = \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} + W \frac{\partial C}{\partial z}. \quad (2.14)$$

Equation (2.13) can then be expressed in terms of the total derivative (2.14) as

$$\frac{DC}{Dt} = \mathcal{D} \nabla^2 C + S(C). \quad (2.15)$$

2.3 Nondimensionalization

All the equations in the previous section are considered to be in dimensional form. In this section, we rewrite these equations in a nondimensional form. The nondimensionalization of equations is effective for several reasons. It reduces the complexity of the equations by lowering the number of unknown parameters. Also, the analytical behaviour of the equations can be studied regardless of the effect of units of the variables. Finally, the nondimensionalization is powerful since it allows us to rescale the equation so that we can compare the order of magnitude of all terms in an equation. This can then help us to know the important terms and the negligible terms in the equation.

To write the equations in nondimensional form, we divide each variable or quantity by a corresponding typical value that has the same units. Denoting a quantity in a dimensional form with “ $\star$ ”, the dimensionless independent spatial and temporal variables can be obtained using the following transformations:

$$x = \frac{x^\star}{L_x}, \quad z = \frac{z^\star}{L_z} \quad \text{and} \quad t = \frac{t^\star}{\tau}, \quad (2.16)$$

where L_x and L_z are typical lengths in the x and z directions. The typical time τ

satisfies the basic physical law given as

$$\tau = \frac{L_x}{\mathcal{U}} = \frac{L_z}{\mathcal{W}}, \quad (2.17)$$

where $\mathcal{U}$ and $\mathcal{W}$ are the typical horizontal and vertical velocities. The dependent state variables Ψ and ρ , as well as the viscous parameter, the diffusion parameter and the constant acceleration due to gravity can similarly be defined in dimensionless form as

$$\Psi = \frac{\Psi^*}{\mathcal{U} L_z} = \frac{\Psi^*}{\mathcal{W} L_x}, \quad \rho = \frac{\rho^*}{D}, \quad \nu = \frac{\nu^*}{\mathcal{M}}, \quad \kappa = \frac{\kappa^*}{\kappa} \quad \text{and} \quad g = \frac{g^* L_z}{\mathcal{U}^2}, \quad (2.18)$$

where D is a typical density, $\mathcal{M}$ is a typical value of the viscous parameter ν^* and κ is a typical value of the thermal diffusivity κ^* . In addition to the scaling transformations (2.16), (2.17) and (2.18), we also have the following transformation

$$\alpha = \frac{\alpha^*}{\mathcal{A}} \quad \text{and} \quad J = \frac{J^*}{\mathcal{H}}, \quad (2.19)$$

where $\mathcal{A}$ and $\mathcal{H}$ are scaling parameters. We can then write the dimensional equation (2.6) in dimensionless form as

$$\frac{1}{\tau} \mathcal{W} L_x \tilde{\nabla}^2 \Psi_t - \frac{\mathcal{W}^2 L_x}{L_z} \Psi_z \tilde{\nabla}^2 \Psi_x + \frac{\mathcal{W}^2 L_x}{L_z} \Psi_x \tilde{\nabla}^2 \Psi_z = - \frac{g \mathcal{U}^2}{\rho_0 L_z L_x} \rho_x + \nu \mathcal{M} \mathcal{W} L_x \tilde{\nabla}^2 (\tilde{\nabla}^2 \Psi), \quad (2.20)$$

where the differential operator is $\tilde{\nabla}^2 = (\frac{1}{L_x^2} \frac{\partial^2}{\partial x^2} + \frac{1}{L_z^2} \frac{\partial^2}{\partial z^2})$. Rearranging based on equation (2.17), then multiplying equation (2.20) by L_z^4 , we get

$$\begin{aligned} \mathcal{W}^2 L_x L_z \nabla^2 \Psi_t - \mathcal{W}^2 L_x L_z \Psi_z \nabla^2 \Psi_x + \mathcal{W}^2 L_x L_z \Psi_x \nabla^2 \Psi_z = & - \mathcal{W}^2 L_x L_z \frac{g}{\rho_0} \rho_x \\ & + \nu \mathcal{M} \mathcal{W} L_x \nabla^2 (\nabla^2 \Psi), \end{aligned} \quad (2.21)$$

where the differential operator is now $\nabla^2 = L_z^2 \tilde{\nabla}^2 = (\delta \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2})$ with $\delta = \frac{L_z^2}{L_x^2}$. The ratio $\frac{L_z}{L_x}$ is called the aspect ratio. Dividing equation (2.21) by $(\mathcal{W}^2 L_x L_z)$, we obtain

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + \frac{\nu \mathcal{M}}{\mathcal{W} L_z} \nabla^2 (\nabla^2 \Psi). \quad (2.22)$$

Similarly, equation (2.7) can be written in dimensionless form as

$$\frac{D}{\tau} \rho_t - \frac{D \mathcal{W}}{L_z} \Psi_z \rho_x + \frac{D \mathcal{W}}{L_z} \Psi_x \rho_z = \kappa \kappa D \left(\frac{1}{L_x^2} \frac{\partial^2}{\partial x^2} + \frac{1}{L_z^2} \frac{\partial^2}{\partial z^2} \right) \rho - \alpha \mathcal{A} \mathcal{H} J. \quad (2.23)$$

Multiplying by L_z^2 , we get

$$D \mathcal{W} L_z \rho_t - D \mathcal{W} L_z \Psi_z \rho_x + D \mathcal{W} L_z \Psi_x \rho_z = \kappa \kappa D \left(\frac{L_z^2}{L_x^2} \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) \rho - L_z^2 \alpha \mathcal{A} \mathcal{H} J, \quad (2.24)$$

which then reduces to

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = \frac{\kappa \kappa}{\mathcal{W} L_z} \nabla^2 \rho - \frac{L_z \alpha \mathcal{A} \mathcal{H}}{D \mathcal{W}} J. \quad (2.25)$$

Therefore the system consisting of equations (2.22) and (2.25) has the form

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + Re^{-1} \nabla^2 (\nabla^2 \Psi) \quad (2.26)$$

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = Re^{-1} Pr^{-1} \nabla^2 \rho - \frac{\tau \alpha \mathcal{A} \mathcal{H}}{D} J, \quad (2.27)$$

where the Reynolds and Prandtl numbers are given respectively as

$$Re = \frac{\mathcal{W} L_z}{\nu \mathcal{M}},$$

$$Pr = \frac{\nu \mathcal{M}}{\kappa \kappa}.$$

The fluid (air) in the atmosphere has low viscosity, and thus the Reynold's num-

ber may be considered to be a large parameter. The Prandtl number for air is approximately 0.71. Thus, in studying gravity waves in the atmosphere, the viscosity and heat conduction terms in (2.26) and (2.27) can be neglected as a first approximation.

In the dimensional chemical transport equation (2.13), C is the mixing ratio which is defined by (2.12). So C is nondimensional, but the independent spatial and temporal variables and the diffusion parameter are dimensional. The source term $S(C)$ is also dimensional since it involves a reaction-rate parameter with unit s^{-1} . We define nondimensional variables by (2.16) and a nondimensional diffusion parameter by $\mathcal{D} = \frac{\mathcal{D}^*}{\mathcal{D}_s}$ where $\mathcal{D}_s$ is a reference value. We also define the nondimensional source term as $S = \left(\frac{S^*}{\tau}\right)$. The nondimensional form of the chemical equation (2.13) is then given as

$$\frac{1}{\tau}C_t + \frac{\mathcal{U}}{L_x}U C_x + \frac{\mathcal{W}}{L_z}W C_z = \mathcal{D}\mathcal{D}_s \left(\frac{1}{L_x^2}C_{xx} + \frac{1}{L_z^2}C_{zz} \right) + \frac{1}{\tau}S(C). \quad (2.28)$$

From (2.17), we have

$$\frac{\mathcal{W}}{L_z}C_t + \frac{\mathcal{W}}{L_z}U C_x + \frac{\mathcal{W}}{L_z}W C_z = \frac{\mathcal{D}\mathcal{D}_s}{L_z^2}(\delta C_{xx} + C_{zz}) + \frac{\mathcal{W}}{L_z}S(C), \quad (2.29)$$

where $\delta = \frac{L_z^2}{L_x^2}$ is the square of the aspect ratio, as before. Multiplying by $\frac{L_z}{\mathcal{W}}$, we obtain the nondimensional equation

$$C_t + U C_x + W C_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + S(C). \quad (2.30)$$

where $\mathcal{D} = \frac{\mathcal{D}\mathcal{D}_s}{\mathcal{W}L_z}$.

2.4 Equations for a gravity wave perturbation

In atmospheric applications where there are propagating waves, it is common, as shown for example by Nappo (2002), to represent the dimensional density ρ^* and dimensional streamfunction Ψ^* in terms of background and perturbation (wave) quantities in the form

$$\Psi^*(x, z, t) = \bar{\psi}^*(z) + \psi^*(x, z, t) \quad \text{and} \quad \rho^*(x, z, t) = \bar{\rho}^*(z) + \rho^*(x, z, t). \quad (2.31)$$

These expressions can be made nondimensional by dividing each quantity by its corresponding reference scale. We define the nondimensional total streamfunction Ψ and density ρ as in (2.18) and define the perturbation quantities in nondimensional forms by $\psi = \frac{\psi^*}{\varphi}$ and $\rho = \frac{\rho^*}{D_p}$ to obtain (2.31) in a nondimensional form written as

$$\Psi(x, z, t) = \bar{\psi}(z) + \varepsilon\psi(x, z, t) \quad \text{and} \quad \rho(x, z, t) = \bar{\rho}(z) + \varepsilon\rho(x, z, t), \quad (2.32)$$

where $\varepsilon = \frac{\varphi}{UL_z} = \frac{D_p}{D}$ gives the magnitude of the perturbations relative to the background flow. We consider the situation where the perturbations are small relative to the background flow quantities and thus $\varepsilon \ll 1$. The background flow is taken to be a horizontal flow with vertical shear— i.e the horizontal component of the background flow velocity is $\bar{u}(z) = -\bar{\psi}'(z)$ — and the vertical component $\bar{w}$ is zero. Substituting (2.32) into (2.26) and (2.27), we obtain

$$\varepsilon \nabla^2 \psi_t - (\bar{\psi}' + \varepsilon\psi_z)\varepsilon \nabla^2 \psi_x + \varepsilon\psi_x(\bar{\psi}''' + \varepsilon \nabla^2 \psi_z) = \frac{\varepsilon g}{\bar{\rho}} \rho_x + \mathbf{v} \nabla^2 (\bar{\psi}'' + \varepsilon \nabla^2 \psi) \quad (2.33)$$

and

$$\varepsilon \rho_t - \varepsilon(\bar{\psi}' + \varepsilon \psi_z) \rho_x + \varepsilon \psi_x (\bar{\rho}' + \varepsilon \rho_z) = \varkappa \bar{\rho}'' + \varkappa \varepsilon \nabla^2 \rho - \frac{\varepsilon \tau \alpha \mathcal{A} \mathcal{H}}{D_p} J, \quad (2.34)$$

where the primes denote the derivative with respect to z , $\mathfrak{v} = Re^{-1}$ and $\varkappa = Re^{-1} Pr^{-1}$. As noted before, we consider an atmospheric flow that is almost inviscid with very weak heat conduction as well. We consider the balance where $\mathfrak{v} \ll \varepsilon^2 \ll \varepsilon$ and $\varkappa \ll \varepsilon^2 \ll \varepsilon$ and hence the effects of viscosity and heat conduction are much less than the nonlinear effects in equations (2.33) and (2.34). Thus, the parameters $\mathfrak{v}$ and $\varkappa$ are very small and are neglected in the analysis. Neglecting the terms involving $\mathfrak{v}$ and $\varkappa$ and dividing (2.33) and (2.34) by ε , we obtain

$$\nabla^2 \psi_t + \bar{u} \nabla^2 \psi_x - \bar{u}'' \psi_x + \varepsilon (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) = -\frac{g}{\bar{\rho}} \rho_x \quad (2.35)$$

and

$$\rho_t + \bar{u} \rho_x + \bar{\rho}' \psi_x + \varepsilon (\psi_x \rho_z - \psi_z \rho_x) = -\mathcal{K} J, \quad (2.36)$$

where $\mathcal{K} = \frac{\tau \alpha \mathcal{A} \mathcal{H}}{D_p}$.

The perturbation vorticity is defined as $\zeta = w_x - u_z = \delta \psi_{xx} + \psi_{zz} = \nabla^2 \psi$. In terms of the perturbation vorticity, equation (2.35) can be written as

$$\zeta_t + \bar{u} \zeta_x - \bar{u}'' \psi_x + \varepsilon (\psi_x \zeta_z - \psi_z \zeta_x) = -\frac{g}{\bar{\rho}} \rho_x. \quad (2.37)$$

Therefore, from (2.37) and (2.36), we obtain equations which define a simple model that we shall use to study gravity waves under the Boussinesq approximation and under the influence of heating from a chemical. These equations are

given as

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\bar{\rho}}\rho_x, \quad (2.38)$$

$$\zeta = \nabla^2\psi, \quad (2.39)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = -\mathcal{K}J. \quad (2.40)$$

These equations can be used to represent gravity waves generated by a source such as convection or topography at some altitude $z = z_1$ in the atmosphere and propagate upwards as $z \rightarrow \infty$. Thus we define the domain to be the semi-infinite rectangular region $z_1 < z < \infty$, $x_1 < x < x_2$. The gravity-wave source can then be approximated by a suitable oscillatory boundary condition at $z = z_1$.

2.5 Configuration of the model

The full model we are studying in this thesis is composed of the gravity wave-equations (2.38), (2.39) and (2.40), coupled with equation (2.30) representing the chemical transport. As shown by Holton (2004) and as will be discussed in more detail in Chapter 6, the heating rate due to the chemical in equation (2.40) is proportional to $(-\frac{DC}{Dt})$ and can be expressed as $J = -\mathcal{H}\frac{DC}{Dt}$, where $\mathcal{H}$ is a parameter related to the chemical under study. An example of such parameter is the latent heat, as in the case of water vapour in Chapter 6. In the chemical-transport equation, the velocity components are $U = \bar{u} + \varepsilon u$ and $W = \varepsilon w$ where $\bar{u}$ is a constant or a function of z and the perturbation quantities $u = -\psi_z$ and $w = \psi_x$. Thus the full model representing gravity waves interacting with a chemical constituent in the atmosphere is given as

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\bar{\rho}}\rho_x, \quad (2.41)$$

$$\zeta = \nabla^2\psi, \quad (2.42)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = \gamma\frac{DC}{Dt}, \quad (2.43)$$

$$\frac{\partial C}{\partial t} + (\bar{u} + \varepsilon u)\frac{\partial C}{\partial x} + \varepsilon w\frac{\partial C}{\partial z} = \mathcal{D}(\delta C_{xx} + C_{zz}) + S(C), \quad (2.44)$$

$$u = -\psi_z \quad \text{and} \quad w = \psi_x, \quad (2.45)$$

where $\gamma = \mathcal{KH}$ is the heating coefficient.

We define the domain to be the rectangular region $z_1 \leq z \leq z_2$, $x_1 \leq x \leq x_2$. The forcing is represented by the lower boundary condition of the streamfunction given as

$$\psi(x, z_1, t) = A(\mu x)e^{ik_0 x} + \text{c.c.}, \quad (2.46)$$

where c.c. represents the complex conjugate. The parameter $\mu \ll 1$, so A is a slowly varying function and $A \rightarrow 0$ as $x \rightarrow \pm\infty$; k_0 is the forcing wavenumber. The boundary condition (2.46) generates a perturbation in the form of a horizontally localized wave packet comprising a spectrum of wavenumbers centred at k_0 . The special case where $A = 1$ gives a boundary condition that generates a monochromatic wave with a single wavenumber k_0 . The nonlinear terms in equations (2.41) and (2.43) mean that other horizontal wavenumbers are generated by a product that involves the wavenumbers k_0 and $-k_0$. The perturbation vorticity ζ and perturbation density ρ are considered zero at the lower boundary z_1 . The initial conditions are defined as $\zeta(x, z, 0) = 0$, $\zeta_t(x, z, 0) = 0$ and $\rho(x, z, 0) = 0$.

The upper boundary condition is the requirement that the waves generated at $z = z_1$ propagate upwards to infinity, so there is no incoming energy from infinity. This means that, as discussed in Appendix D, only waves with upward (positive)

group velocity can be present.

The initial condition for the chemical mixing ratio C is in the form where $C \rightarrow 0$ as $x, z \rightarrow \infty$ and $C \rightarrow \text{constant}$ as $x, z \rightarrow -\infty$. This form of initial profile is shown, for example, by Gille and Lyjak (1986), where the heating released in the atmosphere due to several chemicals is investigated. This initial condition generates a travelling wave, which maintains a profile satisfying these boundary conditions for all time. One possible form of the initial condition for C is the profile satisfying $C \rightarrow 0$ as $x, z \rightarrow \infty$ and $C \rightarrow 1$ as $x, z \rightarrow -\infty$. Another possible form of the initial condition for C is the Gaussian form with $C \rightarrow 0$ as $x, z \rightarrow \pm\infty$. The latter form is more appropriate representation for the chemicals and hence is mostly considered. The former is considered in the analytical discussion where an exact solution corresponding to the choice of the source term $S(C)$ can be found in Chapter 3. These two possible forms of C can be related and can be compared under some conditions as discussed in Chapter 5.

The nonlinear term $S(C)$ is intended to represent reactions of the chemical such as those arising from the effect of ultraviolet radiation as will be seen in Chapter 6. We consider $S(C) = -\sigma C$ with which (2.30) gives the advection-reaction-diffusion equation, and $S(C) = \sigma C(1 - C)$ with which equation (2.30) represents the well-known Fisher's equation. The analytical and numerical solutions of both of these two forms of equations are discussed in Chapter 3.

Chemical heating in (2.43) affects the energy of the atmosphere and hence affects the energy of gravity waves. Gravity waves affect the distribution of the chemical as can be seen in equation (2.44), where the advection speed of the chemical is modified by the gravity wave perturbations. The latter effect is studied analytically in Chapter 3 and numerically in Chapter 5. Analytical approximations of the effect of the chemical heating on gravity waves are obtained in Chapter 4.

Numerical simulations for the full model, which considers both effects, are obtained in Chapter 6.

Chapter 3

The Analytical and Numerical Solutions of the Chemical Equation

In this thesis, we examine situations where gravity waves are affected by chemical heating in the atmosphere and the distribution of a chemical is affected by wave-induced perturbations to the advection speed of the background flow. In this chapter, we give an overview of simple one-dimensional and two-dimensional representations for the concentration of a chemical species in a fluid medium where the advection of the chemical species takes the form of a travelling wave. We introduce some analytical solutions and compare them with the corresponding numerical approximations of the chemical equation. We then consider the solution that arises when the background wind speed is perturbed. This is the situation that arises when gravity-wave interactions generate a wave-induced mean flow as we shall see in the gravity wave numerical simulations in Chapter 4. We first discuss the case where the source term in the chemical-transport equation is linear in Section 3.1. The case where the source term is nonlinear is then discussed in Section 3.2.

The most general form of the equation studied in this chapter is given by equation (2.30),

$$C_t + U(x, z, t) C_x + W(x, z, t) C_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + S(C), \quad (3.1)$$

derived in Chapter 2. In Section 3.1, we consider the case with a linear source term $S(C)$. Section 3.2 is devoted to the discussion of the nonlinear source term. In Section 3.2.1, we consider the case where the advection velocity components U and W are constant. In Section 3.2.2, we consider the perturbed problem where the horizontal advection speed U is a constant plus a z -dependent perturbation quantity and the vertical advection speed W is zero. The numerical solution of equation (3.1) with the nonlinear source term is presented in Section 3.3.

3.1 Linear equation

We first consider the chemical transport equation (3.1) with a linear source term and with the diffusion neglected,

$$C_t + U(x, z, t) C_x + W(x, z, t) C_z = -\sigma C. \quad (3.2)$$

We consider equation (3.2) in the domain $-\infty < x < \infty$, $-\infty < z < \infty$ for $t \geq 0$ and with initial condition $C(x, z, 0) = \bar{C}(x, z)$. The initial condition $\bar{C}(x, z)$ is assumed to be continuous, differentiable and satisfying $\bar{C}(x, z) \rightarrow 1$ as $x, z \rightarrow -\infty$ and $\bar{C}(x, z) \rightarrow 0$ as $x, z \rightarrow \infty$. This is a Cauchy problem, which can be solved using the method of characteristics. We introduce characteristic variables (ξ, η, s)

as a transformation of (x, z, t) ; we then have the characteristic equations

$$\frac{\partial x}{\partial s} = U(x, z, t), \quad (3.3)$$

$$\frac{\partial z}{\partial s} = W(x, z, t), \quad (3.4)$$

$$\frac{\partial t}{\partial s} = 1 \quad (3.5)$$

and

$$\frac{\partial C}{\partial s} = -\sigma C, \quad (3.6)$$

with initial conditions given, respectively, as

$$x(\xi, \eta, 0) = \xi, z(\xi, \eta, 0) = \eta, t(\xi, \eta, 0) = 0, C(\xi, \eta, 0) = \bar{C}(\xi, \eta). \quad (3.7)$$

From equation (3.5) and its corresponding initial condition $t(\xi, \eta, 0) = 0$, we find that $t = s$. If U and W are constant, equation (3.3), with $x(\xi, \eta, 0) = \xi$, is solved to give $x = Ut + \xi$, so we have

$$\xi = x - Ut. \quad (3.8)$$

Similarly, from equation (3.4), along with its initial condition $z(\xi, \eta, 0) = \eta$, we obtain

$$\eta = z - Wt. \quad (3.9)$$

The solution C can be obtained from equation (3.6) along with its initial condition $C(\xi, \eta, 0) = \bar{C}(\xi, \eta)$ as

$$C(\xi, \eta, s) = \bar{C}(\xi, \eta)e^{-\sigma s}. \quad (3.10)$$

In terms of the variables (x, z, t) , the solution C is

$$C(x, z, t) = \bar{C}(x - Ut, z - Wt)e^{-\sigma t}. \quad (3.11)$$

This describes linear transport with velocity components U and W in the x and z directions respectively and with an exponential decay rate of σ .

3.2 Nonlinear Fisher's equation

3.2.1 Analytical solutions

In this section, we discuss a special case of a nonlinear advection-diffusion-reaction equation of the form (3.1) for which we are able to derive exact solutions in the form of a travelling wave that maintains its shape for all time. The equation discussed is known as Fisher's equation, and its properties are well known [Bramson (1983)]. We describe one-dimensional and two-dimensional cases. The two-dimensional Fisher's equation with advection terms is

$$C_t + U C_x + W C_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + \sigma C(1 - C), \quad (3.12)$$

and we consider it in the domain $-\infty < x < \infty$, $-\infty < z < \infty$ for $t \geq 0$. In this section, we consider the case where the advection velocity components U and W are constant.

The one-dimensional case

We start with the one-dimensional case in the x -direction with $U = 0$, so we obtain the well-known Fisher's equation

$$C_t = \tilde{\mathcal{D}}C_{xx} + \sigma C(1 - C), \quad (3.13)$$

where $\tilde{\mathcal{D}} = \delta\mathcal{D}$. Introducing a new independent variable $\xi = x - ct$ and writing $C(\xi) = C(x, t)$, we obtain an ordinary differential equation

$$\tilde{\mathcal{D}}C_{\xi\xi} + cC_{\xi} + \sigma C(1 - C) = 0. \quad (3.14)$$

We rescale ξ by $\tilde{\xi} = \frac{\sqrt{\sigma}}{\sqrt{\tilde{\mathcal{D}}}}\xi$ so that equation (3.14) is rewritten in scaled form as

$$C_{\tilde{\xi}\tilde{\xi}} + \tilde{c}C_{\tilde{\xi}} + C(1 - C) = 0, \quad (3.15)$$

where $\tilde{c} = \frac{c}{\sqrt{\sigma\tilde{\mathcal{D}}}}$. A travelling-wave solution of this scaled equation (3.15) with a certain wave speed $\tilde{c} = \frac{5}{\sqrt{6}}$, as shown by Ablowitz and Zeppetella (1979), has the form

$$C(\tilde{\xi}) = \frac{1}{\left(1 + \exp\left(\frac{\tilde{\xi}}{\sqrt{6}}\right)\right)^2}, \quad (3.16)$$

where $C(\tilde{\xi}) \rightarrow 1$ as $\tilde{\xi} \rightarrow -\infty$ and $C(\tilde{\xi}) \rightarrow 0$ as $\tilde{\xi} \rightarrow \infty$. In terms of the original variables x and t with a wave speed $c = \sqrt{\sigma\tilde{\mathcal{D}}}\tilde{c} = \frac{5\sqrt{\sigma\tilde{\mathcal{D}}}}{\sqrt{6}}$, the solution of equation (3.13) is given as

$$C(x, t) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\tilde{\mathcal{D}}}}(x-ct)}{\sqrt{6}}\right)\right)^2}. \quad (3.17)$$

A plot of this solution as a function of x at different times is shown in Figure 3.1.

Figure 3.1: The solution $C(x, t)$ of Fisher's equation (3.13) at different times with $\tilde{D} = 1$ and $\sigma = 1$.

The solution (3.17) corresponds to the case where the background wind speed is given by $U = 0$. If we consider the background wind speed U to be a nonzero constant, we obtain a modified Fisher's equation given as

$$C_t + U C_x = \tilde{D} C_{xx} + \sigma C(1 - C). \quad (3.18)$$

The analogous equation of (3.15) that corresponds to equation (3.18) has the constant $\left(\tilde{c} - \frac{1}{\sqrt{\sigma\tilde{D}}}U\right)$ as a coefficient of the first derivative $C_{\tilde{\xi}}$. Following the approach shown by Ablowitz and Zeppetella (1979), a travelling-wave solution of (3.18), in terms of the original variables x and t , is

$$C(x, t) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\tilde{D}}}(x-ct)}{\sqrt{6}}\right)\right)^2}, \quad (3.19)$$

with wave speed $c = U + \frac{5\sqrt{\sigma\tilde{D}}}{\sqrt{6}}$.

The two-dimensional equation

In this section, we discuss the two-dimensional Fisher's equation

$$C_t + U C_x + W C_z = \tilde{\mathcal{D}} C_{xx} + \mathcal{D} C_{zz} + \sigma C(1 - C). \quad (3.20)$$

We first start with the case where $U = W = 0$, so equation (3.20) reduces to

$$C_t = \tilde{\mathcal{D}} C_{xx} + \mathcal{D} C_{zz} + \sigma C(1 - C). \quad (3.21)$$

We rescale the variables x , z and t by

$$X = \sqrt{\frac{\sigma}{\tilde{\mathcal{D}}}} x, \quad (3.22)$$

$$Z = \sqrt{\frac{\sigma}{\mathcal{D}}} z \quad (3.23)$$

and

$$T = \sigma t. \quad (3.24)$$

Then equation (3.21) becomes

$$C_T = C_{XX} + C_{ZZ} + C(1 - C). \quad (3.25)$$

Equation (3.25) is solved on the domain $-\infty < X < \infty$ and $-\infty < Z < \infty$ with $C \rightarrow 1$ as $X, Z \rightarrow -\infty$ and $C \rightarrow 0$ as $X, Z \rightarrow \infty$. We consider an initial condition of the form $C(X, Z, 0) = \bar{C}(X, Z)$ where $\bar{C} \rightarrow 1$ as $X, Z \rightarrow -\infty$ and $\bar{C} \rightarrow 0$ as $X, Z \rightarrow \infty$ with wave front tilted at an angle θ . A travelling-wave solution propagating along an axis $\bar{X}$, which is tilted by an angle θ from the X -axis and is perpendicular to the wave front parallel to $\bar{Z}$, can be found following Tyson

and Brazhnik (2000). We apply a rotation-of-variables approach, where the new variables $\bar{X}$ and $\bar{Z}$ are defined as

$$\bar{X} = X \cos(\theta) + Z \sin(\theta),$$

$$\bar{Z} = -X \sin(\theta) + Z \cos(\theta).$$

Using the chain rule, we find the partial derivatives

$$\begin{aligned} C_X &= \frac{\partial C}{\partial \bar{X}} \frac{\partial \bar{X}}{\partial X} + \frac{\partial C}{\partial \bar{Z}} \frac{\partial \bar{Z}}{\partial X} = \cos(\theta) C_{\bar{X}} - \sin(\theta) C_{\bar{Z}} \\ C_{XX} &= \frac{\partial^2 C}{\partial \bar{X}^2} \left(\frac{\partial \bar{X}}{\partial X} \right)^2 + \frac{\partial^2 C}{\partial \bar{X} \partial \bar{Z}} \frac{\partial \bar{Z}}{\partial X} \frac{\partial \bar{X}}{\partial X} + \frac{\partial^2 C}{\partial \bar{Z} \partial \bar{X}} \frac{\partial \bar{X}}{\partial X} \frac{\partial \bar{Z}}{\partial X} + \frac{\partial^2 C}{\partial \bar{Z}^2} \left(\frac{\partial \bar{Z}}{\partial X} \right)^2 \\ &= \cos^2(\theta) C_{\bar{X}\bar{X}} - 2 \cos(\theta) \sin(\theta) C_{\bar{X}\bar{Z}} + \sin^2(\theta) C_{\bar{Z}\bar{Z}}. \end{aligned}$$

Similarly, we find

$$\begin{aligned} C_Z &= \frac{\partial C}{\partial \bar{Z}} \frac{\partial \bar{Z}}{\partial Z} + \frac{\partial C}{\partial \bar{X}} \frac{\partial \bar{X}}{\partial Z} = \cos(\theta) C_{\bar{Z}} + \sin(\theta) C_{\bar{X}} \\ C_{ZZ} &= \frac{\partial^2 C}{\partial \bar{Z}^2} \left(\frac{\partial \bar{Z}}{\partial Z} \right)^2 + \frac{\partial^2 C}{\partial \bar{Z} \partial \bar{X}} \frac{\partial \bar{X}}{\partial Z} \frac{\partial \bar{Z}}{\partial Z} + \frac{\partial^2 C}{\partial \bar{X} \partial \bar{Z}} \frac{\partial \bar{Z}}{\partial Z} \frac{\partial \bar{X}}{\partial Z} + \frac{\partial^2 C}{\partial \bar{X}^2} \left(\frac{\partial \bar{X}}{\partial Z} \right)^2 \\ &= \cos^2(\theta) C_{\bar{Z}\bar{Z}} + 2 \cos(\theta) \sin(\theta) C_{\bar{X}\bar{Z}} + \sin^2(\theta) C_{\bar{X}\bar{X}}. \end{aligned}$$

Equation (3.25) is expressed in terms of the space variables $\bar{X}$ and $\bar{Z}$ as

$$\begin{aligned} C_T &= \cos^2(\theta) C_{\bar{X}\bar{X}} + \sin^2(\theta) C_{\bar{Z}\bar{Z}} + \cos^2(\theta) C_{\bar{Z}\bar{Z}} + \sin^2(\theta) C_{\bar{X}\bar{X}} + C(1 - C) \\ &= C_{\bar{X}\bar{X}} + C_{\bar{Z}\bar{Z}} + C(1 - C). \end{aligned} \tag{3.26}$$

The solution is propagating along the $\bar{X}$ -axis and is constant along the $\bar{Z}$ -axis, so the terms involving derivatives with respect to $\bar{Z}$ in equation (3.26) are zero. In

terms of $\bar{\xi} = \bar{X} - \tilde{c}T$, equation (3.26) is given as

$$\tilde{c}C_{\bar{\xi}} + C_{\bar{\xi}\bar{\xi}} + C(1 - C) = 0, \quad (3.27)$$

which has a travelling-wave solution given as

$$C(\bar{X}, T) = \frac{1}{\left(1 + \exp\left(\frac{\bar{X} - \tilde{c}T}{\sqrt{6}}\right)\right)^2}, \quad (3.28)$$

where $\tilde{c} = \frac{5}{\sqrt{6}}$. Substituting $\bar{X} = X \cos(\theta) + Z \sin(\theta)$, we then get a travelling-wave solution for equation (3.25) given as

$$C(X, Z, T) = \frac{1}{\left(1 + \exp\left(\frac{X \cos(\theta) + Z \sin(\theta) - \tilde{c}T}{\sqrt{6}}\right)\right)^2}. \quad (3.29)$$

In terms of the original variables, x , z and t , with a wave speed $c = \sqrt{\sigma\tilde{\mathcal{D}}}\tilde{c} = \frac{5\sqrt{\sigma\tilde{\mathcal{D}}}}{\sqrt{6}}$, the solution of equation (3.21) is then given as

$$C(x, z, t) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\tilde{\mathcal{D}}}}(x \cos(\theta) + \sqrt{\tilde{\mathcal{D}}}z \sin(\theta) - ct)}{\sqrt{6}}\right)\right)^2}. \quad (3.30)$$

For the two-dimensional equation (3.20) with constant advection speed, we follow the same approach of rotating variables. First, rescaling the variables x , z and t by (3.22), (3.23) and (3.24), respectively, equation (3.20) becomes

$$C_T + \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}}UC_X + \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}}WC_Z = C_{XX} + C_{ZZ} + C(1 - C). \quad (3.31)$$

Rewriting equation (3.31) in terms of $\bar{X}$ and $\bar{Z}$, we get

$$\begin{aligned} C_T + \left(\frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} U \cos(\theta) + \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} W \sin(\theta) \right) C_{\bar{X}} \\ + \left(\frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} W \cos(\theta) - \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} U \sin(\theta) \right) C_{\bar{Z}} = C_{\bar{X}\bar{X}} + C_{\bar{Z}\bar{Z}} + C(1 - C). \end{aligned} \quad (3.32)$$

Again, the solution is propagating along the $\bar{X}$ -axis and is constant along the $\bar{Z}$ -axis, so all terms involving derivatives with respect to $\bar{Z}$ are zero. Introducing $\bar{\xi} = \bar{X} - \tilde{c}T$, equation (3.32) is rewritten as

$$\tilde{c}C_{\bar{\xi}} - \left(\frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} U \cos(\theta) + \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} W \sin(\theta) \right) C_{\bar{\xi}} + C_{\bar{\xi}\bar{\xi}} + C(1 - C) = 0. \quad (3.33)$$

Rearranging, we have

$$(\tilde{c} - \alpha)C_{\bar{\xi}} + C_{\bar{\xi}\bar{\xi}} + C(1 - C) = 0, \quad (3.34)$$

where $\alpha = \left(\frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} U \cos(\theta) + \frac{1}{\sqrt{\sigma\tilde{\mathcal{D}}}} W \sin(\theta) \right)$. A travelling-wave solution for equation (3.34) is then given as

$$C(\bar{X}, T) = \frac{1}{\left(1 + \exp \left(\frac{\bar{X} - \tilde{c}T}{\sqrt{6}} \right) \right)^2}, \quad (3.35)$$

where $\tilde{c} = \frac{5}{\sqrt{6}} + \alpha$. A travelling-wave solution for equation (3.31) is given as

$$C(X, Z, T) = \frac{1}{\left(1 + \exp \left(\frac{X \cos(\theta) + Z \sin(\theta) - \tilde{c}T}{\sqrt{6}} \right) \right)^2}. \quad (3.36)$$

In terms of the original variables x , z and t , the travelling-wave solution of equation

(3.20) is then given as

$$C(x, z, t) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\mathcal{D}}}(x \cos(\theta) + \sqrt{\delta} z \sin(\theta) - ct)}{\sqrt{6}}\right)\right)^2}, \quad (3.37)$$

where $c = \sqrt{\sigma \tilde{\mathcal{D}}} \tilde{c} = \frac{5\sqrt{\sigma \tilde{\mathcal{D}}}}{\sqrt{6}} + U \cos(\theta) + W \sin(\theta)$, where θ is the initial tilt of the wavefront.

The travelling-wave solution (3.37) satisfies equation (3.20) only if the advection speeds U and W are constant. If one of them is perturbed, then (3.37) is not valid. However, the exact solution (3.37) is still useful, as it can be used to satisfy the leading order of the solution of the perturbed problem as discussed in the next subsection.

3.2.2 Perturbed problem

When the advection speeds U and W in equation (3.12) are not constant, equation (3.12) cannot be solved exactly. In this section, we consider a travelling wave moving only in the x -direction; i.e $\theta = 0$ with U being a function of z and with $W = 0$. We consider a situation where the wind speed U can be expressed as the sum of constant and a small z -dependent perturbation. This configuration is analogous to the situation considered in Chapter 5 where the background mean flow of the chemical is perturbed due to the wave-induced mean flow from the gravity waves. Thus we express the wind speed U in (3.12) as

$$U(z) = \bar{u} + \epsilon \tilde{u}(z), \quad (3.38)$$

where $\bar{u}$ is the background wind speed, $\epsilon \ll 1$, and $\tilde{u}(z)$ is a perturbation to the wind speed such as that due to the gravity wave interactions described in Chapters

5 and 6. We consider the case where the background wind speed is slowly varying, so we approximate it by a constant. From the gravity-wave solutions seen in Figure 4.6, the wave-induced mean flow $\tilde{u}(z)$ has a form in which $\tilde{u}(z) \rightarrow 0$ as $z \rightarrow \pm\infty$ and $\tilde{u}(z)$ is maximum near the critical level z_c as we shall see in Chapter 4 (Figure 4.6). For the purpose of carrying out asymptotic analysis in this section, we represent $\tilde{u}(z)$ by a function of the form $\tilde{u}(z) = e^{-b|z-z_c|}$ or $\tilde{u}(z) = e^{-b^2(z-z_c)^2}$, where b is a positive constant and z_c is the critical level for the gravity waves. In this section, we study the equation

$$C_t + (\bar{u} + \epsilon\tilde{u}(z)) C_x = \delta\mathcal{D}C_{xx} + \mathcal{D}C_{zz} + \sigma C(1 - C), \quad (3.39)$$

on the domain $-\infty < x < \infty$ and $-\infty < z < \infty$ and consider the situation where $\epsilon \ll \delta$. Equation (3.39) is solved with an initial condition of the form $C(x, z, 0) = \bar{C}(x)$ corresponding to wavefront with $\theta = 0$, as can be seen in Figure 3.5, and with the following boundary conditions:

$$C(x, z, t) \rightarrow 1 \text{ as } x \rightarrow -\infty, \quad (3.40)$$

and

$$C(x, z, t) \rightarrow 0 \text{ as } x \rightarrow \infty. \quad (3.41)$$

The solution $C(x, z, t)$ is expressed in terms of a perturbation series as

$$C(x, z, t) = C^{(0)}(x, z, t) + \epsilon C^{(1)}(x, z, t) + O(\epsilon^2). \quad (3.42)$$

We substitute this into equation (3.39) and obtain the leading-order equation

$$O(\epsilon^0) : C_t^{(0)} + \bar{u} C_x^{(0)} = \delta\mathcal{D}C_{xx}^{(0)} + \mathcal{D}C_{zz}^{(0)} + \sigma C^{(0)}(1 - C^{(0)}). \quad (3.43)$$

From Section 3.2.1, we saw that the solution of (3.20) is (3.37). Now we are considering the case where $W = 0$ and $\theta = 0$, so equation (3.43) has an exact solution given by (3.37) with $W = 0$ and $\theta = 0$. This travelling-wave solution can be expressed as $C^{(0)}(\xi) = C^{(0)}(x, ct)$, where $\xi = x - ct$ and $c = \frac{5\sqrt{\sigma\delta\mathcal{D}}}{\sqrt{6}} + \bar{u}$, as given by (3.19).

At $O(\epsilon)$, we have

$$O(\epsilon) : C_t^{(1)} + \bar{u} C_x^{(1)} - \delta \mathcal{D} C_{xx}^{(1)} - \sigma C^{(1)}(1 - 2C^{(0)}) - \mathcal{D} C_{zz}^{(1)} = -\tilde{u}(z) C_x^{(0)}, \quad (3.44)$$

with $C^{(1)}(x, z, 0) = 0$ and with the following boundary conditions

$$C^{(1)}(x, z, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty, \quad (3.45)$$

and

$$C^{(1)}(x, z, t) \rightarrow 0 \text{ as } z \rightarrow \pm\infty. \quad (3.46)$$

Since $C^{(0)}$ in (3.19) depends on $(x - ct)$, the solution of (3.44) depends on $(x - ct)$ and z . We set $\xi = x - ct$ and $C^{(1)}(\xi, z) = C^{(1)}(x, z, t)$, then equation (3.44) is rewritten as

$$C_{\xi\xi}^{(1)} + \gamma C_{\xi}^{(1)} - \beta(\xi) C^{(1)} + \frac{1}{\delta} C_{zz}^{(1)} = \tilde{u}(z) f(\xi), \quad (3.47)$$

where $\gamma = \frac{5\sqrt{\sigma}}{\sqrt{6\delta\mathcal{D}}}$, $\beta(\xi) = \frac{\sigma}{\delta\mathcal{D}}(2C^{(0)} - 1)$, $f(\xi) = \frac{C_{\xi}^{(0)}}{\delta\mathcal{D}}$, and $C^{(1)} \rightarrow 0$ as $\xi \rightarrow \pm\infty$ and $C^{(1)} \rightarrow 0$ as $z \rightarrow \pm\infty$. The subscripts denote partial derivatives.

Equation (3.47) can be solved using the method of Fourier transforms. The Fourier transforms $\hat{C}(\xi, \lambda)$ and $\hat{u}(\lambda)$ are defined with respect to z as

$$\hat{C}(\xi, \lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C^{(1)}(\xi, z) e^{-i\lambda z} dz \quad (3.48)$$

and

$$\hat{u}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \tilde{u}(z) e^{-i\lambda z} dz. \quad (3.49)$$

Then $C^{(1)}(\xi, z)$ and $\tilde{u}(z)$ can be represented in terms of inverse Fourier transforms as

$$C^{(1)}(\xi, z) = \int_{-\infty}^{\infty} \hat{C}(\xi, \lambda) e^{i\lambda z} d\lambda \quad (3.50)$$

and

$$\tilde{u}(z) = \int_{-\infty}^{\infty} \hat{u}(\lambda) e^{i\lambda z} d\lambda. \quad (3.51)$$

Taking the Fourier transform of equation (3.47) using the definitions (3.48) and (3.49), the transformed equation, for each Fourier mode λ , is

$$\hat{C}_{\xi\xi}(\xi, \lambda) + \gamma \hat{C}_{\xi}(\xi, \lambda) - \left(\beta(\xi) + \frac{1}{\delta} \lambda^2 \right) \hat{C}(\xi, \lambda) = f(\xi) \hat{u}(\lambda), \quad (3.52)$$

with $\hat{C}(\xi, \lambda) \rightarrow 0$ as $\xi \rightarrow \pm\infty$. Equation (3.52) is a nonhomogenous ordinary differential equation with respect to ξ , and its solution consists of a sum of a linear combination of linearly independent solutions of the corresponding homogenous equation and a particular solution of the corresponding nonhomogenous equation. We first discuss the solution of the corresponding homogenous equation

$$\hat{C}_{\xi\xi} + \gamma \hat{C}_{\xi} - \left(\beta(\xi) + \frac{1}{\delta} \lambda^2 \right) \hat{C} = 0, \quad (3.53)$$

with $\hat{C}(\xi, \lambda) \rightarrow 0$ as $\xi \rightarrow \pm\infty$. This equation cannot be solved exactly, so we use the WKB method (following Bender and Orszag (1999)) to obtain an asymptotic approximations.

We rewrite equation (3.53) in a form that is compatible with the WKB theory by introducing $Q(\xi, \lambda)$ such that, for each λ , we have $\hat{C}(\xi, \lambda) = e^{-\frac{\gamma}{2}\xi} Q(\xi, \lambda)$.

Equation (3.53) can then be written as

$$Q_{\xi\xi}(\xi, \lambda) - \left(\frac{\gamma^2}{4} + \beta(\xi) + \frac{1}{\delta} \lambda^2 \right) Q(\xi, \lambda) = 0. \quad (3.54)$$

Setting $P(\xi, \lambda) = \beta(\xi) + \frac{1}{\delta} \lambda^2 + \frac{\gamma^2}{4}$, equation (3.54) is rewritten as

$$Q_{\xi\xi}(\xi, \lambda) - P(\xi, \lambda)Q(\xi, \lambda) = 0. \quad (3.55)$$

As shown in Appendix C, if $P_\xi \ll P^{\frac{3}{2}}$, then P is slowly varying with respect to ξ , and the WKB method is valid. $P_\xi \ll P^{\frac{3}{2}}$ can be expressed as $\frac{P_\xi}{P^{\frac{3}{2}}} \ll 1$. As $\xi \rightarrow -\infty$, we have

$$\lim_{\xi \rightarrow -\infty} \frac{P_\xi}{2P^{\frac{3}{2}}} = \lim_{\xi \rightarrow -\infty} \frac{\frac{\sigma}{\delta \mathcal{D}} C_\xi^{(0)}(\xi)}{\left(\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} (2C^{(0)}(\xi) - 1) + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} = \frac{\lim_{\xi \rightarrow -\infty} \frac{\frac{\sigma}{\delta \mathcal{D}} \frac{-2}{\sqrt{6}} e^{\frac{\xi}{\sqrt{6}}}}{(1+e^{\frac{\xi}{\sqrt{6}}})^3}}{\left(\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} = 0,$$

where $C^{(0)}$ is given by (3.19). As $\xi \rightarrow \infty$, we have

$$\lim_{\xi \rightarrow \infty} \frac{P_\xi}{2P^{\frac{3}{2}}} = \lim_{\xi \rightarrow \infty} \frac{\frac{\sigma}{\delta \mathcal{D}} C_\xi^{(0)}(\xi)}{\left(\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} (2C^{(0)}(\xi) - 1) + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} = \frac{\lim_{\xi \rightarrow \infty} \frac{\frac{\sigma}{\delta \mathcal{D}} \frac{-2}{\sqrt{6}} e^{\frac{\xi}{\sqrt{6}}}}{(1+e^{\frac{\xi}{\sqrt{6}}})^3}}{\left(\frac{\gamma^2}{4} - \frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} = 0.$$

Thus, we have $\frac{P_\xi}{2P^{\frac{3}{2}}} \ll 1$ as $\xi \rightarrow \pm\infty$, which means that P is slowly varying and the WKB approximation is valid as $\xi \rightarrow \pm\infty$. As $\xi \rightarrow 0$ we find that

$$\lim_{\xi \rightarrow 0} \frac{P_\xi}{2P^{\frac{3}{2}}} = \lim_{\xi \rightarrow 0} \frac{\frac{\sigma}{\delta \mathcal{D}} C_\xi^{(0)}(\xi)}{\left(\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} (2C^{(0)}(\xi) - 1) + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} = \frac{\lim_{\xi \rightarrow 0} \frac{\frac{\sigma}{\delta \mathcal{D}} \frac{-2}{\sqrt{6}} e^{\frac{\xi}{\sqrt{6}}}}{(1+e^{\frac{\xi}{\sqrt{6}}})^3}}{\left(\frac{\gamma^2}{4} - \frac{\sigma}{2\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2 \right)^{\frac{3}{2}}} \neq 0,$$

so as $\xi \rightarrow 0$, P is not slowly varying with respect to ξ and the WKB approximation is not valid around $\xi = 0$.

Since $\frac{P_\xi}{P^{\frac{3}{2}}} \ll 1$ as $\xi \rightarrow \pm\infty$, we note that $P(\xi)$ is slowly varying as $\xi \rightarrow \pm\infty$, and hence, according to Appendix C, the WKB approximations (C.25) and (C.24) are expressed in terms of ξ as

$$Q(\xi, \lambda) \sim \frac{e^{\pm i \int \sqrt{-P(\xi, \lambda)} d\xi}}{(-P(\xi, \lambda))^{\frac{1}{4}}}, \text{ if } P(\xi, \lambda) < 0, \quad (3.56)$$

and

$$Q(\xi, \lambda) \sim \frac{e^{\pm i \int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}}, \text{ if } P(\xi, \lambda) > 0. \quad (3.57)$$

If $P(\xi, \lambda) = 0$ at some point $\xi = \xi_0$, then there is a turning point at $\xi = \xi_0$.

From (3.19), we find that $C^{(0)}(\xi) \rightarrow 1$ as $\xi \rightarrow -\infty$ and $C^{(0)}(\xi) \rightarrow 0$ as $\xi \rightarrow \infty$, and we have

$$\begin{aligned} 1 &> C^{(0)}(\xi) > 0 \\ 2 &> 2C^{(0)}(\xi) > 0 \\ 1 &> 2C^{(0)}(\xi) - 1 > -1 \\ \frac{\sigma}{\delta\mathcal{D}} &> \frac{\sigma}{\delta\mathcal{D}} (2C^{(0)}(\xi) - 1) > -\frac{\sigma}{\delta\mathcal{D}} \\ \frac{\sigma}{\delta\mathcal{D}} + \frac{\gamma^2}{4} + \frac{1}{\delta}\lambda^2 &> \frac{\sigma}{\delta\mathcal{D}} (2C^{(0)}(\xi) - 1) + \frac{\gamma^2}{4} + \frac{1}{\delta}\lambda^2 > -\frac{\sigma}{\delta\mathcal{D}} + \frac{\gamma^2}{4} + \frac{1}{\delta}\lambda^2 \\ L(\lambda) &> P(\xi, \lambda) > R(\lambda) \end{aligned}$$

where $L(\lambda) = \frac{\sigma}{\delta\mathcal{D}} + \frac{\gamma^2}{4} + \frac{1}{\delta}\lambda^2$ is the limit of $P(\xi, \lambda)$ as $\xi \rightarrow -\infty$ and $R(\lambda) = \frac{\gamma^2}{4} + \frac{1}{\delta}\lambda^2 - \frac{\sigma}{\delta\mathcal{D}}$ is the limit of $P(\xi, \lambda)$ as $\xi \rightarrow \infty$. Since the parameters σ , δ and $\mathcal{D}$ are positive, $L(\lambda)$ is always positive. Since $\gamma = \frac{5\sqrt{\sigma}}{\sqrt{6\delta\mathcal{D}}}$, we find that $R(\lambda) = \frac{1}{\delta}\lambda^2 + \frac{\sigma}{24\delta\mathcal{D}}$ which is always positive. Therefore, $P(\xi, \lambda) > 0$ as $\xi \rightarrow \pm\infty$ and hence we have exponential (growth and decay) approximations for $Q(\xi, \lambda)$ given by (3.57).

Since $\hat{C}(\xi, \lambda) = e^{-\frac{\gamma}{2}\xi} Q(\xi, \lambda)$, we then have

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi} + a_2(\lambda) \frac{e^{-\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi} \quad \text{as } \xi \rightarrow \pm\infty. \quad (3.58)$$

The solution of the nonhomogenous equation (3.52) is

$$\hat{C}(\xi, \lambda) = \hat{C}_h(\xi, \lambda) + \hat{C}_p(\xi, \lambda),$$

where $\hat{C}_h(\xi, \lambda)$ is the homogenous solution given by (3.58) and $\hat{C}_p(\xi, \lambda)$ is the particular solution $\hat{C}_p(\xi, \lambda)$. Using the method of variation of parameters, the particular solution can be found as

$$\hat{C}_p(\xi, \lambda) = -\hat{C}_1 \int \frac{\hat{u}(\lambda) \hat{C}_2 f(\xi)}{W(\hat{C}_1, \hat{C}_2)} d\xi + \hat{C}_2 \int \frac{\hat{u}(\lambda) \hat{C}_1 f(\xi)}{W(\hat{C}_1, \hat{C}_2)} d\xi, \quad (3.59)$$

where $\hat{C}_1(\xi, \lambda) = \frac{e^{\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi}$, $\hat{C}_2(\xi, \lambda) = \frac{e^{-\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi}$ and $W(\hat{C}_1, \hat{C}_2)$ is the Wronskian, given by $W(\hat{C}_1, \hat{C}_2) = \hat{C}_1 \hat{C}_2' - \hat{C}_1' \hat{C}_2$.

Since $P(\xi, \lambda) \rightarrow L(\lambda)$ as $\xi \rightarrow -\infty$, the homogenous solution can be approximated as $\xi \rightarrow -\infty$ by

$$\hat{C}_h(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}}, \quad \text{as } \xi \rightarrow -\infty. \quad (3.60)$$

The particular solution then can be approximated as $\xi \rightarrow -\infty$ by

$$\begin{aligned}
\hat{C}_p(\xi, \lambda) &\sim \hat{u} \frac{2e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \int \left(\frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi} e^{\frac{\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi - \hat{u} \frac{2e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \int \left(\frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi} e^{\frac{\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi \\
&\sim -\hat{u} \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \int e^{(-\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi} d\xi + \hat{u} \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \int e^{(\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi} d\xi \\
&\sim -\hat{u} \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \frac{e^{(-\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi}}{\left(-\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}}\right)} + \hat{u} \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \frac{e^{(\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi}}{\left(\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}}\right)} \\
&\sim -\hat{u} \frac{1}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \frac{e^{\frac{\xi}{\sqrt{6}}}}{\left(-\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}}\right)} + \hat{u} \frac{1}{\delta\mathcal{D}\sqrt{6}L^{\frac{1}{2}}} \frac{e^{\frac{\xi}{\sqrt{6}}}}{\left(\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}}\right)} \\
&\sim \frac{\hat{u} e^{\frac{\xi}{\sqrt{6}}}}{\delta\mathcal{D}\sqrt{6}} \left(\frac{-2}{-L+\frac{\gamma}{\sqrt{6}}+\frac{\gamma^2}{4}+\frac{1}{6}} \right).
\end{aligned} \tag{3.61}$$

Thus, the asymptotic solution of the nonhomogenous equation (3.52) as $\xi \rightarrow -\infty$ is

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + \frac{\hat{u} e^{\frac{\xi}{\sqrt{6}}}}{\delta\mathcal{D}\sqrt{6}} \left(\frac{-2}{-L+\frac{\gamma}{\sqrt{6}}+\frac{\gamma^2}{4}+\frac{1}{6}} \right). \tag{3.62}$$

In order to satisfy the boundary condition $\hat{C} \rightarrow 0$ as $\xi \rightarrow -\infty$ given in (3.52), we note that since $\gamma > 0$ we must choose $a_2(\lambda) = 0$, and, for $a_1(\lambda) \neq 0$, we need to have $\sqrt{L} - \frac{\gamma}{2} > 0$. That is, we need

$$\begin{aligned}
\sqrt{\frac{\gamma^2}{4} + \frac{\sigma}{\delta\mathcal{D}} + \frac{1}{\delta}\lambda^2} &> \frac{\gamma}{2} \\
\frac{\gamma^2}{4} + \frac{\sigma}{\delta\mathcal{D}} + \frac{1}{\delta}\lambda^2 &> \frac{\gamma^2}{4} \\
\frac{\sigma}{\delta\mathcal{D}} + \frac{1}{\delta}\lambda^2 &> 0,
\end{aligned}$$

which is always satisfied since the parameters are positive.

The WKB approximation for the homogenous equation (3.53), valid as $\xi \rightarrow \infty$, is

$$\hat{C}_h(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}}, \quad (3.63)$$

and the particular solution can then be approximated, as $\xi \rightarrow \infty$, by

$$\begin{aligned} \hat{C}_p(\xi, \lambda) &\sim \hat{u} \frac{2e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} R^{\frac{1}{2}}} \int \left(\frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi} e^{\frac{-2\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi - \hat{u} \frac{2e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} R^{\frac{1}{2}}} \int \left(\frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi} e^{\frac{-2\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi \\ &\sim \frac{\hat{u} e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-R - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right). \end{aligned} \quad (3.64)$$

Therefore, the asymptotic solution of the nonhomogenous equation (3.52), as $\xi \rightarrow \infty$, is

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + \frac{\hat{u} e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-R - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right). \quad (3.65)$$

We have $\sqrt{R} > 0$ and $\gamma > 0$ and to satisfy the boundary condition $\hat{C} \rightarrow 0$ as $\xi \rightarrow \infty$ given in (3.52), we must choose $a_1(\lambda) = 0$ unless

$$\begin{aligned} \sqrt{R} - \frac{\gamma}{2} &< 0 \\ \sqrt{\frac{\gamma^2}{4} - \frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2} &< \frac{\gamma}{2} \\ \frac{1}{\delta} \lambda^2 &< \frac{\sigma}{\delta \mathcal{D}} \\ \lambda^2 &< \frac{\sigma}{\mathcal{D}}. \end{aligned}$$

In summary, the asymptotic solution of the nonhomogenous equation (3.52) as $\xi \rightarrow -\infty$ is represented by (3.62). As $\xi \rightarrow \infty$, the asymptotic solution of (3.52) is represented by (3.65). That is, we have

$$\hat{C}(\xi, \lambda) \sim \begin{cases} \text{Expression (3.62)}, & \text{as } \xi \rightarrow -\infty \\ \text{Expression (3.65)}, & \text{as } \xi \rightarrow \infty \end{cases}$$

To find $C^{(1)}(\xi, z)$ as $\xi \rightarrow \pm\infty$, we apply the inverse Fourier transform given by (3.50). As $\xi \rightarrow -\infty$, we find

$$C^{(1)}(\xi, z) \sim \int_{-\infty}^{\infty} \left(a_1(\lambda) \frac{e^{(\sqrt{L(\lambda)} - \frac{\gamma}{2})\xi}}{L(\lambda)^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-L(\lambda) + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right) \right) e^{i\lambda z} d\lambda. \quad (3.66)$$

We already know that $\sqrt{L(\lambda)} - \frac{\gamma}{2} > 0$. For wave modes satisfying $\sqrt{L(\lambda)} - \frac{\gamma}{2} > \frac{1}{\sqrt{6}}$, the first term goes to zero as $\xi \rightarrow -\infty$ much faster than the second term. That is for

$$\begin{aligned} \sqrt{L(\lambda)} - \frac{\gamma}{2} &> \frac{1}{\sqrt{6}} \\ \sqrt{L(\lambda)} &> \frac{\gamma}{2} + \frac{1}{\sqrt{6}} \\ \sqrt{\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2} &> \frac{\gamma}{2} + \frac{1}{\sqrt{6}} \end{aligned}$$

this holds if and only if

$$\begin{aligned} \frac{\lambda^2}{\delta} + \frac{\sigma}{\delta \mathcal{D}} &> \frac{\gamma}{\sqrt{6}} + \frac{1}{6} \\ \lambda^2 &> -\frac{\sigma}{\mathcal{D}} + \delta \left(\frac{\gamma}{\sqrt{6}} + \frac{1}{6} \right). \end{aligned} \quad (3.67)$$

For wave modes where the condition (3.67) is satisfied, the second term on the right-hand side of (3.66) is dominant; otherwise the first term is dominant. If the parameters are chosen such as the right hand-side of (3.67) is negative, then the condition (3.67) is satisfied for all λ . In this case, it is reasonable to approximate $C^{(1)}(\xi, z)$ as $\xi \rightarrow -\infty$ by the second term which corresponds to the particular

solution as

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \int_{-\infty}^{\infty} \left(\frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-L(\lambda) + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right) \right) e^{i\lambda z} d\lambda \\
&\sim \frac{-e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \hat{u} \frac{1}{(-\lambda^2 - \frac{\sigma}{\mathcal{D}} + \frac{\delta\gamma}{\sqrt{6}} + \frac{\delta}{6})} e^{i\lambda z} d\lambda \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \hat{u} \frac{1}{(\lambda^2 + \frac{\sigma}{\mathcal{D}} - \frac{\delta\gamma}{\sqrt{6}} - \frac{\delta}{6})} e^{i\lambda z} d\lambda \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} G(\lambda) \hat{u} e^{i\lambda z} d\lambda,
\end{aligned} \tag{3.68}$$

where $G(\lambda) = \frac{1}{(\lambda^2 + a^2)}$ and $a^2 = \frac{\sigma}{\mathcal{D}} - \delta \left(\frac{\gamma}{\sqrt{6}} + \frac{1}{6} \right)$. Comparing with the condition (3.67), we note that a^2 has an opposite sign to the right hand-side of (3.67). Thus the expression for a^2 is positive and a is real. From equation (3.49), we find that Fourier transform for $\tilde{u}(z) = e^{-b|z-z_c|}$ is

$$\hat{u}(\lambda) = \mathcal{F}(\tilde{u}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-b|z-z_c|} e^{-i\lambda z} dz, \tag{3.69}$$

setting $\bar{z} = z - z_c$, we then have

$$\begin{aligned}
\hat{u}(\lambda) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-b|\bar{z}|} e^{-i\lambda(\bar{z}+z_c)} d\bar{z} \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \int_{-\infty}^{\infty} e^{-b|\bar{z}|} e^{-i\lambda\bar{z}} d\bar{z} \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \left(\int_{-\infty}^0 e^{b\bar{z}} e^{-i\lambda\bar{z}} d\bar{z} + \int_0^{\infty} e^{-b\bar{z}} e^{-i\lambda\bar{z}} d\bar{z} \right) \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \left(\int_{-\infty}^0 e^{(b-i\lambda)\bar{z}} d\bar{z} + \int_0^{\infty} e^{-(b+i\lambda)\bar{z}} d\bar{z} \right) \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \left(\left[\frac{e^{(b-i\lambda)\bar{z}}}{(b-i\lambda)} \right]_{-\infty}^0 - \left[\frac{e^{-(b+i\lambda)\bar{z}}}{(b+i\lambda)} \right]_0^{\infty} \right) \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \left(\frac{1}{(b-i\lambda)} + \frac{1}{(b+i\lambda)} \right) \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \left(\frac{2b}{b^2 + \lambda^2} \right)
\end{aligned} \tag{3.70}$$

From the final line in (3.70), we note that it has a similar form to $G(\lambda)$. Thus, $G(\lambda)$ is the Fourier transform of some function $g(z)$. Rearranging $G(\lambda)$, we find

$$G(\lambda) = \frac{1}{(\lambda^2 + a^2)} = \frac{1}{2a} \frac{2a}{(\lambda^2 + a^2)},$$

Comparing with (3.70), we find that

$$G(\lambda) = \frac{1}{2a} \frac{2a}{(\lambda^2 + a^2)} = \frac{1}{2a} \mathcal{F}(e^{-a|z|}),$$

so we have $g(z) = e^{-a|z|}$. The asymptotic approximation (3.68) is then rewritten as

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} G(\lambda) \hat{u} e^{i\lambda z} d\lambda, \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} \mathcal{F}(g) \mathcal{F}(\tilde{u}) e^{i\lambda z} d\lambda,
\end{aligned} \tag{3.71}$$

using the convolution theorem, we find

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\sqrt{6}} \int_{-\infty}^{\infty} \mathcal{F}(g)\mathcal{F}(\tilde{u}) e^{i\lambda z} d\lambda \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \mathcal{F}^{-1}(\mathcal{F}(g)\mathcal{F}(\tilde{u})) \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} (\tilde{u} * g) \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} g(\tau) \tilde{u}(z - \tau) d\tau \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} e^{-a|\tau|} e^{-b|z - \tau - z_c|} d\tau \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} e^{-a|\tau|} e^{-b|\tilde{z} - \tau|} d\tau,
\end{aligned} \tag{3.72}$$

where $\tilde{z} = z - z_c$. For $\tilde{z} \leq 0$, we have

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\int_{-\infty}^{\tilde{z}} e^{a\tau} e^{-b(\tilde{z} - \tau)} d\tau + \int_{\tilde{z}}^0 e^{a\tau} e^{b(\tilde{z} - \tau)} d\tau + \int_0^{\infty} e^{-a\tau} e^{b(\tilde{z} - \tau)} d\tau \right) \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(e^{-b\tilde{z}} \left[\frac{e^{(a+b)\tau}}{a+b} \right]_{-\infty}^{\tilde{z}} + e^{b\tilde{z}} \left[\frac{e^{(a-b)\tau}}{a-b} \right]_{\tilde{z}}^0 - e^{b\tilde{z}} \left[\frac{e^{-(a+b)\tau}}{a+b} \right]_0^{\infty} \right),
\end{aligned} \tag{3.73}$$

For $a > 0$, we have

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\frac{e^{a\tilde{z}}}{a+b} + \frac{e^{b\tilde{z}} - e^{a\tilde{z}}}{a-b} + \frac{e^{b\tilde{z}}}{a+b} \right). \tag{3.74}$$

For $\tilde{z} \geq 0$, we have

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\int_{-\infty}^0 e^{a\tau} e^{-b(\tilde{z}-\tau)} d\tau + \int_0^{\tilde{z}} e^{-a\tau} e^{-b(\tilde{z}-\tau)} d\tau + \int_{\tilde{z}}^{\infty} e^{-a\tau} e^{b(\tilde{z}-\tau)} d\tau \right) \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(e^{-b\tilde{z}} \left[\frac{e^{(a+b)\tau}}{a+b} \right]_{-\infty}^0 + e^{-b\tilde{z}} \left[\frac{e^{(b-a)\tau}}{b-a} \right]_0^{\tilde{z}} - e^{b\tilde{z}} \left[\frac{e^{-(a+b)\tau}}{a+b} \right]_{\tilde{z}}^{\infty} \right) \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\frac{e^{-b\tilde{z}}}{a+b} + \frac{e^{-a\tilde{z}} - e^{-b\tilde{z}}}{b-a} + \frac{e^{-a\tilde{z}}}{a+b} \right).
\end{aligned} \tag{3.75}$$

The asymptotic solution $C^{(1)}(\xi, z)$, as $\xi \rightarrow \infty$, can be approximated as

$$C^{(1)}(\xi, z) \sim \int_{-\infty}^{\infty} \left(a_2(\lambda) \frac{e^{-(\sqrt{R} + \frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{-2\xi}{\sqrt{6}}}}{\delta\mathcal{D}\sqrt{6}} \left(\frac{-2}{-R(\lambda) - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right) \right) e^{i\lambda z} d\lambda \tag{3.76}$$

Comparing the exponentials, we note that the second term is dominant if the condition $-\sqrt{R} - \frac{\gamma}{2} < \frac{-2}{\sqrt{6}}$ is satisfied for all λ . That is, if

$$\begin{aligned}
-\sqrt{R} - \frac{\gamma}{2} &< \frac{-2}{\sqrt{6}} \\
\sqrt{\frac{\lambda^2}{\delta} + \frac{\sigma}{24\delta\mathcal{D}}} &> \frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6}\delta\mathcal{D}}.
\end{aligned} \tag{3.77}$$

If $\frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6}\delta\mathcal{D}} < 0$, then (3.77) is satisfied for all λ . Otherwise, if $\frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6}\delta\mathcal{D}} > 0$, then (3.77) holds if and only if

$$\begin{aligned}
\frac{\lambda^2}{\delta} + \frac{\sigma}{24\delta\mathcal{D}} &> \frac{25\sigma}{24\delta\mathcal{D}} - \frac{10\sqrt{\sigma}}{6\sqrt{\delta\mathcal{D}}} + \frac{4}{6} \\
\lambda^2 &> \frac{\sigma}{\mathcal{D}} + \delta \left(\frac{4}{6} - \frac{10\sqrt{\sigma}}{6\sqrt{\delta\mathcal{D}}} \right).
\end{aligned} \tag{3.78}$$

If the condition (3.78) is satisfied for all λ , we can approximate $C^{(1)}(\xi, z)$ as $\xi \rightarrow \infty$

by

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{-\frac{2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \frac{1}{(-\frac{\lambda^2}{\delta} + \frac{\sigma}{\delta \mathcal{D}} - \frac{2\gamma}{\sqrt{6}} + \frac{2}{3})} \hat{u} e^{i\lambda z} d\lambda \\
&\sim \frac{e^{-\frac{2\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \frac{1}{\lambda^2 - \frac{\sigma}{\mathcal{D}} + \delta \left(\frac{2\gamma}{\sqrt{6}} - \frac{2}{3} \right)} \hat{u} e^{i\lambda z} d\lambda \\
&\sim \frac{e^{-\frac{2\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \tilde{G}(\lambda) \hat{u} e^{i\lambda z} d\lambda,
\end{aligned} \tag{3.79}$$

where $\tilde{G}(\lambda) = \frac{1}{(\lambda^2 + \tilde{a}^2)}$ and $\tilde{a}^2 = -\frac{\sigma}{\mathcal{D}} + \delta \left(\frac{2\gamma}{\sqrt{6}} - \frac{2}{3} \right)$. According to the condition (3.78), $\tilde{a}^2$ is positive. We follow the same approach and use the convolution theorem where $\tilde{G}(\lambda)$ is expressed as

$$\tilde{G}(\lambda) = \frac{1}{2\tilde{a}} \frac{2\tilde{a}}{(\lambda^2 + \tilde{a}^2)} = \frac{1}{2\tilde{a}} \mathcal{F}(e^{-\tilde{a}|z|}).$$

For $\tilde{z} \leq 0$, (3.79) is approximated as

$$C^{(1)}(\xi, z) \sim \frac{e^{-\frac{2\xi}{\sqrt{6}}}}{2\tilde{a}\mathcal{D}\sqrt{6}} \left(\frac{e^{\tilde{a}\tilde{z}}}{\tilde{a} + b} + \frac{e^{b\tilde{z}} - e^{\tilde{a}\tilde{z}}}{\tilde{a} - b} + \frac{e^{b\tilde{z}}}{\tilde{a} + b} \right), \tag{3.80}$$

and for $\tilde{z} \geq 0$, we have

$$C^{(1)}(\xi, z) \sim \frac{e^{-\frac{2\xi}{\sqrt{6}}}}{2\tilde{a}\mathcal{D}\sqrt{6}} \left(\frac{e^{-b\tilde{z}}}{\tilde{a} + b} + \frac{e^{-\tilde{a}\tilde{z}} - e^{-b\tilde{z}}}{b - \tilde{a}} + \frac{e^{-\tilde{a}\tilde{z}}}{\tilde{a} + b} \right). \tag{3.81}$$

The asymptotic approximations of $C^{(1)}(\xi, z)$ as $\xi \rightarrow \pm\infty$ were obtained so far with $\tilde{u} = e^{-b|z-z_c|}$. We now consider the other possible form of $\tilde{u}$ given by $\tilde{u} = e^{-b^2(z-z_c)^2}$. From equation (3.49), we find that for $\tilde{u} = e^{-b^2(z-z_c)^2}$ we have

$$\hat{u}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-b^2(z-z_c)^2} e^{-i\lambda z} dz, \tag{3.82}$$

Setting $\bar{z} = z - z_c$, we then have

$$\begin{aligned}
\hat{u}(\lambda) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-b^2 \bar{z}^2} e^{-i\lambda(\bar{z}+z_c)} d\bar{z} \\
&= \frac{e^{-i\lambda z_c}}{2\pi} \int_{-\infty}^{\infty} e^{-b^2 \bar{z}^2} e^{-i\lambda \bar{z}} d\bar{z} \\
&= \frac{e^{-i\lambda z_c}}{2b\sqrt{\pi}} e^{\frac{-\lambda^2}{4b^2}}.
\end{aligned} \tag{3.83}$$

The asymptotic approximation of $C^{(1)}(\xi, z)$, as $\xi \rightarrow -\infty$, is

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2b\mathcal{D}\sqrt{\pi}\sqrt{6}} \int_{-\infty}^{\infty} G(\lambda) e^{\frac{-\lambda^2}{4b^2}} e^{-i\lambda z_c} e^{i\lambda z} d\lambda. \tag{3.84}$$

From (3.84), we note that the Gaussian $e^{\frac{-\lambda^2}{4b^2}}$ is the dominant part for small b , and most of the contribution to the integral is around $\lambda = 0$ where the Gaussian is maximum. Thus, we expand $G(\lambda)$ about $\lambda = 0$ in (3.84) and obtain

$$\begin{aligned}
C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}b\sqrt{\pi}\sqrt{6}} \int_{-\infty}^{\infty} \left(\frac{1}{a^2} - \frac{1}{a^4} \lambda^2 + \frac{1}{a^6} \lambda^4 + O(\lambda^6) \right) e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda \\
&\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}b\sqrt{\pi}\sqrt{6}} \left[\frac{1}{a^2} \int_{-\infty}^{\infty} e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda - \frac{1}{a^4} \int_{-\infty}^{\infty} \lambda^2 e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda \right. \\
&\quad \left. + \frac{1}{a^6} \int_{-\infty}^{\infty} \lambda^4 e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda + O(\lambda^6) \right].
\end{aligned} \tag{3.85}$$

From the table of integrals, we find that

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}, \tag{3.86}$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2+bx} dx = \frac{\sqrt{\pi}(2a+b^2)}{4a^{5/2}} e^{\frac{b^2}{4a}}, \tag{3.87}$$

and

$$\int_{-\infty}^{\infty} x^4 e^{-ax^2+bx} dx = \frac{\sqrt{\pi}(12a^2 + 12ab^2 + b^4)}{16a^{9/2}} e^{\frac{b^2}{4a}}. \quad (3.88)$$

Evaluating the integrals in (3.85) using (3.86), (3.87) and (3.88), (3.85) becomes

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}b\sqrt{\pi}\sqrt{6}} \left[\frac{1}{a^2} 2b\sqrt{\pi} e^{-b^2(z-z_c)^2} - \frac{1}{a^4} \left(\frac{\sqrt{\pi} e^{-b^2(z-z_c)^2} \left(\frac{1}{2b^2} - (z-z_c)^2 \right)}{4 \left(\frac{1}{2b} \right)^5} \right) \right. \\ &\quad \left. + \frac{1}{a^6} \left(\frac{\sqrt{\pi} e^{-b^2(z-z_c)^2} \left(\frac{6}{8b^4} - \frac{12}{4b^2} (z-z_c)^2 + (z-z_c)^4 \right)}{16 \left(\frac{1}{2b} \right)^9} \right) + \dots \right] \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}} e^{-b^2(z-z_c)^2}}{\mathcal{D}b\sqrt{6}} \left[\frac{2b}{a^2} - \frac{1}{a^4} \left(\frac{\frac{1}{2b^2} - (z-z_c)^2}{4 \left(\frac{1}{2b} \right)^5} \right) \right. \\ &\quad \left. + \frac{1}{a^6} \left(\frac{\frac{6}{8b^4} - \frac{12}{4b^2} (z-z_c)^2 + (z-z_c)^4}{16 \left(\frac{1}{2b} \right)^9} \right) + \dots \right]. \end{aligned} \quad (3.89)$$

Similarly, following the same approach we used to find (3.89), we find that the asymptotic solution $C^{(1)}(\xi, z)$, as $\xi \rightarrow \infty$, can be approximated as

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{-2\xi}{\sqrt{6}}} e^{-b^2(z-z_c)^2}}{\mathcal{D}b\sqrt{6}} \left[\frac{2b}{\tilde{a}^2} - \frac{1}{\tilde{a}^4} \left(\frac{\frac{1}{2b^2} - (z-z_c)^2}{4 \left(\frac{1}{2b} \right)^5} \right) \right. \\ &\quad \left. + \frac{1}{\tilde{a}^6} \left(\frac{\frac{6}{8b^4} - \frac{12}{4b^2} (z-z_c)^2 + (z-z_c)^4}{16 \left(\frac{1}{2b} \right)^9} \right) + \dots \right]. \end{aligned} \quad (3.90)$$

The asymptotic solutions for $C^{(1)}(\xi, z)$ as $\xi \rightarrow \pm\infty$ are obtained with two different forms of $\tilde{u}$. In both cases, we note that $C^{(1)}(\xi, z) \rightarrow 0$, as $\xi \rightarrow \pm\infty$ and is proportional to a Gaussian in the vertical direction. The qualitative behaviour of the total solution $C(\xi, z)$ in the vertical direction follows that of the first-order approximations $C^{(1)}(\xi, z)$. The first-order $C^{(1)}(\xi, z)$ is proportional to a Gaussian in the vertical direction following the form of the perturbation to the wind speed $\tilde{u}(z)$. This agrees with the numerical results obtained in the next section. This is also consistent with the results obtained in Chapter 5, where the effect of gravity

waves on the chemical equation is discussed.

Using the WKB method, we found asymptotic solutions for $C^{(1)}(\xi, z)$ as $\xi \rightarrow \pm\infty$. However, away from the boundaries where the WKB is not valid, we do not have asymptotic approximations. Thus, we use numerical methods in order to approximate the solution for the whole domain as discussed in the next section.

3.3 Numerical solutions

In this section, we describe the numerical solution of the problem that was presented in Section 3.2.2. The numerical results are compared with the exact solution for the case with constant advection speed and with the qualitative behaviour of the asymptotic solution for the case where the advection speed depends on z .

Description of the numerical method

We consider the two-dimensional Fisher's equation

$$C_t + U(x, z, t) C_x + W(x, z, t) C_z = \tilde{\mathcal{D}} C_{xx} + \mathcal{D} C_{zz} + \sigma C(1 - C), \quad (3.91)$$

where $C(x, z, t)$ represents the chemical concentration; $U(x, z, t)$ and $W(x, z, t)$ are the vertical and horizontal components of the wind velocity; $\tilde{\mathcal{D}} = \delta\mathcal{D}$ where $\mathcal{D}$ denotes the diffusion rate.

Equation (3.91) is solved in the domain $-\infty < x < \infty$, $-\infty < z < \infty$, $0 < t < \infty$ and with the initial condition that corresponds to the travelling-wave exact solution for constant advection given by (3.37). The boundary conditions then satisfy $C \rightarrow 1$ as $x, z \rightarrow -\infty$ and $C \rightarrow 0$ as $x, z \rightarrow \infty$. For the numerical solution, we use a computational domain $x_0 \leq x \leq x_1$ and $z_0 \leq z \leq z_1$. The waves are travelling across the domain in the x and z directions and are allowed to

propagate through the boundaries, so at the computational boundaries $x = x_0, x_1$ and $z = z_0, z_1$, we discretize equation (3.91) using one-sided forward and backward finite difference approximations following the approach given by Fornberg (1988).

Before we proceed with numerical methods to solve equation (3.91), we discuss the numerical methods for solving the one dimensional equation

$$C_t + U(x, t) C_x = \tilde{\mathcal{D}} C_{xx} + \sigma C(1 - C), \quad (3.92)$$

where C is a function of x and t defined in the domain $-\infty < x < \infty$ and $0 < t < \infty$ where $C \rightarrow 1$ as $x \rightarrow -\infty$ and $C \rightarrow 0$ as $x \rightarrow \infty$. For the numerical solution, we use a computational domain $x_0 \leq x \leq x_1$ where $x_0 < 0 < x_1$.

In order to study the stability of the numerical method, we initially discuss equation (3.92) without the source term $\sigma C(1 - C)$ and with constant advection U . This gives the advection diffusion equation

$$C_t + U C_x = \tilde{\mathcal{D}} C_{xx}. \quad (3.93)$$

The forward-time central-space FTCS scheme to solve equation (3.93) is given as

$$C_i^{n+1} = C_i^n + \Delta t U \frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} + \Delta t \tilde{\mathcal{D}} \frac{C_{i-1}^n - 2C_i^n + C_{i+1}^n}{\Delta x^2}. \quad (3.94)$$

It is well known that (3.94) is unconditionally unstable if $\tilde{\mathcal{D}} = 0$ (advection equation). However, when $\tilde{\mathcal{D}} \neq 0$, the FTCS scheme is conditionally stable. The CFL stability conditions obtained from the von Neumann stability analysis for a constant U are given as

$$\left(\frac{U \Delta t}{\Delta x} \right)^2 \leq 2 \frac{\tilde{\mathcal{D}} \Delta t}{\Delta x^2} \quad \text{and} \quad 2 \frac{\tilde{\mathcal{D}} \Delta t}{\Delta x^2} \leq 1, \quad (3.95)$$

as can be seen in Clancy (1981) and Brasseur and Jacob (2017). Although CFL stability conditions are for the case where the nonlinear term is neglected and the advection is constant, we still consider these conditions as a minimum requirement when solving equation (3.92) when the nonlinear term is included and the advection is not constant. However, from the first condition in (3.95), we note that $\Delta t \leq \frac{2\tilde{D}}{U^2}$, so the time step Δt has to be very small when U is large. Since U could be large in our computations, we then use Crank–Nicolson scheme which is unconditionally stable for equation (3.93).

Discretizing the full equation (3.92) using the implicit Crank–Nicolson method for the advection and diffusion terms and the forward Euler method for the nonlinear term, we obtain, for $2 < i < M - 1$,

$$\begin{aligned} \frac{C_i^{n+1} - C_i^n}{\Delta t} + U_i^n \frac{C_{i+1}^{n+1} - C_{i-1}^{n+1} + C_{i+1}^n - C_{i-1}^n}{4\Delta x} \\ = \tilde{D} \frac{C_{i-1}^{n+1} - 2C_i^{n+1} + C_{i+1}^{n+1} + C_{i-1}^n - 2C_i^n + C_{i+1}^n}{2\Delta x^2} + \sigma C_i^n (1 - C_i^n). \end{aligned} \quad (3.96)$$

Rearranging we get

$$\begin{aligned} -(\alpha + \beta)C_{i-1}^{n+1} + (1 + 2\beta)C_i^{n+1} + (\alpha - \beta)C_{i+1}^{n+1} &= (\alpha + \beta)C_{i-1}^n + (1 - 2\beta)C_i^n \\ &+ (\beta - \alpha)C_{i+1}^n + \Delta t \sigma C_i^n (1 - C_i^n), \end{aligned} \quad (3.97)$$

where $\alpha = \frac{U_i^n \Delta t}{4\Delta x}$ and $\beta = \frac{\tilde{D} \Delta t}{2\Delta x^2}$. At the boundary $x = x_0$, we discretize equation (3.92) using the implicit method (3.96) where the advection and the diffusion terms are discretized using the one-sided second-order finite difference approximation

following Fornberg (1988) as

$$\begin{aligned}
& \frac{C_1^{n+1} - C_1^n}{\Delta t} + U_1^n \frac{-3C_1^{n+1} + 4C_2^{n+1} - C_3^{n+1} - 3C_1^n + 4C_2^n - C_3^n}{4\Delta x} \\
&= \tilde{\mathcal{D}} \frac{2C_1^{n+1} - 5C_2^{n+1} + 4C_3^{n+1} - C_4^{n+1} + 2C_1^n - 5C_2^n + 4C_3^n - C_4^n}{2\Delta x^2} + \sigma C_1^n (1 - C_1^n).
\end{aligned} \tag{3.98}$$

Similarly, at the boundary $x = x_1$, we discretize equation (3.92) using the implicit method (3.96) where the advection and diffusion terms are discretized using the one-sided second-order finite difference approximations as

$$\begin{aligned}
& \frac{C_M^{n+1} - C_M^n}{\Delta t} + U_M^n \frac{3C_M^{n+1} - 4C_{M-1}^{n+1} + C_{M-2}^{n+1} + 3C_M^n - 4C_{M-1}^n + C_{M-2}^n}{4\Delta x} \\
&= \tilde{\mathcal{D}} \frac{2C_M^{n+1} - 5C_{M-1}^{n+1} + 4C_{M-2}^{n+1} - C_{M-3}^{n+1} + 2C_M^n - 5C_{M-1}^n + 4C_{M-2}^n - C_{M-3}^n}{2\Delta x^2} \\
&\quad + \sigma C_M^n (1 - C_M^n).
\end{aligned} \tag{3.99}$$

With the discretization at the computational boundaries in (3.98) and (3.99) being included, equation (3.97) can be written in matrix vector form as

$$AC^{(n+1)} = BC^{(n)} + F, \tag{3.100}$$

where

$$C^{(n+1)} = \begin{pmatrix} C_1^{(n+1)} \\ C_2^{(n+1)} \\ \vdots \\ C_M^{(n+1)} \end{pmatrix}, C^{(n)} = \begin{pmatrix} C_1^{(n)} \\ C_2^{(n)} \\ \vdots \\ C_M^{(n)} \end{pmatrix},$$

$$F = \sigma \Delta t C^{(n)} (1 - C^{(n)})$$

and

[illegible]

$$B = \begin{bmatrix} 1 + 3\alpha + 2\beta & -4\alpha - 5\beta & 4\beta + \alpha & -\beta \\ (\alpha + \beta) & (1 - 2\beta) & (\beta - \alpha) & \vdots \\ \vdots & \vdots & \vdots & (\alpha + \beta) & (1 - 2\beta) & (\beta - \alpha) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & -\beta & 4\beta - \alpha & 4\alpha - 5\beta & 1 - 3\alpha + 2\beta \end{bmatrix}. \quad (3.102)$$

Now we consider the original two-dimensional equation (3.91), which has the form

$$C_t + U(x, z, t) C_x + W(x, z, t) C_z = \tilde{\mathcal{D}} C_{xx} + \mathcal{D} C_{zz} + \sigma C(1 - C). \quad (3.103)$$

Throughout this thesis, we are interested in situations where the initial background flow velocity has a horizontal component $\bar{u}$ and a zero vertical component, and the horizontal and vertical components of the flow velocity are modified by gravity waves, which have amplitude of $O(\epsilon)$. In this context, the horizontal velocity component is $U(x, z, t) = \bar{u} + O(\epsilon)$ where $\bar{u}$ is $O(1)$ and the vertical component is $W(x, z, t) = O(\epsilon)$ and is thus much smaller than $U(x, z, t)$. Also, the vertical diffusion $\mathcal{D}$ is larger than the horizontal diffusion $\tilde{\mathcal{D}} = \delta \mathcal{D}$, where $\delta \ll 1$. In the x -direction because of the $O(1)$ advection speed and the diffusion $\tilde{\mathcal{D}}$ is small, the CFL condition for the explicit FTCS requires very small Δt and hence the implicit

Crank–Nicolson scheme is used instead. In the z -direction, however, since $W \ll 1$ and the diffusion $\mathcal{D}$ is relatively large, we use the FTCS scheme.

We discretize equation (3.103) as follows, for $i = 2, \dots, M - 1$ and $j = 2, \dots, N - 1$, we have

$$\begin{aligned} & \frac{C_{i,j}^{n+1} - C_{i,j}^n}{\Delta t} + U_{i,j}^n \frac{C_{i+1,j}^{n+1} - C_{i-1,j}^{n+1} + C_{i+1,j}^n - C_{i-1,j}^n}{4\Delta x} + W_{i,j}^n \frac{C_{i,j+1}^n - C_{i,j-1}^n}{2\Delta z} \\ &= \tilde{\mathcal{D}} \frac{(C_{i-1,j}^{n+1} - 2C_{i,j}^{n+1} + C_{i+1,j}^{n+1} + C_{i-1,j}^n - 2C_{i,j}^n + C_{i+1,j}^n)}{2\Delta x^2} + \mathcal{D} \frac{C_{i,j-1}^n - 2C_{i,j}^n + C_{i,j+1}^n}{\Delta z^2} \\ & \quad + \sigma C_{i,j}^n (1 - C_{i,j}^n). \end{aligned}$$

Rearranging, we get

$$\begin{aligned} & -(\alpha + \beta)C_{i-1,j}^{n+1} + (1 + 2\beta)C_{i,j}^{n+1} + (\alpha - \beta)C_{i+1,j}^{n+1} = (\alpha + \beta)C_{i-1,j}^n + (1 - 2\beta)C_{i,j}^n + (\beta - \alpha)C_{i+1,j}^n \\ & + \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} + \frac{W_{i,j}^n \Delta t}{2\Delta z}\right)C_{i,j-1}^n - \frac{2\mathcal{D}\Delta t}{\Delta z^2}C_{i,j}^n + \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} - \frac{W_{i,j}^n \Delta t}{2\Delta z}\right)C_{i,j+1}^n + \sigma \Delta t C_{i,j}^n (1 - C_{i,j}^n). \end{aligned} \quad (3.104)$$

Since the scheme is explicit in the z -direction, we note that, for each fixed value in z , we can write equation (3.104) in a system form

$$AC_j^{(n+1)} = BC_j^{(n)} + \mathcal{F} + \tilde{\mathcal{F}}, \quad \text{for } j = 2, \dots, N - 1, \quad (3.105)$$

where A, B are defined as in (3.101) and (3.102); $\mathcal{F}$ is a vector that contains the advection and diffusion terms in the z -direction and is given by

$$\mathcal{F} = \begin{pmatrix} \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} + \frac{W_{1,j}^n \Delta t}{2\Delta z}\right)C_{1,j-1}^n - \frac{2\mathcal{D}\Delta t}{\Delta z^2}C_{1,j}^n + \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} - \frac{W_{1,j}^n \Delta t}{2\Delta z}\right)C_{1,j+1}^n \\ \vdots \\ \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} + \frac{W_{M,j}^n \Delta t}{2\Delta z}\right)C_{M,j-1}^n - \frac{2\mathcal{D}\Delta t}{\Delta z^2}C_{M,j}^n + \left(\frac{\mathcal{D}\Delta t}{\Delta z^2} - \frac{W_{M,j}^n \Delta t}{2\Delta z}\right)C_{M,j+1}^n \end{pmatrix}$$

and

$$\tilde{\mathcal{F}} = \sigma \Delta t C_j^n (1 - C_j^n).$$

For $j = 1$ (at the lower boundary), we compute the solution using (3.105) with $\mathcal{F}$ being replaced by the second-order finite difference approximations given as

$$\mathcal{F}_L = \begin{pmatrix} (\frac{2\mathcal{D}\Delta t}{\Delta z^2} + \frac{3W_{1,1}^n \Delta t}{2\Delta z})C_{1,1}^n - (\frac{2W_{1,1}^n \Delta t}{\Delta z} + \frac{5\mathcal{D}\Delta t}{\Delta z^2})C_{1,2}^n + (\frac{4\mathcal{D}\Delta t}{\Delta z^2} + \frac{W_{1,1}^n \Delta t}{2\Delta z})C_{1,3}^n - \frac{\mathcal{D}\Delta t}{\Delta z^2}C_{1,4}^n \\ \vdots \\ (\frac{2\mathcal{D}\Delta t}{\Delta z^2} + \frac{3W_{M,1}^n \Delta t}{2\Delta z})C_{M,1}^n - (\frac{2W_{M,1}^n \Delta t}{\Delta z} + \frac{5\mathcal{D}\Delta t}{\Delta z^2})C_{M,2}^n + (\frac{4\mathcal{D}\Delta t}{\Delta z^2} + \frac{W_{M,1}^n \Delta t}{2\Delta z})C_{M,3}^n - \frac{\mathcal{D}\Delta t}{\Delta z^2}C_{M,4}^n \end{pmatrix}.$$

Similarly, at the upper boundary, we compute the solution using (3.105) with $\mathcal{F}$ being replaced by the second-order finite difference approximations given as

$$\mathcal{F}_U = \begin{pmatrix} -\frac{\mathcal{D}\Delta t}{\Delta z^2}C_{1,N-3}^n + (\frac{4\mathcal{D}\Delta t}{\Delta z^2} - \frac{W_{1,N}^n \Delta t}{2\Delta z})C_{1,N-2}^n + (\frac{2W_{1,N}^n \Delta t}{\Delta z} - \frac{5\mathcal{D}\Delta t}{\Delta z^2})C_{1,N-1}^n + (\frac{2\mathcal{D}\Delta t}{\Delta z^2} - \frac{3W_{1,N}^n \Delta t}{2\Delta z})C_{1,N}^n \\ \vdots \\ -\frac{\mathcal{D}\Delta t}{\Delta z^2}C_{M,N-3}^n + (\frac{4\mathcal{D}\Delta t}{\Delta z^2} - \frac{W_{M,N}^n \Delta t}{2\Delta z})C_{M,N-2}^n + (\frac{2W_{M,N}^n \Delta t}{\Delta z} - \frac{5\mathcal{D}\Delta t}{\Delta z^2})C_{M,N-1}^n + (\frac{2\mathcal{D}\Delta t}{\Delta z^2} - \frac{3W_{M,N}^n \Delta t}{2\Delta z})C_{M,N}^n \end{pmatrix}.$$

For each point in z , system (3.105) is solved to find the solution for all points in x . This process is repeated for all points in the z -direction.

The choice of the grid size is based on grid sensitivity analysis. For the choice of grid size in the vertical direction, we repeated the solution with several Δz by comparing solution with $2\Delta z$, $4\Delta z$ and so on. With the choice of $\Delta z = 0.025$, the maximum error of solutions computed with this Δz compared with the corresponding ones computed with $2\Delta z$ was found to be 9×10^{-4} which is small enough and lies within the tolerance we want. Following the same procedure of grid sensitivity analysis, we decided to choose $\Delta x = 0.025$, where the maximum difference of solutions computed with this Δx compared with the corresponding ones computed with $2\Delta x$ was found to be 3×10^{-3} .

Numerical results

The numerical solution and the exact solution of the one-dimensional equation (3.92) with constant advection speed are shown in Figure 3.2. The graphs show that the numerical solution is almost identical to the exact solution. The maximum relative error is found to be 5×10^{-4} . The maximum relative error is computed in the middle region away from boundaries to avoid the situations where the solution is very close to zero, which gives invalid maximum relative error due to the division by zero. We compute the relative errors over all points in the interval considered for each time step and consider the maximum. We eventually consider the maximum relative error to be the maximum over all time steps.

Figure 3.2: Numerical solution and exact solution (3.19) of Fisher's equation (3.92) at different times with $U = 1$, $\tilde{D} = 0.4$ and $\sigma = 1$.

The initial condition used to compute the numerical solution of the two-dimensional Fisher's equation (3.103) is shown in Figure 3.3. It corresponds to $t = 0$ in the analytical solution given in (3.37). Figure 3.4 illustrates the comparison between the numerical solution of (3.103) as well as the corresponding analytical solution (3.37) at several different times. These solutions correspond to constant advection speed U and W for which we were able to find analytical solution given by (3.37).

The remaining figures concern the numerical solution of (3.103) with advection speeds of the form $U = \bar{u} + \epsilon \tilde{u}$ and $W = 0$, and these figures are obtained with initial condition that corresponds to $\theta = 0$ in (3.37). This configuration corresponds to the asymptotic analysis in Subsection 3.2.2, where $\bar{u}$ is constant and $\tilde{u}$ is a function of z . Figure 3.5 shows the initial condition and the numerical solution where the horizontal advection is taken to be constant plus a perturbation $\tilde{u} = \exp(-0.5(z - 5)^2)$. In this figure, we find that solutions are propagating in the x -direction and solutions are modified around $z = 5$ due to the perturbation. To see the effect of the perturbation, we show numerical results corresponding to $C^{(1)}$, which is approximated in Section 3.2.2 using the WKB method. We compute $C^{(1)}$ numerically by subtracting the exact solution $C^{(0)}$, which corresponds to the solution of (3.103) with constant advection, from the numerical solution C for the perturbed problem. Figure 3.6 illustrates the numerical solution C of the perturbed problem at fixed z point, whereas Figure 3.8 shows the perturbation solution $C^{(1)}$ at that fixed point. We observe from Figure 3.8 that the solution $C^{(1)}$ approaches zero as $x \rightarrow -\infty$. This is consistent with asymptotic approximation given by (3.62). As $x \rightarrow \infty$, we note from Figure 3.8 that the solution $C^{(1)}$ approaches zero, which is also in agreement with the asymptotic approximation (3.65). From Figure 3.7, we note that the z -direction of the solution of the per-

turbed problem is proportional to the Gaussian perturbation $\tilde{u}$. These figures are consistent with the analytical observations given in equations (3.89) and (3.90).

For the choice of input parameters in numerical results shown in this section, we find from the asymptotic approximation (Section 3.2.2) that the dominant behaviour is

$$C^{(1)} \sim e^{0.4\xi} \text{ as } \xi \rightarrow -\infty \quad \text{and} \quad C^{(1)} \sim e^{-2.7\xi} \text{ as } \xi \rightarrow \infty$$

This shows that the decay is faster on the right which is consistent with numerics as shown in Figure 3.8.

Figure 3.9 shows a comparison between the solution C , the leading order $C^{(0)}$ and the perturbation $\epsilon C^{(1)}$ as a function of x and at $z = 5$, $t = 1$. We observe from the figure that the difference between the curves corresponding to C and $C^{(0)}$ is consistent with the curve corresponding to $\epsilon C^{(1)}$. This shows that the solution $C \sim C^{(0)} + \epsilon C^{(1)}$ as suggested by the perturbation series in the asymptotic discussion in Section 3.2.2.

The numerical solutions with $\bar{u} = \tanh(z - 5)$ and a perturbation are shown in Figures 3.10 and 3.11. This corresponds to the case where the mean flow is not constant, as shall be seen in the discussion of the effect of gravity waves on the chemical equation in Chapter 5.

Figure 3.3: The initial condition $C(x, z, 0)$ considered for the numerical solution. It is the analytical solution (3.37) at $t = 0$.

(a)

(b)

(c)

(d)

Figure 3.4: The contour plots of the numerical and exact solution of the two-dimensional Fisher's equation with $U = 1$, $W = 0.3$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$ and $\sigma = 1$. Numerical solution at times (a) $t = 0.5$ and (c) $t = 1$. Exact solution (3.37) at times (b) $t = 0.5$ and (d) $t = 1$.

(a)

(b)

(c)

(d)

(e)

(f)

Figure 3.5: Numerical solution of the two-dimensional Fisher's equation with $U = 0.5 + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\hat{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.7$ and $\sigma = 1$. The initial condition is shown in (a) and (b), numerical solutions at $t = 0.5$ are shown in (c) and (d) and numerical solutions at $t = 1$ are shown in (e) and (f).

Figure 3.6: The numerical solution of the two-dimensional Fisher's equation with $U = 0.5 + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.7$ and $\sigma = 1$. The plot is for $C(x, 5)$ at several times.

Figure 3.7: The numerical solution of the two-dimensional Fisher's equation with $U = 0.5 + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.7$ and $\sigma = 1$. The plot is for C at $x = 0$ as a function of z at times $t = 0$, $t = 0.5$ and $t = 1$.

Figure 3.8: The numerical solution of the two-dimensional Fisher's equation with $U = 0.5 + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.7$ and $\sigma = 1$. The plot is for $C^{(1)}(x, 5)$ at times $t = 0.5$ and $t = 1$.

Figure 3.9: The numerical solution of the two-dimensional Fisher's equation with $U = 0.5 + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.7$ and $\sigma = 1$. The plot is comparison between $C(x, 5)$, $C^{(0)}(x, 5)$ and the perturbation $\epsilon C^{(1)}(x, 5)$ at time $t = 1$.

(a)

(b)

Figure 3.10: The contour plots of the numerical solution of the two-dimensional Fisher's equation with $U = \tanh(z - 5)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$ and $\sigma = 1$ at times (a) $t = 1$ and (b) $t = 3$.

(a)

(b)

Figure 3.11: The contour plots of the numerical solution of the two-dimensional Fisher's equation with $U = \tanh(z - 5) + \epsilon \exp(-0.5(z - 5)^2)$, $W = 0$, $\tilde{\mathcal{D}} = 0.2$, $\mathcal{D} = 0.5$, $\epsilon = 0.1$ and $\sigma = 1$ at times (a) $t = 1$ and (b) $t = 3$.

Chapter 4

Linear and Weakly-Nonlinear Analysis of the Equations for Gravity Waves Influenced by Chemical Heating

In Chapter 3, we discussed analytical and numerical solutions of the chemical transport equation in a situation where the mean flow is modified by a vertically varying perturbation of the form that could arise from gravity-wave interactions. We now focus on studying the effect that the presence of a chemical species in the atmosphere could have on gravity waves. In this chapter, we carry out linear and nonlinear analysis of gravity waves affected by the presence of a chemical constituent in the atmosphere.

4.1 Linear analysis

As a starting point, we consider a situation where the gravity wave amplitude is small enough relative to the background flow (i.e., $\varepsilon \ll 1$) that we can neglect the nonlinear terms with the factor of ε in equations (2.41) and (2.43), but we maintain the term representing the effect of the chemical species in the gravity wave density in (2.43). The more general nonlinear configuration will be considered next in Section 4.2.

The linearized equations of (2.41)–(2.45) are

$$\nabla^2 \psi_t + \bar{u} \nabla^2 \psi_x - \bar{u}'' \psi_x + \frac{g}{\bar{\rho}} \rho_x = 0, \quad (4.1)$$

$$\rho_t + \bar{u} \rho_x + \bar{\rho}' \psi_x = \gamma \frac{D C}{D t}, \quad (4.2)$$

$$\frac{D C}{D t} = C_t + \bar{u} C_x. \quad (4.3)$$

We examine these equations on a rectangular domain $-\infty < x < \infty$ and $0 \leq z < \infty$. At the lower boundary, we impose a boundary condition that generates a gravity wave or a gravity-wave packet within the domain. If we impose an oscillatory boundary condition at $z = 0$, such as $\psi(x, z, t) = \cos(kx)$ or $\psi(x, z, t) = e^{ikx} + \text{c.c.}$ for $0 < x < 2\pi/k$, where c.c. denotes the complex conjugate, we obtain a solution in the form of monochromatic waves of the form $\psi(x, z, t) = \hat{\psi}(z) e^{ikx} + \text{c.c.}$ with a single wavenumber k . A more realistic formulation is obtained by considering an infinite domain $-\infty < x < \infty$ with a lower boundary condition of the form $\psi(x, 0, t) = A(\mu x) e^{ik_0 x} + \text{c.c.}$ where μ is constant and $\mu \ll 1$, A is a slowly varying function of x , $A \rightarrow 0$ as $x \rightarrow \pm\infty$ and k_0 is a fixed wavenumber. This gives a solution that describes a horizontally localized wave packet, with a continuous spectrum of wavenumbers k centred at the forced wavenumber k_0 . The

wave packet forcing is more realistic than the monochromatic forcing, since the latter is considered reasonable only if the wavelength of the generated waves has a magnitude that is comparable with the circumference of the earth [Campbell and Maslowe (2003)].

In the analysis given here, we consider the Gaussian profile $A(\mu x) = e^{-\mu^2 x^2}$, so the boundary condition of the streamfunction is

$$\psi(x, 0, t) = e^{-\mu^2 x^2} (e^{ik_0 x} + e^{-ik_0 x}). \quad (4.4)$$

The upper boundary condition is the requirement that the waves generated at $z = 0$ propagate upwards to infinity, so there is no incoming energy from infinity. This means that only waves with upward (positive) group velocity can be present. The mean density is considered as $\bar{\rho} = e^{-\frac{z}{h}}$. The mean flow u is considered to be constant in Subsection 4.1.1. In Subsection 4.1.2, the mean flow is considered to be $u(z)$, representing a mean flow with a vertical shear. In the horizontal direction, we have the boundary conditions that $\psi \rightarrow 0$ as $x \rightarrow \pm\infty$ and $\rho \rightarrow 0$ as $x \rightarrow \pm\infty$.

Regarding the specification of the profile of the chemical distribution, we refer to previous observational studies. For example, Gille and Lyjak (1986) studied the heating in the atmosphere due to the effect of several chemicals including ozone and water vapour. In their observations, they show that the initial profile of ozone and water vapour have a form which is localized around the equator in the horizontal direction and localized around some vertical level in the vertical direction. This suggests that the initial condition of the chemical can be specified in the form

$$C(x, z, 0) = \mathcal{G}(ax)\mathcal{H}(bz),$$

where a and b are positive constants, $a \ll 1$, $b \ll 1$, $\mathcal{G} \rightarrow 0$ as $x \rightarrow \pm\infty$ and

$\mathcal{H} \rightarrow 0$ as $z \rightarrow \pm\infty$. The function $\mathcal{H}$ is centred at some level $z = z_1$ where we choose $z_1 \gg 1$ so that, at $z = 0$, $\mathcal{H}$ is small enough that we can set it to zero in the analysis. We will consider the profile $\mathcal{G}(ax) = e^{-a^2x^2}$. The function $\mathcal{H}(bz)$ can be represented by the Gaussian form as $\mathcal{H}(bz) = e^{-b^2(z-z_1)^2}$ or the exponential form as $\mathcal{H}(bz) = e^{-b|z-z_1|}$.

In this section, we consider a steady-state chemical and a steady-amplitude solution for ψ and ρ as a first approximation. The time-dependent problem will be considered in Section 4.2.

From this point and throughout the thesis, the functions ψ , ρ and C are represented in terms of their Fourier transforms in the x -direction. Following Champeney (1987), the Fourier transform of a function $f(x)$ exists, if f is absolutely integrable. That is, if f is absolutely integrable satisfying

$$\int_{-\infty}^{\infty} |f(x)| dx < \infty, \quad (4.5)$$

which means that $f(x) \in L_1$, then the Fourier transform $\hat{f}(k)$ exists, $\hat{f}(k)$ is continuous and $\hat{f}(k) \rightarrow 0$ as $k \rightarrow \pm\infty$. Conversely, if $\hat{f}(k)$ is absolutely integrable, then its inverse transform $f(x)$ exists as a function of x and $f(x)$ is continuous and $f(x) \rightarrow 0$ as $x \rightarrow \pm\infty$.

The functions ψ , ρ and C are smooth and continuously differentiable and from the boundary conditions, we know that $\psi \rightarrow 0$ as $x \rightarrow \pm\infty$, $\rho \rightarrow 0$ as $x \rightarrow \pm\infty$ and $C \rightarrow 0$ as $x \rightarrow \pm\infty$. Thus the functions ψ , ρ and C are absolutely integrable and therefore their Fourier transforms exist. The functions ψ , ρ and C can then be represented in terms of the inverse Fourier transform as

$$\psi(x, z, t) = \int_{-\infty}^{\infty} \hat{\psi}(k, z) e^{ikx} dk, \quad (4.6)$$

$$\rho(x, z, t) = \int_{-\infty}^{\infty} \hat{\rho}(k, z) e^{ikx} dk, \quad (4.7)$$

$$C(x, z, t) = \int_{-\infty}^{\infty} \hat{C}(k, z) e^{ikx} dk. \quad (4.8)$$

The Fourier transform of the streamfunction boundary condition is then given as

$$\hat{\psi}(k, 0) = \frac{\sqrt{\pi}}{2\pi\mu} \left(e^{-\frac{(k+k_0)^2}{4\mu^2}} + e^{-\frac{(k-k_0)^2}{4\mu^2}} \right). \quad (4.9)$$

We consider $\mu \ll 1$ so that the Gaussian profiles $e^{-\frac{(k+k_0)^2}{4\mu^2}}$ and $e^{-\frac{(k-k_0)^2}{4\mu^2}}$ do not overlap. In this case, both functions are small enough at $k = 0$ that $e^{-\frac{(k-k_0)^2}{4\mu^2}}$ can be set to zero for $k < 0$ and $e^{-\frac{(k+k_0)^2}{4\mu^2}}$ can be set to zero for $k > 0$. Thus the Fourier transform of the streamfunction boundary condition given in (4.9) can be rewritten as

$$\hat{\psi}(k, 0) \approx \begin{cases} \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k+k_0)^2}{4\mu^2}}, & \text{if } k \leq 0 \\ \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k-k_0)^2}{4\mu^2}}, & \text{if } k \geq 0. \end{cases} \quad (4.10)$$

The Fourier transform of the initial condition of the chemical is

$$\hat{C}(k, z) = \mathcal{F}[e^{-a^2 x^2}] \mathcal{H}(bz) = \mathcal{H}(bz) \left(\frac{\sqrt{\pi}}{2\pi a} e^{-\frac{k^2}{4a^2}} \right).$$

Since $\mathcal{H}$ is close to zero as $z \rightarrow 0$ and $\mathcal{H} \rightarrow 0$ as $z \rightarrow \infty$, $\hat{C} \rightarrow 0$ at $z = 0$ and as $z \rightarrow \infty$.

Taking the Fourier transform of each term in (4.1) and (4.2) and dividing by ik gives

$$\bar{u} \hat{\psi}_{zz} - \delta k^2 \bar{u} \hat{\psi} - \bar{u}'' \hat{\psi} + \frac{g}{\bar{\rho}} \hat{\rho} = 0 \quad (4.11)$$

$$\bar{u} \hat{\rho} + \bar{\rho}' \hat{\psi} = \gamma \bar{u} \hat{C}. \quad (4.12)$$

From (4.12), we find

$$\hat{\rho} = \gamma \hat{C} - \frac{\bar{\rho}' \hat{\psi}}{\bar{u}}.$$

Substituting this into equation (4.11), we obtain

$$\bar{u} \hat{\psi}_{zz} - \delta k^2 \bar{u} \hat{\psi} - \bar{u}'' \hat{\psi} + \frac{g}{\bar{\rho}} \left(\gamma \hat{C} - \frac{\bar{\rho}' \hat{\psi}}{\bar{u}} \right) = 0 \quad (4.13)$$

Rearranging, we obtain

$$\hat{\psi}_{zz} + \left(\frac{N^2}{\bar{u}^2} - \delta k^2 - \frac{\bar{u}''}{\bar{u}} \right) \hat{\psi} = -\frac{g\gamma \hat{C}}{\bar{\rho}\bar{u}}, \quad (4.14)$$

where $N^2 = \frac{-g\bar{\rho}'}{\bar{\rho}}$ which is the buoyancy frequency, N^2 is constant since $\bar{\rho} = e^{-z/h}$.

The corresponding homogenous equation is the Taylor–Goldstein equation, which is discussed in Appendix D, where a Frobenius series is used to approximate the solution. Substituting for $\bar{\rho}$ and $\hat{C}$, equation (4.14) becomes

$$\hat{\psi}_{zz} + \left(\frac{N^2}{\bar{u}^2} - \delta k^2 - \frac{\bar{u}''}{\bar{u}} \right) \hat{\psi} = f(k, z). \quad (4.15)$$

where $f(k, z) = \mathcal{R}(k) \frac{e^{z/h} \mathcal{H}(bz)}{\bar{u}}$ and $\mathcal{R}(k) = -g\gamma \mathcal{F}[e^{-a^2 x^2}] = -g\gamma \left(\frac{\sqrt{\pi}}{2\pi a} e^{-\frac{k^2}{4a^2}} \right)$. The general solution $\hat{\psi}$ is given as

$$\hat{\psi} = \hat{\psi}_h + \hat{\psi}_p,$$

where $\hat{\psi}_p$ is a particular solution and $\hat{\psi}_h$ is a linear combination of two linearly independent solutions of the corresponding homogenous equation.

We first consider the case where $\bar{u}$ is constant. The more general situation of a flow with vertical shear, where $\bar{u}$ depends on z , is considered in Subsection 4.1.2.

4.1.1 Constant mean flow speed

If background flow speed $\bar{u}$ is constant, then equation (4.15) reduces to

$$\hat{\psi}_{zz} + \left(\frac{N^2}{\bar{u}^2} - \delta k^2 \right) \hat{\psi} = f(k, z). \quad (4.16)$$

If $\frac{N^2}{\bar{u}^2} < \delta k^2$, the homogenous equation has exponentially growing and decaying solutions. However, in the atmosphere the aspect ratio $\frac{L_z}{L_x}$ is small, so $\delta = \frac{L_z}{L_x}$ is considered to be a small parameter ($\delta \ll 1$). This corresponds to the wave type of solutions where $\frac{N^2}{\bar{u}^2} > \delta k^2$. Since $\mu \ll 1$ and $\delta \ll 1$, we observe from (4.10) that for wave modes satisfying $\frac{N^2}{\bar{u}^2} < \delta k^2$, the boundary condition (4.10) is close to zero. Thus on the Fourier spectrum, we consider only the domain of k such that $\frac{N^2}{\bar{u}^2} > \delta k^2$. This means that the general solution of the homogenous equation is given as

$$\hat{\psi}_h(k, z) = A_1(k)e^{im(k)z} + A_2(k)e^{-im(k)z}, \quad (4.17)$$

where, following the group velocity argument of Booker and Bretherton (1967) given in Appendix D, we fix the sign of m to be the same of $\bar{u}$, so we have $m(k) = \text{sgn}(\bar{u})\sqrt{\frac{N^2}{\bar{u}^2} - \delta k^2}$.

Configuration 1:

On the right-hand side of equation (4.16), we have $f(k, z) = \mathcal{R}(k)\frac{e^{z/h}\mathcal{H}(bz)}{\bar{u}}$. We first consider the case where $\mathcal{H}(bz) = e^{-b^2(z-z_1)^2}$, where $z_1 \gg 1$ so that $\mathcal{H} \rightarrow 0$ as $z \rightarrow 0$. Using the method of variation of parameters and choosing the lower limit so that $\hat{\psi}_p(k, 0) = 0$ to satisfy the boundary condition at $z = 0$, we find that the

particular solution is

$$\hat{\psi}_p(k, z) = -\hat{\psi}_1 \left(\int_0^z \frac{\hat{\psi}_2(k, \tilde{z}) f(k, \tilde{z})}{W(\hat{\psi}_1(k, \tilde{z}), \hat{\psi}_2(k, \tilde{z}))} d\tilde{z} \right) + \hat{\psi}_2 \left(\int_0^z \frac{\hat{\psi}_1(k, \tilde{z}) f(k, \tilde{z})}{W(\hat{\psi}_1(k, \tilde{z}), \hat{\psi}_2(k, \tilde{z}))} d\tilde{z} \right), \quad (4.18)$$

where $\hat{\psi}_1 = e^{im(k)z}$, $\hat{\psi}_2 = e^{-im(k)z}$, $f(k, z) = \mathcal{R}(k) \frac{e^{\frac{\bar{z}}{h}} e^{-b^2(z-z_1)^2}}{\bar{u}}$ and $W(\hat{\psi}_1, \hat{\psi}_2)$ is the Wronskian given as $W(\hat{\psi}_1, \hat{\psi}_2) = \hat{\psi}_1 \hat{\psi}_2' - \hat{\psi}_1' \hat{\psi}_2 = -2im(k)$. The integrals are evaluated as

$$\int_0^z \frac{\hat{\psi}_2(k, \tilde{z}) f(k, \tilde{z})}{W(\hat{\psi}_1(k, \tilde{z}), \hat{\psi}_2(k, \tilde{z}))} d\tilde{z} = \frac{-\mathcal{R}(k)}{2im(k)\bar{u}} \underbrace{\left\{ \int_0^z e^{-im(k)\tilde{z}} e^{\frac{\bar{z}}{h}} e^{-b^2(\tilde{z}-z_1)^2} d\tilde{z} \right\}}_I. \quad (4.19)$$

Setting $\bar{z} = \tilde{z} - z_1$, we then have

$$I = e^{-im(k)z_1} e^{\frac{z_1}{h}} \int_{-z_1}^{z-z_1} e^{-im(k)\bar{z}} e^{\frac{\bar{z}}{h}} e^{-b^2\bar{z}^2} d\bar{z}, \quad (4.20)$$

and completing the square for the exponents in the integrand, we obtain

$$I = e^{-im(k)z_1} e^{\frac{z_1}{h}} e^{\frac{\left(\frac{1}{h}-im(k)\right)^2}{4b^2}} \int_{-z_1}^{z-z_1} e^{-b^2\left(\bar{z}-\frac{\left(\frac{1}{h}-im(k)\right)}{2b^2}\right)^2} d\bar{z}. \quad (4.21)$$

This integral cannot be evaluated exactly, but it can be expressed in terms of the error function as

$$\begin{aligned} I &= e^{-im(k)z_1} e^{\frac{z_1}{h}} e^{\frac{\left(\frac{1}{h}-im(k)\right)^2}{4b^2}} \left[\int_0^{z-z_1} e^{-b^2\left(\bar{z}-\frac{\left(\frac{1}{h}-im(k)\right)}{2b^2}\right)^2} d\bar{z} - \int_0^{-z_1} e^{-b^2\left(\bar{z}-\frac{\left(\frac{1}{h}-im(k)\right)}{2b^2}\right)^2} d\bar{z} \right] \\ &= \frac{\sqrt{\pi} e^{-im(k)z_1} e^{\frac{z_1}{h}} e^{\frac{\left(\frac{1}{h}-im(k)\right)^2}{4b^2}}}{2b} \left[\operatorname{erf} \left(\frac{2b^2h(z-z_1) + im(k)h - 1}{2hb} \right) \right. \\ &\quad \left. - \operatorname{erf} \left(\frac{im(k)h - 2b^2hz_1 - 1}{2hb} \right) \right]. \end{aligned} \quad (4.22)$$

Substituting (4.22) into (4.19), we obtain

$$\begin{aligned}
& \int_0^z \frac{\hat{\psi}_2(k, \tilde{z}) f(k, \tilde{z})}{W(\hat{\psi}_1(k, \tilde{z}), \hat{\psi}_2(k, \tilde{z}))} d\tilde{z} \\
&= \frac{-\sqrt{\pi} \mathcal{R}(k) e^{-im(k)z_1} e^{\frac{z_1}{h}} e^{\left(\frac{1}{h} - im(k)\right)^2 \frac{1}{4b^2}}}{4b im(k) \bar{u}} \left[\operatorname{erf} \left(\frac{2b^2 h(z - z_1) + im(k)h - 1}{2hb} \right) \right. \\
&\quad \left. - \operatorname{erf} \left(\frac{im(k)h - 2b^2 h z_1 - 1}{2hb} \right) \right]. \tag{4.23}
\end{aligned}$$

Similarly, following the same approach used to find (4.23), we have

$$\begin{aligned}
& \int_0^z \frac{\hat{\psi}_1(k, \tilde{z}) f(k, \tilde{z})}{W(\hat{\psi}_1(k, \tilde{z}), \hat{\psi}_2(k, \tilde{z}))} d\tilde{z} \\
&= \frac{-\sqrt{\pi} \mathcal{R}(k) e^{im(k)z_1} e^{\frac{z_1}{h}} e^{\left(\frac{1}{h} + im(k)\right)^2 \frac{1}{4b^2}}}{4b im(k) \bar{u}} \left[\operatorname{erf} \left(\frac{2b^2 h z_1 + im(k)h + 1}{2hb} \right) \right. \\
&\quad \left. - \operatorname{erf} \left(\frac{2b^2 h(z_1 - z) + im(k)h + 1}{2hb} \right) \right]. \tag{4.24}
\end{aligned}$$

Substituting (4.23) and (4.24) into (4.18), we obtain

$$\hat{\psi}_p(k, z) = \frac{\sqrt{\pi} \mathcal{R}(k) e^{\frac{z_1}{h}}}{4b \bar{u}} G(k, z), \tag{4.25}$$

where

$$\begin{aligned}
G(k, z) = & \frac{e^{im(k)(z-z_1)} e^{\frac{(\frac{1}{h}-im(k))^2}{4b^2}}}{im(k)} \left[\operatorname{erf} \left(b(z-z_1) + \frac{im(k)h-1}{2hb} \right) \right. \\
& \left. - \operatorname{erf} \left(\frac{im(k)h-1}{2hb} - bz_1 \right) \right] \\
& - \frac{e^{im(k)(z_1-z)} e^{\frac{(\frac{1}{h}+im(k))^2}{4b^2}}}{im(k)} \left[\operatorname{erf} \left(bz_1 + \frac{im(k)h+1}{2hb} \right) \right. \\
& \left. - \operatorname{erf} \left(b(z_1-z) + \frac{im(k)h+1}{2hb} \right) \right]
\end{aligned} \tag{4.26}$$

The general solution of equation (4.16) is then given as

$$\hat{\psi}(k, z) = A_1(k)e^{im(k)z} + A_2(k)e^{-im(k)z} + \hat{\psi}_p(k, z). \tag{4.27}$$

For $k > 0$, the function $e^{im(k)z}$ in (4.27) corresponds to a wave with upward group velocity while the function $e^{-im(k)z}$ corresponds to a wave with negative downward group velocity, as discussed in Appendix D. The requirement that there can only be upward propagating waves to satisfy the upper boundary condition means that for $k > 0$ we must have $A_2(k) = 0$ in (4.27). But, for $k < 0$, we must have $A_1(k) = 0$. Applying the lower boundary condition (4.10), we find that $\hat{\psi}_p(k, 0) = 0$ and for $k > 0$ we have

$$A_1(k) = \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k-k_0)^2}{4\mu^2}},$$

and for $k < 0$, we have

$$A_2(k) = \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k+k_0)^2}{4\mu^2}}.$$

To find the solution $\psi(x, z)$, we use the inverse Fourier transform taking into account that, for $k < 0$, we have $A_2(k) \neq 0$, whereas for $k > 0$, we have $A_1(k) \neq 0$.

We obtain

$$\begin{aligned}
\psi(x, z) &= \int_{-\infty}^{\infty} \hat{\psi}(k, z) e^{ikx} dk \\
&= \frac{\sqrt{\pi}}{2\pi\mu} \left[\int_{-\infty}^0 e^{-\frac{(k+k_0)^2}{4\mu^2}} e^{-im(k)z} e^{ikx} dk + \int_0^{\infty} e^{-\frac{(k-k_0)^2}{4\mu^2}} e^{im(k)z} e^{ikx} dk \right] \\
&\quad + \int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk \\
&= \frac{\sqrt{\pi}}{2\pi\mu} \left[\underbrace{\int_{-\infty}^0 e^{-\frac{(k+k_0)^2}{4\mu^2}} e^{-im(k)z} e^{ikx} dk}_{I_1} + \underbrace{\int_0^{\infty} e^{-\frac{(k-k_0)^2}{4\mu^2}} e^{im(k)z} e^{ikx} dk}_{I_2} \right] \\
&\quad + \underbrace{\int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk}_{I_3}. \tag{4.28}
\end{aligned}$$

For the integrals I_1 and I_2 , we note that since $\mu \ll 1$, the dominant contribution is around $(k + k_0)$. We define $F(k, z) = e^{-im(k)z}$ and expand it about $(k + k_0)$. Integrating about $\bar{k} = k + k_0$, we obtain an asymptotic approximation comprising the first two terms

$$I_1 \sim e^{-ik_0x} \left(F(-k_0, z) \int_{-\infty}^{k_0} e^{-\frac{(\bar{k})^2}{4\mu^2}} e^{i\bar{k}x} d\bar{k} + \frac{\partial F}{\partial k}(-k_0, z) \int_{-\infty}^{k_0} e^{-\frac{(\bar{k})^2}{4\mu^2}} e^{i\bar{k}x} \bar{k} d\bar{k} \right). \tag{4.29}$$

The Gaussian $e^{-\frac{(\bar{k})^2}{4\mu^2}}$ is centred at zero and, since $\mu \ll 1$, it is close to zero at $\bar{k} \rightarrow k_0$. Thus the integral I_1 can be written as

$$\begin{aligned}
I_1 &\sim e^{-ik_0x} \left(F(-k_0, z) \int_{-\infty}^{\infty} e^{-\frac{(\bar{k})^2}{4\mu^2}} e^{i\bar{k}x} d\bar{k} + \frac{\partial F}{\partial k}(-k_0, z) \int_{-\infty}^{\infty} e^{-\frac{(\bar{k})^2}{4\mu^2}} e^{i\bar{k}x} \bar{k} d\bar{k} \right) \\
&\sim e^{-ik_0x} \left(2\mu\sqrt{\pi}e^{-\mu^2x^2} F(-k_0, z) + 4\mu^3ix\sqrt{\pi}e^{-\mu^2x^2} \frac{\partial F}{\partial k}(-k_0, z) \right), \tag{4.30}
\end{aligned}$$

for $\mu \ll 1$. Similarly, we set $\tilde{F}(k, z) = e^{im(k)z}$ and expand about $(k - k_0)$. Following

the same approach as in I_1 we find

$$I_2 \sim e^{ik_0x} \left(2\mu\sqrt{\pi}e^{-\mu^2x^2}\tilde{F}(k_0, z) + 4\mu^3ix\sqrt{\pi}e^{-\mu^2x^2}\frac{\partial\tilde{F}}{\partial k}(k_0, z) \right), \quad (4.31)$$

where we note that I_2 is the complex conjugate of I_1 . The last integral, I_3 , in (4.28) is $\psi_p(x, z) = \mathcal{F}^{-1}[\hat{\psi}_p(k, z)]$, where $\hat{\psi}_p(k, z)$ is the particular solution given in (4.25). Thus $I_3 = \psi_p(x, z)$ is

$$\psi_p(x, z) = \frac{-g\gamma e^{\frac{z_1}{h}}}{8ab\bar{u}} \int_{-\infty}^{\infty} e^{ikx - \frac{k^2}{4a}} G(k, z) dk, \quad (4.32)$$

where $G(k, z)$ is given by (4.26). We note that, since a is small, the dominant contribution in (4.32) is around $k = 0$, so we expand $G(k, z)$ about $k = 0$ and integrate to obtain

$$\psi_p(x, z) \sim \frac{-g\gamma e^{\frac{z_1}{h}}}{8ab\bar{u}} \left(2a\sqrt{\pi}e^{-a^2x^2}G(0, z) + 4a^3ix\sqrt{\pi}e^{-a^2x^2}\frac{\partial G}{\partial k}(0, z) \right). \quad (4.33)$$

Substituting (4.30), (4.31) and (4.33) into (4.28), we obtain

$$\begin{aligned} \psi(x, z) \sim & e^{-\mu^2x^2} e^{-ik_0x} \left(F(-k_0, z) + 2\mu^2ix\frac{\partial F}{\partial k}(-k_0, z) \right) \\ & + e^{-\mu^2x^2} e^{ik_0x} \left(\tilde{F}(k_0, z) + 2\mu^2ix\frac{\partial \tilde{F}}{\partial k}(k_0, z) \right) \\ & - \frac{\sqrt{\pi}e^{-a^2x^2}g\gamma e^{\frac{z_1}{h}}}{4b\bar{u}} \left(G(0, z) + 2a^2ix\frac{\partial G}{\partial k}(0, z) \right). \end{aligned} \quad (4.34)$$

Rearranging, equation (4.34) can be written as

$$\begin{aligned} \psi(x, z) \sim & e^{ik_0x} e^{-\mu^2x^2} [p_1(z) + \mu^2x p_2(z)] \\ & + \text{c.c.} + e^{-a^2x^2} [q_1(z) + a^2x q_2(z)], \end{aligned} \quad (4.35)$$

where $p_1(z) = \tilde{F}(k_0, z)$, $p_2(z) = 2i \frac{\partial \tilde{F}}{\partial k}(k_0, z)$, c.c. is the complex conjugate of the first line of (4.35), $q_1(z) = -\frac{\sqrt{\pi} g \gamma e^{z_1/h}}{4b\bar{u}} G(0, z)$ and $q_2(z) = -\frac{2i\sqrt{\pi} g \gamma e^{z_1/h}}{4b\bar{u}} \frac{\partial G}{\partial k}(0, z)$.

In the absence of the chemical constituent, equation (4.16) is homogeneous, and the solution simply describes upward-propagating gravity waves given by (4.17). In this case, the asymptotic approximation of $\psi(x, z)$ takes the form (4.35) without the terms $q_1(z)$ and $q_2(z)$. When the chemical is present, equation (4.16) is non-homogenous, and the asymptotic approximation for $\psi(x, z)$ takes the form (4.35) with the terms $q_1(z)$ and $q_2(z)$ being included. The terms $q_1(z)$ and $q_2(z)$ are complicated functions that depend on error functions involving complex variables. In this case, the behaviour of the particular solution and hence the behaviour of the solution of the nonhomogenous equation is not well understood. This will be better understood in Configuration 2, where the absolute value form of the function $\mathcal{H}(bz)$ is considered.

Configuration 2:

We now consider the other possible form of the function $\mathcal{H}(bz)$ given by $\mathcal{H}(bz) = e^{-b|z-z_1|}$ so that $f(k, z) = \mathcal{R}(k) \frac{e^{z/h} e^{-b|z-z_1|}}{\bar{u}}$ in equation (4.16). We solve (4.16) with same boundary conditions as in Configuration 1. The homogenous solution is given by (4.17), just as in Configuration 1, whereas the particular solution is different. Following the same approach as in (4.18), the particular solution corresponding to $f(k, z) = \mathcal{R}(k) \frac{e^{z/h} e^{-b|z-z_1|}}{\bar{u}}$ is

$$\hat{\psi}_p(k, z) = \frac{e^{im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \int_0^z e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b|\tilde{z}-z_1|} d\tilde{z} - \frac{e^{-im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \int_0^z e^{im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b|\tilde{z}-z_1|} d\tilde{z}, \quad (4.36)$$

where the homogenous solutions are the same as in Configuration 1 and hence the Wronskian is the same as in (4.18). For $z < z_1$, we note that the exponential $e^{-b|\tilde{z}-z_1|}$ in both integrals in (4.36) becomes $e^{b(\tilde{z}-z_1)}$. The particular solution for

$z < z_1$ is then

$$\begin{aligned}
\hat{\psi}_p &= \frac{e^{-bz_1} e^{im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \int_0^z e^{(-im(k)+\frac{1}{h}+b)\tilde{z}} d\tilde{z} - \frac{e^{-bz_1} e^{-im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \int_0^z e^{(im(k)+\frac{1}{h}+b)\tilde{z}} d\tilde{z} \\
&= \frac{e^{-bz_1} e^{im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \frac{(e^{(-im(k)+\frac{1}{h}+b)z} - 1)}{(-im(k) + \frac{1}{h} + b)} - \frac{e^{-bz_1} e^{-im(k)z} \mathcal{R}(k)}{2im(k)\bar{u}} \frac{(e^{(im(k)+\frac{1}{h}+b)z} - 1)}{(im(k) + \frac{1}{h} + b)} \\
&= \frac{\mathcal{R}(k)}{2im(k)\bar{u}} \left\{ \frac{2im(k)e^{\frac{z}{h}} e^{b(z-z_1)}}{m(k)^2 + (\frac{1}{h} + b)^2} - \frac{e^{-bz_1} e^{im(k)z}}{(-im(k) + \frac{1}{h} + b)} + \frac{e^{-bz_1} e^{-im(k)z}}{(im(k) + \frac{1}{h} + b)} \right\}.
\end{aligned} \tag{4.37}$$

For $z \geq z_1$, however, we note that the first integral in (4.36) can be evaluated as a sum of two integrals as

$$\begin{aligned}
\int_0^z e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b|\tilde{z}-z_1|} d\tilde{z} &= \int_0^{z_1} e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{b(\tilde{z}-z_1)} d\tilde{z} + \int_{z_1}^z e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b(\tilde{z}-z_1)} d\tilde{z} \\
&= \int_0^{z_1} e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{b(\tilde{z}-z_1)} d\tilde{z} + \int_{z_1}^z e^{-im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b(\tilde{z}-z_1)} d\tilde{z} \\
&= e^{-bz_1} \int_0^{z_1} e^{(-im(k)+\frac{1}{h}+b)\tilde{z}} d\tilde{z} + e^{bz_1} \int_{z_1}^z e^{(-im(k)+\frac{1}{h}-b)\tilde{z}} d\tilde{z} \\
&= e^{-bz_1} \frac{(e^{(-im(k)+\frac{1}{h}+b)z_1} - 1)}{(-im(k) + \frac{1}{h} + b)} + e^{bz_1} \frac{e^{(-im(k)+\frac{1}{h}-b)z}}{(-im(k) + \frac{1}{h} - b)} \\
&\quad - e^{bz_1} \frac{e^{(-im(k)+\frac{1}{h}-b)z_1}}{(-im(k) + \frac{1}{h} - b)}.
\end{aligned} \tag{4.38}$$

We follow the same procedure for the second integral in (4.36) and obtain

$$\begin{aligned}
\int_0^z e^{im(k)\tilde{z}} e^{\frac{\tilde{z}}{h}} e^{-b|\tilde{z}-z_1|} d\tilde{z} &= e^{-bz_1} \frac{(e^{(im(k)+\frac{1}{h}+b)z_1} - 1)}{(im(k) + \frac{1}{h} + b)} + e^{bz_1} \frac{e^{(im(k)+\frac{1}{h}-b)z}}{(im(k) + \frac{1}{h} - b)} \\
&\quad - e^{bz_1} \frac{e^{(im(k)+\frac{1}{h}-b)z_1}}{(im(k) + \frac{1}{h} - b)}.
\end{aligned} \tag{4.39}$$

Substituting (4.38) and (4.39) into (4.36), the particular solution for $z \geq z_1$ is

$$\begin{aligned}
\hat{\psi}_p &= \frac{\mathcal{R}(k)}{2im(k)\bar{u}} \left[\frac{e^{im(k)z} \left(e^{(-im(k)+\frac{1}{h})z_1} - e^{-bz_1} \right)}{(-im(k) + \frac{1}{h} + b)} + \frac{e^{bz_1} e^{(\frac{1}{h}-b)z}}{(-im(k) + \frac{1}{h} - b)} \right. \\
&\quad - \frac{e^{im(k)z} e^{(-im(k)+\frac{1}{h})z_1}}{(-im(k) + \frac{1}{h} - b)} - \frac{e^{-im(k)z} \left(e^{(im(k)+\frac{1}{h})z_1} - e^{-bz_1} \right)}{(im(k) + \frac{1}{h} + b)} - \frac{e^{bz_1} e^{(\frac{1}{h}-b)z}}{(im(k) + \frac{1}{h} - b)} \\
&\quad \left. + \frac{e^{-im(k)z} e^{(im(k)+\frac{1}{h})z_1}}{(im(k) + \frac{1}{h} - b)} \right] \\
&= \frac{\mathcal{R}(k)}{2im(k)\bar{u}} \left[\frac{-2b e^{im(k)(z-z_1)} e^{\frac{z_1}{h}}}{(im(k) - \frac{1}{h})^2 - b^2} + \frac{2im(k) e^{-b(z-z_1)} e^{\frac{z}{h}}}{m(k)^2 + (\frac{1}{h} - b)^2} + \frac{2b e^{-im(k)(z-z_1)} e^{\frac{z_1}{h}}}{(im(k) + \frac{1}{h})^2 - b^2} \right. \\
&\quad \left. - \frac{e^{im(k)z} e^{-bz_1}}{(-im(k) + \frac{1}{h} + b)} + \frac{e^{-im(k)z} e^{-bz_1}}{(im(k) + \frac{1}{h} + b)} \right], \tag{4.40}
\end{aligned}$$

where $\mathcal{R}(k) = -g\gamma \left(\frac{\sqrt{\pi}}{2\pi a} e^{\frac{-k^2}{4a^2}} \right)$, as before.

With this particular solution corresponding to this choice of exponential form of $e^{-b|z-z_1|}$, the solution $\psi(x, z)$ given in (4.28) still holds except that the particular solution $\psi_p(x, z)$ is now in terms of the Fourier particular solution (4.37) and (4.40).

If $z < z_1$, then

$$\psi_p(x, z) = \frac{-\gamma\sqrt{\pi}g}{2\pi a\bar{u}} \int_{-\infty}^{\infty} e^{ikx - \frac{k^2}{4a^2}} M(k, z) dk,$$

where

$$M(k, z) = \frac{1}{2im(k)} \left\{ \frac{2im(k) e^{\frac{z}{h}} e^{b(z-z_1)}}{m(k)^2 + (\frac{1}{h} + b)^2} - \frac{e^{-bz_1} e^{im(k)z}}{(-im(k) + \frac{1}{h} + b)} + \frac{e^{-bz_1} e^{-im(k)z}}{(im(k) + \frac{1}{h} + b)} \right\}$$

We follow the same approach we did before by expanding $M(k, z)$ about $k = 0$ and integrating to obtain

$$\psi_p(x, z) \sim \frac{-\gamma\sqrt{\pi}g}{2\pi a\bar{u}} \left(2a\sqrt{\pi} e^{-a^2 x^2} M(0, z) + 4a^3 ix\sqrt{\pi} e^{-a^2 x^2} \frac{\partial M}{\partial k}(0, z) \right).$$

If $z \geq z_1$, then

$$\psi_p(x, z) = \frac{-\gamma\sqrt{\pi}g}{2\pi a\bar{u}} \int_{-\infty}^{\infty} e^{ikx - \frac{k^2}{4a^2}} N(k, z) dk,$$

where

$$N(k, z) = \frac{1}{2im(k)} \left[\frac{-2b e^{im(k)(z-z_1)} e^{\frac{z_1}{h}}}{\left(im(k) - \frac{1}{h}\right)^2 - b^2} + \frac{2im(k) e^{-b(z-z_1)} e^{\frac{z}{h}}}{m(k)^2 + \left(\frac{1}{h} - b\right)^2} + \frac{2b e^{-im(k)(z-z_1)} e^{\frac{z_1}{h}}}{\left(im(k) + \frac{1}{h}\right)^2 - b^2} - \frac{e^{im(k)z} e^{-bz_1}}{\left(-im(k) + \frac{1}{h} + b\right)} + \frac{e^{-im(k)z} e^{-bz_1}}{\left(im(k) + \frac{1}{h} + b\right)} \right].$$

Expanding $N(k, z)$ about $k = 0$ and integrating we obtain

$$\psi_p(x, z) \sim \frac{-\gamma\sqrt{\pi}g}{2\pi a\bar{u}} \left(2a\sqrt{\pi} e^{-a^2x^2} N(0, z) + 4a^3ix\sqrt{\pi} e^{-a^2x^2} \frac{\partial N}{\partial k}(0, z) \right).$$

From equation (4.28), we obtain an approximation of $\psi(x, z)$ given as

$$\begin{aligned} \psi(x, z) \sim e^{ik_0x} e^{-\mu^2x^2} [p_1(z) + \mu^2x p_2(z)] \\ + \text{c.c.} + e^{-a^2x^2} [\tilde{q}_1(z) + a^2x \tilde{q}_2(z)], \end{aligned} \quad (4.41)$$

where $p_1(z) = \tilde{F}(k_0, z)$, $p_2(z) = 2i \frac{\partial \tilde{F}}{\partial k}(k_0, z)$, as before, c.c. is the complex conjugate of the first line of (4.41), $\tilde{q}_1(z)$ is

$$\tilde{q}_1(z) = \begin{cases} \frac{-\gamma g}{\bar{u}} M(0, z) & \text{if } z < z_1 \\ \frac{-\gamma g}{\bar{u}} N(0, z) & \text{if } z \geq z_1 \end{cases}$$

and $\tilde{q}_2(z)$ is

$$\tilde{q}_2(z) = \begin{cases} \frac{-2i\gamma g}{\bar{u}} \frac{\partial M}{\partial k}(0, z) & \text{if } z < z_1 \\ \frac{-2i\gamma g}{\bar{u}} \frac{\partial N}{\partial k}(0, z) & \text{if } z \geq z_1. \end{cases}$$

Figure 4.1 shows a contour plot of the asymptotic approximation for $\psi(x, z)$

given by (4.41). The background mean flow is set to $\bar{u} = -1$. This choice of $\bar{u}$ is shown for comparison with the asymptotic approximation presented in Subsection 4.1.2, where $\bar{u}$ is taken to be $\bar{u} = \tanh(z - z_c)$ and $\bar{u} \approx -1$ in the lower half of the domain. In Figure 4.1 (a), the chemical is centred at $z_1 = 5$, which corresponds to the location of the critical level z_c used in Subsection 4.1.2. In the absence of the chemical constituent, equation (4.16) is homogeneous, and the solution simply describes upward-propagating gravity waves given by the solution (4.17). In this case, the asymptotic approximation of $\psi(x, z)$ takes the form (4.41) without the terms $\tilde{q}_1(z)$ and $\tilde{q}_2(z)$. This case is shown in Figure 4.1 (b). The gravity waves take the form of spatially localized wave packet generated by the lower boundary forcing (4.4). The asymptotic approximation of $\psi(x, z)$ corresponding to the solution of the nonhomogenous equation (4.16), where the chemical forcing is present, takes the form (4.41) with the terms $\tilde{q}_1(z)$ and $\tilde{q}_2(z)$ being included in addition to other terms. This case is shown in Figure 4.1 (d). Figure 4.1 (c) shows the asymptotic approximation for the particular solution $\psi_p(x, z)$, which takes the form (4.41), where only the terms $\tilde{q}_1(z)$ and $\tilde{q}_2(z)$ are present. We observe from Figure 4.1 (d) that gravity waves are affected by the presence of the chemical concentration and the qualitative behaviour of the gravity waves affected by the chemical corresponds to the behaviour of the particular solution shown in Figure 4.1 (c).

Figure 4.1: The concentration of the chemical $C(x, z)$ is shown in (a). The approximation of $\psi(x, z)$ corresponding to the solution of the corresponding homogenous equation (no chemical) is shown in (b), and the solution of the nonhomogenous equation is shown in (d). Figure (c) shows the particular solution $\psi_p(x, z)$. The parameters are $a = 0.08$, $b = 0.8$, $\mu = 0.2$, $\delta = 0.2$, $h = 4.9$, $\gamma = 0.5$ and $k_0 = 2$.

4.1.2 Mean flow with vertical shear

When the mean flow is not constant and includes vertical shear— i.e. $\bar{u} = \bar{u}(z)$ — then equation (4.15) is a nonhomogeneous Taylor–Goldstein equation for $0 < z < \infty$. We consider the case where $\bar{u}(z) = 0$ at $z = z_c$, equation (4.15) is singular and there is a critical level at $z = z_c$. As in Subsection 4.1.1, the lower boundary condition at $z = 0$ is given by (4.10), and the upper boundary condition as $z \rightarrow \infty$ is that only waves with upward group velocity are considered. In the

right-hand side of (4.15), we consider the Gaussian form for the chemical, which corresponds to Configuration 1 in Subsection 4.1.1, and consider the situation where the chemical is centred at the critical level, so we choose $z_1 = z_c$. As before, the general solution of (4.15) is given as

$$\hat{\psi}(k, z) = \hat{\psi}_h(k, z) + \hat{\psi}_p(k, z).$$

The solution of the corresponding homogenous equation, as derived in Appendix D using Frobenius series, has the form

$$\hat{\psi}_h(k, z) \sim a_0(k)\phi_a(k, z) + b_0(k)\phi_b(k, z) \quad (4.42)$$

as $z \rightarrow z_c$, where

$$\phi_a(k, z) = (z - z_c)^{\frac{1}{2} + i\beta} [1 + a_1(k)(z - z_c) + a_2(k)(z - z_c)^2]$$

and

$$\phi_b(k, z) = (z - z_c)^{\frac{1}{2} - i\beta} [1 + b_1(k)(z - z_c) + b_2(k)(z - z_c)^2],$$

where $\beta = (Ri_c - \frac{1}{4})^{\frac{1}{2}}$ and Ri_c is the Richardson number at the critical level. The coefficients are

$$a_1(k) = \frac{(1 + Ri)\bar{u}_c''}{2\alpha\bar{u}_c'},$$

where $\bar{u}_c' = \bar{u}'(z_c)$, $\bar{u}_c'' = \bar{u}''(z_c)$ and

$$a_2(k) = \frac{\left(\frac{\bar{u}_c''^2}{2} + \bar{u}_c'\bar{u}_c''' + \delta k^2\bar{u}_c'^2\right) - a_1\bar{u}_c\bar{u}_c''(\alpha^2 + \alpha - 1)}{(\alpha^2 + 3\alpha + 2)\bar{u}_c'^2 + N^2},$$

where $\alpha = \frac{1}{2} + i\beta$. The coefficients $b_1(k)$ and $b_2(k)$ follow the same definitions of $a_1(k)$ and $a_2(k)$ except that α is taken as $(\frac{1}{2} - i\beta)$. The coefficients $a_0(k)$ and $b_0(k)$ can be found from the boundary conditions (4.10) at $z = 0$ and the upward group velocity condition at $z \rightarrow \infty$.

The particular solution of equation (4.15) with $f(k, z) = \mathcal{R}(k) \frac{e^{\frac{z}{h}} e^{-b^2(z-z_c)^2}}{\bar{u}(z)}$ is given as

$$\begin{aligned} \hat{\psi}_p(k, z) \sim & \frac{(z - z_c)^{\frac{1}{2} + i\beta} \mathcal{R}(k)}{2i\beta} \left(\int_0^z \frac{(\tilde{z} - z_c)^{\frac{1}{2} - i\beta} e^{\frac{\tilde{z}}{h} - b^2(\tilde{z} - z_c)^2}}{\bar{u}(\tilde{z})} d\tilde{z} \right) \\ & - \frac{(z - z_c)^{\frac{1}{2} - i\beta} \mathcal{R}(k)}{2i\beta} \left(\int_0^z \frac{(\tilde{z} - z_c)^{\frac{1}{2} + i\beta} e^{\frac{\tilde{z}}{h} - b^2(\tilde{z} - z_c)^2}}{\bar{u}(\tilde{z})} d\tilde{z} \right). \end{aligned} \quad (4.43)$$

In the derivation of the homogenous solution (4.42), $\bar{u}(z)$ is approximated by its Taylor expansion in powers of $(z - z_c)$. We follow the same approach and approximate $\bar{u}(\tilde{z})$ in (4.43) as

$$\bar{u}(\tilde{z}) \sim (\tilde{z} - z_c) \bar{u}'_{z_c}.$$

We also expand $e^{\frac{\tilde{z}}{h} - b^2(\tilde{z} - z_c)^2}$ about $(\tilde{z} - z_c)$, so the integrals in (4.43) are evaluated as

$$\begin{aligned} & \int_0^z (\tilde{z} - z_c)^{\frac{1}{2} - i\beta} e^{\frac{\tilde{z}}{h} - b^2(\tilde{z} - z_c)^2} d\tilde{z} \\ & \sim \int_0^z \frac{(\tilde{z} - z_c)^{\frac{1}{2} - i\beta}}{(\tilde{z} - z_c) \bar{u}'_{z_c}} \left\{ e^{\frac{\tilde{z}_c}{h}} + (\tilde{z} - z_c) \left(\frac{1}{h} \right) e^{\frac{\tilde{z}_c}{h}} - \frac{1}{2} (\tilde{z} - z_c)^2 \left(\frac{1}{h} \right)^2 (2b^2 h^2 - 1) e^{\frac{\tilde{z}_c}{h}} \right\} d\tilde{z} \\ & \sim \frac{e^{\frac{z_c}{h}}}{\bar{u}'_{z_c}} \left\{ \frac{(z - z_c)^{\frac{1}{2} - i\beta}}{(\frac{1}{2} - i\beta)} + \frac{(z - z_c)^{\frac{3}{2} - i\beta}}{h(\frac{3}{2} - i\beta)} - (2b^2 h^2 - 1) \frac{(z - z_c)^{\frac{5}{2} - i\beta}}{2h^2(\frac{5}{2} - i\beta)} - \frac{(-z_c)^{\frac{1}{2} - i\beta}}{(\frac{1}{2} - i\beta)} \right. \\ & \quad \left. - \frac{(-z_c)^{\frac{3}{2} - i\beta}}{h(\frac{3}{2} - i\beta)} + (2b^2 h^2 - 1) \frac{(-z_c)^{\frac{5}{2} - i\beta}}{2h^2(\frac{5}{2} - i\beta)} \right\}, \end{aligned} \quad (4.44)$$

as $z \rightarrow z_c$, and

$$\begin{aligned}
& \int_0^z (\tilde{z} - z_c)^{\frac{1}{2}+i\beta} e^{\frac{\tilde{z}}{h} - b^2(\tilde{z}-z_c)^2} d\tilde{z} \\
& \sim \frac{e^{\frac{z_c}{h}}}{\bar{u}'_{z_c}} \left\{ \frac{(z - z_c)^{\frac{1}{2}+i\beta}}{(\frac{1}{2} + i\beta)} + \frac{(z - z_c)^{\frac{3}{2}+i\beta}}{h(\frac{3}{2} + i\beta)} - (2b^2h^2 - 1) \frac{(z - z_c)^{\frac{5}{2}+i\beta}}{2h^2(\frac{5}{2} + i\beta)} - \frac{(-z_c)^{\frac{1}{2}+i\beta}}{(\frac{1}{2} + i\beta)} \right. \\
& \quad \left. - \frac{(-z_c)^{\frac{3}{2}+i\beta}}{h(\frac{3}{2} + i\beta)} + (2b^2h^2 - 1) \frac{(-z_c)^{\frac{5}{2}+i\beta}}{2h^2(\frac{5}{2} + i\beta)} \right\},
\end{aligned} \tag{4.45}$$

as $z \rightarrow z_c$. We substitute (4.44) and (4.45) into (4.43) to obtain the particular solution $\hat{\psi}_p(k, z)$ as

$$\begin{aligned}
\hat{\psi}_p(k, z) \sim & \frac{e^{\frac{z_c}{h}} \mathcal{R}(k)}{2i\beta \bar{u}'_{z_c}} \left\{ \frac{(z - z_c)}{(\frac{1}{2} - i\beta)} + \frac{(z - z_c)^2}{h(\frac{3}{2} - i\beta)} - (2b^2h^2 - 1) \frac{(z - z_c)^3}{2h^2(\frac{5}{2} - i\beta)} \right. \\
& - \frac{(z - z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{1}{2}-i\beta}}{(\frac{1}{2} - i\beta)} - \frac{(z - z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{3}{2}-i\beta}}{h(\frac{3}{2} - i\beta)} \\
& + (2b^2h^2 - 1) \frac{(z - z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{5}{2}-i\beta}}{2h^2(\frac{5}{2} - i\beta)} \left. \right\} - \frac{e^{\frac{z_c}{h}} \mathcal{R}(k)}{2i\beta \bar{u}'_{z_c}} \left\{ \frac{(z - z_c)}{(\frac{1}{2} + i\beta)} \right. \\
& + \frac{(z - z_c)^2}{h(\frac{3}{2} + i\beta)} - (2b^2h^2 - 1) \frac{(z - z_c)^3}{2h^2(\frac{5}{2} + i\beta)} - \frac{(z - z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{1}{2}+i\beta}}{(\frac{1}{2} + i\beta)} \\
& \left. - \frac{(z - z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{3}{2}+i\beta}}{h(\frac{3}{2} + i\beta)} + (2b^2h^2 - 1) \frac{(z - z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{5}{2}+i\beta}}{2h^2(\frac{5}{2} + i\beta)} \right\},
\end{aligned} \tag{4.46}$$

where $\mathcal{R}(k) = -g\gamma \left(\frac{\sqrt{\pi}}{2\pi a} e^{\frac{-k^2}{4a^2}} \right)$, as before.

The general solution can be written as

$$\hat{\psi}(k, z) = a_0(k)\phi_a(k, z) + b_0(k)\phi_b(k, z) + \hat{\psi}_p(k, z). \tag{4.47}$$

From the upper boundary condition, we require waves with only upward group

velocity. This means that, for $k > 0$, we must have $b_0(k) = 0$ in order to avoid the solution with negative sign, which has downward group velocity. For $k < 0$, it is the opposite, so we must have $a_0(k) = 0$ when $k < 0$. By applying the lower boundary condition (4.10), we find that if $k > 0$, then

$$\hat{\psi}(k, 0) = a_0(k)\phi_a(k, 0) + \hat{\psi}_p(k, 0) \sim \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k-k_0)^2}{4\mu^2}}, \quad (4.48)$$

and if $k < 0$, then

$$\hat{\psi}(k, 0) = b_0(k)\phi_b(k, 0) + \hat{\psi}_p(k, 0) \sim \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k+k_0)^2}{4\mu^2}}. \quad (4.49)$$

Since the particular solution goes to zero as $z \rightarrow 0$, we then find that if $k > 0$, then

$$a_0(k) \sim \frac{\sqrt{\pi}}{2\pi\mu \phi_a(k, 0)} e^{-\frac{(k-k_0)^2}{4\mu^2}},$$

and for $k < 0$, we have

$$b_0(k) \sim \frac{\sqrt{\pi}}{2\pi\mu \phi_b(k, 0)} e^{-\frac{(k+k_0)^2}{4\mu^2}}.$$

The general solution $\hat{\psi}(k, z)$ for $k > 0$ is then given as

$$\hat{\psi}(k, z) \sim \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k-k_0)^2}{4\mu^2}} H_a(k, z) + \hat{\psi}_p(k, z), \quad (4.50)$$

where

$$H_a(k, z) = \frac{\phi_a(k, z)}{\phi_a(k, 0)} = \frac{(z - z_c)^{\frac{1}{2}+i\beta} + a_1(z - z_c)^{\frac{3}{2}+i\beta} + a_2(k)(z - z_c)^{\frac{5}{2}+i\beta}}{(-z_c)^{\frac{1}{2}+i\beta} + a_1(-z_c)^{\frac{3}{2}+i\beta} + a_2(k)(-z_c)^{\frac{5}{2}+i\beta}}.$$

Similarly, for $k < 0$, we have

$$\hat{\psi}(k, z) \sim \frac{\sqrt{\pi}}{2\pi\mu} e^{-\frac{(k+k_0)^2}{4\mu^2}} H_b(k, z) + \hat{\psi}_p(k, z), \quad (4.51)$$

where

$$H_b(k, z) = \frac{(z - z_c)^{\frac{1}{2}-i\beta} + b_1(z - z_c)^{\frac{3}{2}-i\beta} + b_2(k)(z - z_c)^{\frac{5}{2}-i\beta}}{(-z_c)^{\frac{1}{2}-i\beta} + b_1(-z_c)^{\frac{3}{2}-i\beta} + b_2(k)(-z_c)^{\frac{5}{2}-i\beta}}.$$

To find the solution $\psi(x, z, t)$, we use the inverse Fourier transform:

$$\begin{aligned} \psi(x, z) &= \int_{-\infty}^{\infty} \hat{\psi}(k, z) e^{ikx} dk \\ &\sim \frac{\sqrt{\pi}}{2\pi\mu} \int_{-\infty}^0 e^{-\frac{(k+k_0)^2}{4\mu^2}} H_b(k, z) e^{ikx} dk + \frac{\sqrt{\pi}}{2\pi\mu} \int_0^{\infty} e^{-\frac{(k-k_0)^2}{4\mu^2}} H_a(k, z) e^{ikx} dk \\ &\quad + \int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk \end{aligned} \quad (4.52)$$

The first two integrals corresponding to the homogenous equation are approximated following the same approach as in Subsection 4.1.1. The first integral is approximated as

$$\begin{aligned} \int_{-\infty}^0 e^{-\frac{(k+k_0)^2}{4\mu^2}} H_b(k, z) e^{ikx} dk &\sim e^{-ik_0x} \left((2\mu\sqrt{\pi}e^{-\mu^2x^2}) H_b(-k_0, z) \right. \\ &\quad \left. + 4\mu^3ix\sqrt{\pi}e^{-\mu^2x^2} \frac{\partial H_b}{\partial k}(-k_0, z) \right). \end{aligned} \quad (4.53)$$

Similarly, the second integral is

$$\begin{aligned} \int_0^{\infty} e^{-\frac{(k-k_0)^2}{4\mu^2}} H_a(k, z) e^{ikx} dk &\sim e^{ik_0x} \left((2\mu\sqrt{\pi}e^{-\mu^2x^2}) H_a(k_0, z) \right. \\ &\quad \left. + 4\mu^3ix\sqrt{\pi}e^{-\mu^2x^2} \frac{\partial H_a}{\partial k}(k_0, z) \right). \end{aligned} \quad (4.54)$$

We substitute the particular solution $\hat{\psi}_p(k, z)$ given in (4.46) into the third term in (4.52) and obtain

$$\begin{aligned}
& \int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk \\
& \sim \frac{g\gamma\sqrt{\pi}}{4i\pi a\beta\bar{u}'_{z_c}} e^{\frac{z_c}{h}} \left\{ -\frac{(z-z_c)}{(\frac{1}{2}-i\beta)} - \frac{(z-z_c)^2}{h(\frac{3}{2}-i\beta)} + (2b^2h^2-1) \frac{(z-z_c)^3}{2h^2(\frac{5}{2}-i\beta)} \right. \\
& \quad + \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{1}{2}-i\beta}}{(\frac{1}{2}-i\beta)} + \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{3}{2}-i\beta}}{h(\frac{3}{2}-i\beta)} \\
& \quad - (2b^2h^2-1) \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{5}{2}-i\beta}}{2h^2(\frac{5}{2}-i\beta)} + \frac{(z-z_c)}{(\frac{1}{2}+i\beta)} + \frac{(z-z_c)^2}{h(\frac{3}{2}+i\beta)} \\
& \quad - (2b^2h^2-1) \frac{(z-z_c)^3}{2h^2(\frac{5}{2}+i\beta)} - \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{1}{2}+i\beta}}{(\frac{1}{2}+i\beta)} - \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{3}{2}+i\beta}}{h(\frac{3}{2}+i\beta)} \\
& \quad \left. + (2b^2h^2-1) \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{5}{2}+i\beta}}{2h^2(\frac{5}{2}+i\beta)} \right\} \int_{-\infty}^{\infty} e^{\frac{-k^2}{4a^2}} e^{ikx} dk.
\end{aligned} \tag{4.55}$$

Evaluating the integral in the last line of (4.55) as before, we obtain

$$\begin{aligned}
& \int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk \\
& \sim \frac{g\gamma\sqrt{\pi}}{4i\pi a\beta\bar{u}'_{z_c}} e^{\frac{z_c}{h}} \left\{ -\frac{(z-z_c)}{(\frac{1}{2}-i\beta)} - \frac{(z-z_c)^2}{h(\frac{3}{2}-i\beta)} + (2b^2h^2-1) \frac{(z-z_c)^3}{2h^2(\frac{5}{2}-i\beta)} \right. \\
& \quad + \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{1}{2}-i\beta}}{(\frac{1}{2}-i\beta)} + \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{3}{2}-i\beta}}{h(\frac{3}{2}-i\beta)} \\
& \quad - (2b^2h^2-1) \frac{(z-z_c)^{\frac{1}{2}+i\beta}(-z_c)^{\frac{5}{2}-i\beta}}{2h^2(\frac{5}{2}-i\beta)} + \frac{(z-z_c)}{(\frac{1}{2}+i\beta)} + \frac{(z-z_c)^2}{h(\frac{3}{2}+i\beta)} \\
& \quad - (2b^2h^2-1) \frac{(z-z_c)^3}{2h^2(\frac{5}{2}+i\beta)} - \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{1}{2}+i\beta}}{(\frac{1}{2}+i\beta)} - \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{3}{2}+i\beta}}{h(\frac{3}{2}+i\beta)} \\
& \quad \left. + (2b^2h^2-1) \frac{(z-z_c)^{\frac{1}{2}-i\beta}(-z_c)^{\frac{5}{2}+i\beta}}{2h^2(\frac{5}{2}+i\beta)} \right\} \left(2a\sqrt{\pi} e^{-a^2x^2} \right).
\end{aligned} \tag{4.56}$$

This can be written as

$$\begin{aligned}
& \int_{-\infty}^{\infty} \hat{\psi}_p(k, z) e^{ikx} dk \\
& \sim \frac{g\gamma e^{-a^2 x^2} e^{\frac{z_c}{h}}}{\bar{u}'_{z_c}} \left\{ -\frac{(z - z_c)}{(\frac{1}{4} + \beta^2)} - \frac{(z - z_c)^2}{h(\frac{9}{4} + \beta^2)} + \frac{(2b^2 h^2 - 1)(z - z_c)^3}{2h^2(\frac{25}{4} + \beta^2)} \right. \\
& \quad + \frac{(z - z_c)^{\frac{1}{2} + i\beta}}{2i\beta} \left[\frac{(-z_c)^{\frac{1}{2} - i\beta}}{(\frac{1}{2} - i\beta)} + \frac{(-z_c)^{\frac{3}{2} - i\beta}}{h(\frac{3}{2} - i\beta)} - \frac{(2b^2 h^2 - 1)(-z_c)^{\frac{5}{2} - i\beta}}{2h^2(\frac{5}{2} - i\beta)} \right] \\
& \quad \left. + \frac{(z - z_c)^{\frac{1}{2} - i\beta}}{2i\beta} \left[-\frac{(-z_c)^{\frac{1}{2} + i\beta}}{(\frac{1}{2} + i\beta)} - \frac{(-z_c)^{\frac{3}{2} + i\beta}}{h(\frac{3}{2} + i\beta)} + \frac{(2b^2 h^2 - 1)(-z_c)^{\frac{5}{2} + i\beta}}{2h^2(\frac{5}{2} + i\beta)} \right] \right\}.
\end{aligned} \tag{4.57}$$

Therefore, the general solution $\psi(x, z)$ given in (4.52) can be written as

$$\begin{aligned}
\psi(x, z) & \sim e^{ik_0 x} e^{-\mu^2 x^2} [\tilde{p}_1(z) + \mu^2 x \tilde{p}_2(z)] \\
& + \text{c.c.} + e^{-a^2 x^2} \tilde{q}(z),
\end{aligned} \tag{4.58}$$

where $\tilde{p}_1(z) = H_a(k_0, z)$, $\tilde{p}_2(z) = 2i \frac{\partial H_a}{\partial k}(k_0, z)$, c.c. is the complex conjugate of the first line of (4.58) and $\tilde{q}(z)$ is

$$\begin{aligned}
\tilde{q}(z) & = \frac{g\gamma e^{\frac{z_c}{h}}}{\bar{u}'_{z_c}} \left\{ -\frac{(z - z_c)}{(\frac{1}{4} + \beta^2)} - \frac{(z - z_c)^2}{h(\frac{9}{4} + \beta^2)} + \frac{(2b^2 h^2 - 1)(z - z_c)^3}{2h^2(\frac{25}{4} + \beta^2)} \right. \\
& \quad + \frac{(z - z_c)^{\frac{1}{2} + i\beta}}{2i\beta} \left[\frac{(-z_c)^{\frac{1}{2} - i\beta}}{(\frac{1}{2} - i\beta)} + \frac{(-z_c)^{\frac{3}{2} - i\beta}}{h(\frac{3}{2} - i\beta)} - \frac{(2b^2 h^2 - 1)(-z_c)^{\frac{5}{2} - i\beta}}{2h^2(\frac{5}{2} - i\beta)} \right] \\
& \quad \left. + \frac{(z - z_c)^{\frac{1}{2} - i\beta}}{2i\beta} \left[-\frac{(-z_c)^{\frac{1}{2} + i\beta}}{(\frac{1}{2} + i\beta)} - \frac{(-z_c)^{\frac{3}{2} + i\beta}}{h(\frac{3}{2} + i\beta)} + \frac{(2b^2 h^2 - 1)(-z_c)^{\frac{5}{2} + i\beta}}{2h^2(\frac{5}{2} + i\beta)} \right] \right\}.
\end{aligned} \tag{4.59}$$

Figure 4.2: The concentration of the chemical $C(x, z)$ is shown in (a). The approximation of $\psi(x, z)$ where the solution of the corresponding homogenous equation (no chemical) is shown in (b), and the solution of the nonhomogenous equation is shown in (d). Figure (c) shows the particular solution $\psi_p(x, z)$. The parameters are $a = 0.08$, $b = 0.8$, $\mu = 0.2$, $\delta = 0.2$, $h = 4.9$, $\gamma = 0.5$ and $k_0 = 2$.

The asymptotic approximation of $\psi(x, z)$ given by (4.58) is shown in Figure 4.2. The background shear flow is considered to be $\bar{u}(z) = \tanh(z - 5)$, so we have a critical level at $z_c = 5$ and the chemical is centred at $z_c = 5$. The contour plot of the chemical concentration is shown in Figure 4.2 (a). The asymptotic approximation of $\psi(x, z)$ that corresponds to the homogenous equation of (4.15) where there is no chemical effect is shown in Figure 4.2 (b). In this case, the asymptotic approximation of $\psi(x, z)$ takes the form (4.58) without the term $\tilde{q}(z)$. This gives upward-propagating gravity waves as shown in Figure 4.2 (b). We note

in this figure that the waves are absorbed at $z = 5$ due to the presence of the critical level at $z = 5$. This behaviour at the critical level is consistent with the periodic case as shown in Figure D.1 in Appendix D, and generally consistent with the critical layer theory as shall be discussed in Section 4.3. The approximation of $\psi(x, z)$ corresponding to the solution of the nonhomogenous equation (4.15) is shown in Figure 4.2 (d). This shows the effect of the chemical on gravity waves, which can be seen around the critical level where the chemical is centred. It can be seen in Figure 4.2 (d) that the behaviour of gravity waves around the critical level follows that of the particular solution that corresponds to the chemical forcing, which is shown in Figure 4.2 (c). In Chapter 6, when we consider the full nonlinear equations for gravity waves, we shall see that more effect can be seen as the waves are not totally absorbed at the critical level as in the linear case.

4.2 Weakly-nonlinear analysis

In this section, we carry out a weakly-nonlinear analysis of equations (2.41)–(2.45) in a configuration of the form studied in Section 4.1. We evaluate the horizontal average over the streamfunction equation and density equations. This gives us insight into the behaviour of the wave-induced mean flow streamfunction as well as the wave-induced mean flow density, which then can be compared with the corresponding numerical results obtained in Chapter 6.

As in Section 4.1, the domain is considered to be $-\infty < x < \infty$ and $0 \leq z < \infty$, and the lower boundary condition is in the form of the wave packet forcing $\psi(x, 0, t) = A(\mu x)e^{ik_0 x}$. The function A is a slowly varying function of x , which satisfies $A \rightarrow 0$ as $x \rightarrow \pm\infty$. The upper boundary condition as $z \rightarrow \infty$ is that only waves with upward group velocity are considered. We impose the conditions that ψ , ψ_x and ψ_z all go to zero as $x \rightarrow \pm\infty$. We also have the boundary conditions

$\rho \rightarrow 0$ as $x \rightarrow \pm\infty$ and $C(x, z, t) \rightarrow 0$ as $x \rightarrow \pm\infty$.

The amplitude A varies slowly over x and is different over each horizontal wavelength; thus we cannot define the mean by averaging the solution over a horizontal wavelength. Following Campbell and Maslowe (2003), the horizontal average is taken over the length of the packet L , which in the numerical computations chosen to be the length of the computational domain. We consider the horizontal average over some function $q(x, z, t)$ as

$$\bar{q} = \frac{1}{L} \int_{-\infty}^{\infty} q(x, z, t) dx. \quad (4.60)$$

The streamfunction $\psi(x, z, t)$ can be represented in terms of its inverse Fourier transform as

$$\psi(x, z, t) = \int_{-\infty}^{\infty} \hat{\psi}(k, z, t) e^{ikx} dk, \quad (4.61)$$

where $\hat{\psi}(k, z, t)$ is the Fourier transform of $\psi(x, z, t)$. The zero wavenumber component of $\hat{\psi}(k, z, t)$ is

$$\hat{\psi}(0, z, t) = \int_{-\infty}^{\infty} \psi(x, z, t) dx. \quad (4.62)$$

Since the wave-induced mean flow corresponds to the zero wavenumber, the wave-induced mean streamfunction that corresponds to the definition of the horizontal average (4.60) is $\bar{\psi}_0(z, t) = \frac{\varepsilon}{L} \hat{\psi}(0, z, t)$. The wave-induced horizontal velocity is then defined as $\bar{u}_0 = -\bar{\psi}_{0z}(z, t)$.

The vertical flux of horizontal momentum is defined, as shown by Holton (2004), as $F = -\overline{uw}$. From (4.60), the averaged vertical momentum flux is given as

$$F = -\frac{1}{L} \int_{-\infty}^{\infty} u w dx, \quad (4.63)$$

where $u = -\psi_z$ and $w = \psi_x$.

4.2.1 Wave-induced mean streamfunction

From equations (2.41)–(2.45) representing the interaction of a chemical constituent with gravity waves, the streamfunction equation can be expressed as

$$\nabla^2 \psi_t + \bar{u} \nabla^2 \psi_x - \bar{u}'' \psi_x + \varepsilon (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) = -\frac{g}{\rho} \rho_x, \quad (4.64)$$

where ψ , ρ and their derivatives are all continuous. Taking the average by applying the integral $\int_{-\infty}^{\infty} (\cdots) dx$, we obtain

$$\int_{-\infty}^{\infty} \nabla^2 \psi_t dx + \varepsilon \int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx = 0. \quad (4.65)$$

which reduces to

$$\int_{-\infty}^{\infty} \psi_{zzt} dx + \varepsilon \int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx = 0. \quad (4.66)$$

Rearranging, we get

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \psi_{zz} dx = -\varepsilon \int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx. \quad (4.67)$$

The right-hand side of equation (4.67) can be written as

$$\int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx = \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} + \delta \psi_x \psi_{zxx} - \delta \psi_z \psi_{xxx} - \psi_z \psi_{xzz}) dx. \quad (4.68)$$

From integration by parts, we find that

$$\int_{-\infty}^{\infty} \psi_x \psi_{zxx} dx = [\psi_x \psi_{zx}]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi_{zx} \psi_{xx} dx = - \int_{-\infty}^{\infty} \psi_{zx} \psi_{xx} dx.$$

Similarly, we have

$$\int_{-\infty}^{\infty} \psi_z \psi_{xxx} dx = [\psi_z \psi_{xx}]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi_{zx} \psi_{xx} dx = - \int_{-\infty}^{\infty} \psi_{zx} \psi_{xx} dx.$$

Thus equation (4.68) can be written as

$$\begin{aligned} \int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx &= \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} - \delta \psi_{zx} \psi_{xx} + \delta \psi_{zx} \psi_{xx} - \psi_z \psi_{xzz}) dx \\ &= \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} - \psi_z \psi_{xzz}) dx. \end{aligned} \quad (4.69)$$

Equation (4.69) can be written as

$$\begin{aligned} \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} - \psi_z \psi_{xzz}) dx &= \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} + \psi_z \psi_{xzz} - \psi_z \psi_{xzz} - \psi_z \psi_{xzz}) dx \\ &= \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} + \psi_z \psi_{xzz}) dx - 2 \int_{-\infty}^{\infty} \psi_z \psi_{xzz} dx \end{aligned} \quad (4.70)$$

The last integral on the right-hand side of (4.70) is evaluated as

$$\int_{-\infty}^{\infty} \psi_z \psi_{xzz} dx = [\psi_z \psi_{zz}]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \psi_{zx} \psi_{zz} dx = - \int_{-\infty}^{\infty} \psi_{zx} \psi_{zz} dx.$$

Therefore, equation (4.68) can be written as

$$\begin{aligned} \int_{-\infty}^{\infty} (\psi_x \nabla^2 \psi_z - \psi_z \nabla^2 \psi_x) dx &= \int_{-\infty}^{\infty} (\psi_x \psi_{zzz} + \psi_z \psi_{xzz} + 2\psi_{zx} \psi_{zz}) dx \\ &= \int_{-\infty}^{\infty} \frac{\partial^2}{\partial z^2} (\psi_z \psi_x) dx \\ &= \frac{\partial^2}{\partial z^2} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right). \end{aligned} \quad (4.71)$$

Equation (4.67) can be written as

$$\frac{\partial}{\partial t} \hat{\psi}_{zz}(0, z, t) = -\varepsilon \frac{\partial^2}{\partial z^2} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right). \quad (4.72)$$

Integrating with respect to z , we obtain

$$\frac{\partial}{\partial t} \hat{\psi}_z(0, z, t) = -\varepsilon \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right). \quad (4.73)$$

Since the wave-induced mean flow is $\bar{u}_0 = -\frac{\varepsilon}{L} \hat{\psi}_z(0, z, t)$, we then have

$$\frac{\partial}{\partial t} \bar{u}_0 = \varepsilon^2 \frac{\partial}{\partial z} F, \quad (4.74)$$

where F is the vertical flux of the horizontal momentum given as

$$F = \frac{1}{L} \int_{-\infty}^{\infty} \psi_z \psi_x dx.$$

This is the standard equation for the evaluation of a gravity-wave-induced mean flow. Equation (4.74) indicates that the change of the wave-induced mean flow with time is proportional to the vertical gradient of the momentum flux. The right-hand-side of equation (4.74) represents gravity-wave drag. This could be used in a parameterization scheme. We note that, although in our configuration waves are modified by a chemical forcing, the effect of the chemical forcing does not appear in this equation since the chemical forcing term is in the density perturbation equation only.

4.2.2 Wave-induced mean density

Applying the integral over the density equation (2.43) in system (2.41)–(2.45), representing the interaction of a chemical constituent with gravity waves, we ob-

tain

$$\int_{-\infty}^{\infty} \rho_t dx + \int_{-\infty}^{\infty} \varepsilon(\psi_x \rho_z - \psi_z \rho_x) dx = \gamma \int_{-\infty}^{\infty} \frac{D C}{D t} dx. \quad (4.75)$$

Rearranging, we obtain

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \rho dx = -\varepsilon \int_{-\infty}^{\infty} (\psi_x \rho_z - \psi_z \rho_x) dx + \gamma \int_{-\infty}^{\infty} \frac{D C}{D t} dx. \quad (4.76)$$

The nonlinear Jacobian term can be rewritten as

$$\begin{aligned} \int_{-\infty}^{\infty} (\psi_x \rho_z - \psi_z \rho_x) dx &= \int_{-\infty}^{\infty} \left(\psi_x \rho_z - \left(\frac{\partial}{\partial x} (\psi_z \rho) - \rho \psi_{zx} \right) \right) dx \\ &= \int_{-\infty}^{\infty} (\psi_x \rho_z + \rho \psi_{zx}) dx \\ &= \int_{-\infty}^{\infty} \frac{\partial}{\partial z} (\psi_x \rho) dx. \end{aligned} \quad (4.77)$$

Multiplying equation (4.76) by $(\frac{\varepsilon}{L})$, we obtain

$$\frac{\partial}{\partial t} \rho_0(z, t) = -\frac{\varepsilon^2}{L} \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_x \rho dx \right) + \frac{\varepsilon \gamma}{L} \int_{-\infty}^{\infty} \frac{D C}{D t} dx. \quad (4.78)$$

The wave-induced density $\rho_0(z, t) = \frac{\varepsilon}{L} \int_{-\infty}^{\infty} \rho dx$ is given in terms of the zero wavenumber component $\hat{\rho}(0, z, t)$ as $\rho_0(z, t) = \frac{\varepsilon}{L} \hat{\rho}(0, z, t)$. The last term in the right-hand side of equation (4.78) is evaluated as

$$\int_{-\infty}^{\infty} \frac{D C}{D t} dx = \int_{-\infty}^{\infty} \left(\frac{\partial C}{\partial t} + (\bar{u} + \varepsilon u) \frac{\partial C}{\partial x} + \varepsilon w \frac{\partial C}{\partial z} \right) dx. \quad (4.79)$$

The middle term goes to zero since $C(x, z, t) \rightarrow 0$ as $x \rightarrow \pm\infty$, so (4.79) simplifies to

$$\int_{-\infty}^{\infty} \frac{D C}{D t} dx = \int_{-\infty}^{\infty} \left(\frac{\partial C}{\partial t} + \varepsilon w \frac{\partial C}{\partial z} \right) dx. \quad (4.80)$$

Therefore, equation (4.78) can be rewritten as

$$\frac{\partial}{\partial t} \rho_0(z, t) = -\frac{\varepsilon^2}{L} \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_x \rho dx \right) + \frac{\gamma \varepsilon}{L} \int_{-\infty}^{\infty} \left(\frac{\partial C}{\partial t} + \varepsilon w \frac{\partial C}{\partial z} \right) dx. \quad (4.81)$$

This equation describes the change in energy or temperature, which is represented by the density in the Boussinesq model, resulting from a gradient in the vertical flux of energy (density) and from chemical heating. Equation (4.81) shows that the wave-induced mean density is significantly affected by the chemical heating. Equation (4.81) could be considered in a parameterization scheme. The effect of the chemical on the gravity-wave mean density is greater when the chemical is changing with time, as we shall see in Chapter 6. In the case of a steady-state chemical as in Section 4.1, the second term of the right-hand side of (4.81) is zero, and the effect of the chemical heating on the mean flow density will reduce to be of order $O(\varepsilon)$.

4.3 Numerical results for gravity wave equations

In this section, we present a description of the numerical method to solve the gravity-wave equations under the Boussinesq approximation, as well as the results of numerical computations. The discussion in this section concerns the equations of gravity waves with no chemical effect. The numerical results for the case where the chemical interaction is present are shown in Chapter 6. In this section, we present numerical solutions for the linear and nonlinear equations, which can be used for comparison with the results obtained in the case of the interaction with the chemical equation. From equations (2.38), (2.39) and (2.40), the gravity-wave

equations under the Boussinesq approximation are

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\bar{\rho}}\rho_x, \quad (4.82)$$

$$\zeta = \nabla^2\psi, \quad (4.83)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = 0. \quad (4.84)$$

We solve the equations (4.82), (4.83) and (4.84) on the two dimensional spatial domain $-x_1 \leq x \leq x_2$ in the horizontal direction and $0 \leq z \leq z_2$ in the vertical direction. The initial conditions are ζ and ρ are zero for $0 \leq z \leq z_2$ and $\psi = 0$ for $0 < z \leq z_2$. The vorticity ζ and density ρ are considered zero at the lower boundary $z = 0$. The forcing lower boundary condition is

$$\psi(x, 0, t) = \frac{e^{-\mu^2 x^2}}{2} (e^{ik_0 x} + e^{-ik_0 x}). \quad (4.85)$$

We study gravity waves under the Boussinesq approximation in a configuration where there is a background shear flow with a critical level z_c . We choose $z_c = \frac{z_2}{2}$ so the critical level is at half the height of the domain. We consider the background shear flow to be $\bar{u} = \tanh(z - z_c)$ and the background density $\bar{\rho} = \rho_0 e^{-z/h}$. Because there is a critical level at $z = z_c$, the waves do not reach the upper boundary. The wave amplitude remains so small at the upper boundary that it is sufficient to simply set zero upper boundary conditions for ψ , ζ and ρ . In addition, we impose the boundary conditions that ψ_z , ζ_z and ρ_z are zero at $z = 0$ and $z = z_2$, which ensures that the Jacobian term is zero at the boundaries. We also impose the conditions that ψ , ψ_x , ρ and ψ_z all go to zero as $x \rightarrow x_1, x_2$.

This configuration of gravity waves with background shear flow has been studied by numerous investigators in the past few decades; e.g., Booker and Bretherton

(1967), Brown and Stewartson (1980, 1982a,b) and more recently by Campbell and Maslowe (2003). Booker and Bretherton (1967) studied the linearized equations of internal gravity waves with a background shear flow. They found that the waves are reduced by a factor of $\exp(-2\pi\sqrt{\text{Ri} - \frac{1}{4}})$ as they cross the critical level, and the mean flow is enhanced at the critical level. Analogous linear analysis was carried out for the Rossby waves, and analytical solutions were obtained by Dickinson (1970). These solutions were reexamined by Warn and Warn (1976), and it was found that at a specific time, $t = O(\epsilon^{\frac{-1}{2}})$, the critical level becomes nonlinear and thus nonlinearity should be considered for investigating the critical level as shown by Warn and Warn (1978). Analytical and numerical investigation of the linearized equations of Rossby waves forced by a horizontally localized wave packet were studied by Campbell and Maslowe (1998). It was found that the waves are absorbed at the critical level and that induced-mean flow is proportional to the length of the wave packet. Campbell (2004) carried out a nonlinear numerical and analytical analysis of Rossby waves forced by a zonally localized wave packet. It was found that the waves are absorbed at the critical level at early time and reflected at later time when the nonlinearity becomes non-negligible. However, it was found that the absorption is dominant compared to the reflection.

Brown and Stewartson (1980, 1982a,b) extended the work of Booker and Bretherton (1967) by including the nonlinear terms in the internal gravity wave equations to study the behaviour at the critical level. They found that the waves at the critical level are absorbed at early time and reflected at later time. Campbell and Maslowe (2003) carried out a detailed numerical investigation of the nonlinear critical level evolution for internal gravity waves with a horizontally localized wave packet forcing as well as monochromatic forcing. It was found that, at early time, the waves are absorbed as suggested by linear critical theory and at later

time, as the nonlinear terms become important at the critical level, the waves can be reflected. However, it was found that there is more absorption in the case of wave packet forcing compared to that with monochromatic forcing. Numerical and analytical analysis of internal gravity waves forced by a horizontally localized wave packet were studied by Campbell and Nikitina (2014), where consistent analytical as well as numerical results obtained showing that the waves could either be absorbed or reflected.

In this section, we carry out numerical computation of the equations (4.82), (4.83) and (4.84) for comparison with the results obtained by Campbell and Maslowe (2003). These numerical results are then considered for comparison in later chapters when the chemical term is present.

As discussed in Section 4.1, the functions ψ , ζ and ρ are smooth and continuously differentiable and they are absolutely integrable (L_1) due to the form of boundary condition (4.85) which leads to expressing each function in (4.82), (4.83) and (4.84) in an integral form as

$$\hat{\psi}(k, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x, z, t) e^{-ikx} dx, \quad (4.86)$$

$$\hat{\zeta}(k, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \zeta(x, z, t) e^{-ikx} dx, \quad (4.87)$$

$$\hat{\rho}(k, z, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \rho(x, z, t) e^{-ikx} dx, \quad (4.88)$$

and the corresponding inverse Fourier transforms are

$$\psi(x, z, t) = \int_{-\infty}^{\infty} \hat{\psi}(k, z, t) e^{ikx} dk, \quad (4.89)$$

$$\zeta(x, z, t) = \int_{-\infty}^{\infty} \hat{\zeta}(k, z, t) e^{ikx} dk, \quad (4.90)$$

$$\rho(x, z, t) = \int_{-\infty}^{\infty} \hat{\rho}(k, z, t) e^{ikx} dk. \quad (4.91)$$

Taking the Fourier transform of (4.82), (4.83) and (4.84), we obtain the transformed equations

$$\hat{\zeta}_t + ik\bar{u}\hat{\zeta} - ik\bar{u}''\hat{\psi} + ik\frac{g}{\rho}\hat{\rho} + \varepsilon\mathcal{F}[\psi_x\zeta_z - \psi_z\zeta_x] = 0, \quad (4.92)$$

$$\hat{\rho}_t + ik\bar{u}\hat{\rho} + ik\bar{\rho}'\hat{\psi} + \varepsilon\mathcal{F}[\psi_x\rho_z - \psi_z\rho_x] = 0, \quad (4.93)$$

$$\hat{\psi}_{zz} - \delta k^2\hat{\psi} = \hat{\zeta}. \quad (4.94)$$

We solve the first two equations for $\hat{\zeta}$ and $\hat{\rho}$ using the fourth-order Adams–Bashforth method for the time discretization and solve for $\hat{\psi}$ at each time level using the second-order central finite difference approximation to represent $\hat{\psi}_{zz}$.

We define k as $k_m = k_0 + m\Delta k$ for $m = 0 \dots N-1$ and x is defined as $x = x_0 + j\Delta x$ for $j = 0 \dots N-1$. The Fourier integral can be computed numerically in a form of summation as

$$\begin{aligned} \hat{\psi}(k, z, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x, z, t) e^{-ikx} dx \\ &\approx \frac{\Delta x}{2\pi} \sum_{x=-\infty}^{\infty} \psi(x, z, t) e^{-ikx} \\ &= \frac{\Delta x}{2\pi} \sum_{j=0}^{N-1} \psi(x, z, t) e^{-i(k_0+m\Delta k)(x_0+j\Delta x)}. \end{aligned} \quad (4.95)$$

Rearranging, we get

$$\hat{\psi}(k, z, t) = \frac{\Delta x}{2\pi} e^{-ikx_0} \sum_{j=0}^{N-1} \psi(x, z, t) e^{-ik_0j\Delta x} e^{-imj\Delta k\Delta x}. \quad (4.96)$$

Computing these summations is computationally expensive, so we instead use the Fast Fourier Transform (FFT) algorithm. However, the equation should be written

in a form that is compatible with the FFT algorithm and satisfy its conditions. Thus we choose Δk and Δx such that the condition

$$\Delta k \Delta x = \frac{2\pi}{N}$$

is satisfied.

The pseudo-spectral method is used to compute the nonlinear terms at each time step. This means that, at each time level, the x and z derivatives of ψ , ζ and ρ are computed for each x_j , $j = 0, \dots, N-1$, by evaluating the inverse Fourier transforms of $\hat{\psi}_z$, $\hat{\zeta}_z$, $\hat{\rho}_z$, $ik\hat{\psi}$, $ik\hat{\zeta}$ and $ik\hat{\rho}$. We then compute the nonlinear Jacobian functions $(\psi_x \zeta_z - \psi_z \zeta_x)$ and $(\psi_x \rho_z - \psi_z \rho_x)$ and then take the Fourier transform of each function to add to the numerical computations at the next time step.

Grid size is chosen based on grid sensitivity analysis. In the vertical direction, we computed the solution with several Δz . With the choice of $\Delta z = 0.025$, the maximum error of solutions computed with this Δz compared with the corresponding ones computed with $2\Delta z$ was found to be 3×10^{-2} which is small enough and lies within the tolerance we want.

As discussed before, the choice of Δx and Δk is chosen such that $\Delta k \Delta x = \frac{2\pi}{N}$ in order to use the FFT. For efficiency reasons, it is preferable for the FFT that the number of points N is a power of 2. Following the same procedure of grid sensitivity analysis, as before, we decided to choose $N = 1024$ which gives $\Delta k = 0.0625$, where the maximum error of solutions computed with this Δk compared with the corresponding ones computed with $2\Delta k$ corresponding to $N = 512$ was found to be 3.8×10^{-3} . With $\Delta k = 0.0625$ and from $\Delta k \Delta x = \frac{2\pi}{N}$, we have $\Delta x = 0.09$, where the maximum error of solutions computed with this Δx compared with $2\Delta x$ is 2.5×10^{-3} .

4.3.1 Physical configuration

In this subsection, we discuss the choice of input parameters δ , ε that are used in the numerical computations. The meridional circumference of earth is approximately 40000 km, which means that the length between the north and south poles is about 20000 km. This corresponds to the full-dimensional horizontal coordinate x^* . As given in equation (2.16), the nondimensional horizontal variable x is defined as $x = \frac{x^*}{L_x}$, where L_x is a reference dimensional scale. Similarly, the nondimensional vertical variable z is defined as $z = \frac{z^*}{L_z}$, where L_z is a reference dimensional scale. In the computations shown, we fix L_z and consider different values of the parameter $\delta = \left(\frac{L_z}{L_x}\right)^2$. If we define our domain to be $-50 \leq x \leq 50$ on the horizontal direction; and $0 \leq z \leq 10$ on the vertical direction and consider $L_z = 3$ km so that $0 \leq z^* \leq 30$, then the horizontal reference scale L_x is defined as

$$L_x = \begin{cases} 30 \text{ km} & \text{if } \delta = 0.01 \longrightarrow -1500 \leq x^* \leq 1500 \text{ km} \\ 6.7 \text{ km} & \text{if } \delta = 0.2 \longrightarrow -335 \leq x^* \leq 335 \text{ km.} \end{cases}$$

When L_z is fixed, large values of the horizontal reference scale L_x corresponds to small values of δ . We consider a range of δ given as $0.01 \leq \delta \leq 0.2$, which corresponds to a reasonable dimensional scale.

We carried out several numerical experiments and found that very small values of δ cause numerical instabilities. For the linear equations, where $\varepsilon = 0$, the smallest stable δ is 0.01, which also give stable result with $\varepsilon = 0.01$. For the larger choice $\varepsilon = 0.05$, we found that the smallest stable δ is 0.2.

In Subsection 4.3.2, we show numerical results with $\delta = 0.01$ and $\delta = 0.2$ for $\varepsilon = 0.01$. For $\varepsilon = 0.05$, we fix δ to be 0.2. In all computations, the background density $\bar{\rho} = \rho_0 e^{-z/h}$, where $\rho_0 = 1$ and $h = 4.9$.

4.3.2 Numerical results

The numerical results for the equations (4.82), (4.83) and (4.84) are shown in this subsection. Figure 4.3 shows the results of the horizontal velocity perturbation u with $\delta = 0.2$ and $\varepsilon = 0.05$, while Figure 4.4 and Figure 4.5 show the numerical results with $\varepsilon = 0.01$ for the two different values of δ , $\delta = 0.01$ and $\delta = 0.2$, at two different times $t = 10$ and $t = 40$.

The behaviour of the solutions at early time is similar to that in the analytical linear case as shown by Figure 4.2, where the disturbance is almost entirely absorbed at the critical level. Above the critical level where $z > 5$, the wave amplitude is close to zero. At late time, however, where the effect of wave-wave interactions coming from the nonlinear terms becomes evident, we note that the solutions experience a different behaviour around the critical level. We note that the incident waves are reflected and the reflected waves are superimposed on the incident ones, as found by Campbell and Maslowe (2003). The zero wavenumber components $\hat{\psi}(k = 0, z, t)$, $\hat{\zeta}(k = 0, z, t)$ and $\hat{\rho}(k = 0, z, t)$ correspond to changes in the mean flow streamfunction, vorticity and density, respectively. The corresponding change in the mean flow velocity is $-\hat{\psi}_z(k = 0, z, t)$.

The perturbed mean flow resulting from the nonlinear interaction and corresponds to zero-wavenumber $k = 0$ component of the perturbation is shown in Figure 4.6. We note that the mean flow velocity is modified around the critical level. This is consistent with the analytical observation by Booker and Bretherton (1967), suggesting that the momentum of the absorbed gravity waves is transferred to the mean flow. From the analysis of the streamfunction mean flow in Section 4.2.1, we found, as in (4.74), that the change in the induced mean flow with respect to time is proportional to the change in the vertical momentum flux with respect to z . Comparing this analytical observation with Figure 4.6, we ob-

serve that the vertical momentum flux is constant away from the critical level and is changing only in the vicinity of the critical level.

In Chapter 5, we consider a simple model for chemical transport comprising an advection diffusion reaction equation and corresponding initial and boundary conditions. We first present numerical solutions for this problem where no advection is present, as well as with mean flow advection speed. We then modify the advection speed by considering the gravity wave perturbations that calculated as described in this Chapter.

Figure 4.3: The horizontal velocity perturbation $u(x, z, t)$ at (a) $t = 10$ and (b) $t = 40$ with $\delta = 0.2$ and $\varepsilon = 0.05$.

Figure 4.4: The horizontal velocity perturbation $u(x, z, t)$ with $\delta = 0.01$ and $\varepsilon = 0.01$ at (a) $t = 10$ and (b) $t = 40$.

Figure 4.5: The horizontal velocity perturbation $u(x, z, t)$ with $\delta = 0.2$ and $\varepsilon = 0.01$ at (a) $t = 10$ and (b) $t = 40$.

Figure 4.6: Wave-induced mean flow $\bar{u}_0(z, t)$ at different times.

Chapter 5

Gravity-Wave Effects on the Distribution of a Chemical Species

In Chapter 3, we considered a configuration where the concentration of a chemical is modelled by a nonlinear advection-diffusion-reaction equation and the constant advection speed is modified and thus affects the distribution of the chemical. The modification of the background flow was of a form similar to what occurs as a result of nonlinear gravity-wave interactions. The resulting perturbation of the profile of the chemical concentration was evaluated approximately using a perturbation analysis with the WKB method.

In this chapter, we carry out numerical computations to study the effect of gravity waves on a chemical in the atmosphere modelled by a nonlinear advection diffusion reaction equation represented by Fisher's equation. In this configuration, the gravity waves affect the distribution of the chemical by modifying the advection velocity of the chemical. In this chapter, it is assumed that there is no chemical heating and hence the presence of the chemical does not have an impact on the

gravity waves. First, we present a numerical solution of the chemical equation with no gravity-wave effects. The effect of the gravity wave on the distribution of the chemical concentration is investigated in Section 5.3.

In Chapter 3, we considered the special case of Fisher's equation (3.13) with an initial condition $C(x, 0) = C_0(x)$ in the form of wave front where $C_0 \rightarrow 1$ as $x \rightarrow -\infty$ and $C_0 \rightarrow 0$ as $x \rightarrow \infty$ as shown in Figure 3.1. This initial function gives a travelling-wave solution as $t \rightarrow \infty$. The conditions under which a travelling-wave solution of Fisher's equation can be obtained, are given by Theorem 5.1 in Section 5.1.

Chemical concentration in the atmosphere is often localized around some latitude and altitude. This can be seen, for example, in the work of Gille and Lyjak (1986), where they studied the heating in the atmosphere due to the effect of several chemicals including ozone and water vapour. In their observations, they show that the initial profile of ozone and water vapour have a form that is localized around the equator in the horizontal direction and localized around some vertical level in the vertical direction. This suggests that the initial condition of the chemical can be represented by a Gaussian form. Thus it is more appropriate to consider a Gaussian initial condition for the chemical concentration. Under certain conditions, a solution with initial condition of a Gaussian form can converge to a travelling-wave solution according to Bramson (1983). In the next section, we illustrate these conditions by stating the convergence theorem as shown by Bramson (1983).

5.1 The convergence theorem

In this section, we start by stating the convergence theorem for the travelling-wave solution of Fisher's equation and then apply that on the Gaussian initial condition

to check whether it satisfies the conditions for a travelling-wave solution. The conditions are stated in the following theorem as given by Bramson (1983).

Theorem 5.1. *Let $C(x, t)$ be a solution of the nonlinear reaction-diffusion equation*

$$C_t = \frac{1}{2}C_{xx} + F(C), \quad (5.1)$$

where $0 \leq C(x, 0) \leq 1$,

$$F(0) = 0 = F(1), \quad F(C) > 0 \text{ for } 0 < C < 1 \text{ and } F \in C^1[0, 1] \quad (5.2)$$

and

$$F'(0) = 1, \quad F'(C) \leq 1 \text{ for } 0 < C \leq 1 \text{ and } 1 - F'(C) = O(C^p) \text{ for } p > 0. \quad (5.3)$$

In addition, suppose that, for $h > 0$,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log \left[\int_t^{t(1+h)} C(y, 0) dy \right] = -b, \quad (5.4)$$

where $b < \sqrt{2}$, and suppose that, for some $\eta > 0$, $M > 0$ and $N > 0$,

$$\int_x^{x+N} C(y, 0) dy > \eta \text{ for } x \leq -M. \quad (5.5)$$

Then, for some $m(t)$ and $s > \sqrt{2}$,

$$C(x + m(t), t) \longrightarrow W^s(X) \text{ uniformly in } x \text{ as } t \rightarrow \infty,$$

where $s = \frac{b^2+2}{2b}$ and $W^s(X)$ is a travelling-wave solution that satisfies

$$\frac{1}{2}W_{XX}^s + sW_X^s + F(W^s) = 0.$$

Theorem 5.1 is stated for the specific choice of diffusion $\mathcal{D} = \frac{1}{2}$. In this case s was found to be $s = \frac{b}{2} + \frac{1}{b}$. However, Theorem 5.1 could be generalized to general $\mathcal{D}$. For a general diffusion $\mathcal{D}$, s takes the form $s = \mathcal{D}b + \frac{1}{b}$. The convergence theorem (Theorem 5.1) gives the required conditions for a given initial function to converge to a travelling-wave solution $W^s(X)$.

We apply Theorem 5.1 to equation (3.13) with the Gaussian initial condition $C(x, 0) = e^{-a^2 x^2}$, where $0 < a < 1$, which satisfies $0 \leq C(x, 0) \leq 1$. Equation (3.13) given in Chapter 3 has the form

$$C_t = \tilde{D}C_{xx} + \sigma C(1 - C), \quad (5.6)$$

We note that Theorem 5.1 is given for equation (5.1). In order to apply Theorem 5.1 to (5.6), we rescale (5.6) to have the form of (5.1) using the rescaling variables $\bar{x} = \sqrt{\frac{\sigma}{2\tilde{D}}}x$ and $\bar{t} = \sigma t$ as we have done in Chapter 3. With this rescaling, the initial condition has the form $C(x, 0) = e^{-\tilde{a}^2 \bar{x}^2}$, where $\tilde{a}^2 = \frac{2\tilde{D}a^2}{\sigma}$.

Applying Theorem 5.1 to the rescaled equation with the initial condition $C(x, 0) = e^{-\tilde{a}^2 x^2}$, we find that the conditions (5.2) and (5.3) on $F(C) = C(1 - C)$ are clearly satisfied. It remains to confirm conditions (5.4) and (5.5). As $y \rightarrow \infty$, we have $C(y, 0) = e^{-\tilde{a}^2 y^2} \ll e^{-\tilde{a}^2 y}$ since $\lim_{y \rightarrow \infty} \frac{e^{-\tilde{a}^2 y^2}}{e^{-\tilde{a}^2 y}} = 0$. Applying condition (5.4) on $e^{-\tilde{a}^2 y}$, we find

$$\int_t^{t(1+h)} e^{-\tilde{a}^2 y} dy = \left[\frac{e^{-\tilde{a}^2 y}}{-\tilde{a}^2} \right]_t^{t(1+h)} = \frac{e^{-\tilde{a}^2 t(1+h)}}{-\tilde{a}^2} + \frac{e^{-\tilde{a}^2 t}}{\tilde{a}^2} \quad (5.7)$$

$$\sim \frac{e^{-\tilde{a}^2 t}}{\tilde{a}^2} \quad \text{as } t \rightarrow \infty. \quad (5.8)$$

It follows that

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log \left[\frac{e^{-\tilde{a}^2 t}}{\tilde{a}^2} \right] = -\tilde{a}^2; \quad (5.9)$$

condition (5.4) is satisfied for the function $e^{-\tilde{a}^2 y}$ provided that $\tilde{a}^2 < \sqrt{2}$. That is, provided that the parameters a , $\tilde{D}$ and σ are chosen such that $\tilde{a}^2 < \sqrt{2}$, then condition (5.4) is satisfied. Thus, we could choose the parameters a , $\tilde{D}$ and σ in $\tilde{a}^2$ such that $\tilde{a}^2 < \sqrt{2}$ in order to satisfy condition (5.4). Since $e^{-\tilde{a}^2 y^2} \ll e^{-\tilde{a}^2 y}$ as $y \rightarrow \infty$ and since

$$\lim_{y \rightarrow \infty} \int_t^{t(1+h)} e^{-\tilde{a}^2 y^2} dy = 0$$

and

$$\lim_{y \rightarrow \infty} \int_t^{t(1+h)} e^{-\tilde{a}^2 y} dy = 0,$$

we then have

$$\int_t^{t(1+h)} e^{-\tilde{a}^2 y^2} dy \ll \int_t^{t(1+h)} e^{-\tilde{a}^2 y} dy \text{ as } y \rightarrow \infty. \quad (5.10)$$

Similarly, we find that

$$\log \left[\int_t^{t(1+h)} e^{-\tilde{a}^2 y^2} dy \right] \ll \log \left[\int_t^{t(1+h)} e^{-\tilde{a}^2 y} dy \right] \text{ as } y \rightarrow \infty. \quad (5.11)$$

It follows that

$$\lim_{t \rightarrow \infty} \frac{1}{t} \log \left[\int_t^{t(1+h)} e^{-\tilde{a}^2 y^2} dy \right] < \lim_{t \rightarrow \infty} \frac{1}{t} \log \left[\int_t^{t(1+h)} e^{-\tilde{a}^2 y} dy \right] = -\tilde{a}^2. \quad (5.12)$$

Condition (5.4) is satisfied for the initial function $C(y, 0) = e^{-\tilde{a}^2 y^2}$ provided that the parameters a , $\tilde{D}$ and σ are chosen such that $\tilde{a}^2 < \sqrt{2}$, as before.

Now we discuss the condition (5.5). We know that $0 \leq C(y, 0) \leq 1$, and for y close to zero where the Gaussian is centred, we have a constant r such that, for $0 < r < 1$, we have

$$r < C(y, 0) < 1. \quad (5.13)$$

For $M > 0$, $N > 0$ and $x \leq -M$, N can be chosen as $N < M$ so that $x + N < 0$. Then, integrating (5.13) with respect to y from x to $x + N$, we obtain

$$rN < \int_x^{x+N} C(y, 0) dy < N \quad \text{for } x \leq -M. \quad (5.14)$$

Thus η can be chosen as $\eta = rN$ and the condition (5.5) is satisfied. Therefore, we conclude from the theorem that the Gaussian solution of equation (3.13) converges to a travelling-wave solution.

A numerical illustration is shown in Figure 5.1, where the one-dimensional Fisher's equation (3.13) is solved numerically with an initial condition in the form of a Gaussian, $C(x, 0) = e^{-x^2}$, and compared with the analytical solution (3.17) corresponding to the travelling-wave initial condition. In Figure 5.1 (a), the initial form of the exact travelling-wave solution is (3.17) at $t = 0$ and centred at $x = 1.2$, so it matches the right wave front of the Gaussian initial condition. The wave speed corresponding to the exact solution (3.17) is $c = \frac{5\sqrt{\sigma\mathcal{D}}}{\sqrt{6}}$. We note that if the initial wave fronts (3.17) and e^{-x^2} are initially matched, they continue to propagate at comparable speed. In Figure 5.1 (b), the travelling-wave solution, which is travelling to the left side with a negative wave speed $c = \frac{-5\sqrt{\sigma\mathcal{D}}}{\sqrt{6}}$, is matched with the left wave front of the Gaussian initial condition. We note that the left wave front of the Gaussian solution propagates at comparable speed compared with the exact travelling-wave solution (3.17).

These experiments illustrate the fact that the Gaussian initial condition gives a travelling-wave solution as shown by Theorem 5.1 and that if the initial wave front of the Gaussian matches the initial condition from (3.17), then this travelling-wave solution travels with approximately the same speed as the solution (3.17). This information is useful for verifying that the numerical computations in Sections 5.2 and 5.3 give solutions with the correct propagation speed.

Figure 5.1: The solution of the one-dimensional Fisher's equation (3.13) with $\sigma = 0.5$, $\tilde{D} = 0.01$ at $t = 0$, $t = 10$, and $t = 20$. The circle, square and diamond curves represent the numerical solution of (3.13) with the Gaussian initial condition $C(x, 0) = e^{-x^2}$ at different times. The solid, dashed and dashed-dotted lines represent the exact solution of (3.13) at different times. The exact solution is given in (3.17), which corresponds to the travelling-wave initial condition travelling to the right in (a) and to the left in (b).

5.2 Solving the chemical equation using spectral method

In this section, we solve the two-dimensional chemical transport equation (3.91), which has the form

$$C_t + U(x, z, t) C_x + W(x, z, t) C_z = \delta \mathcal{D} C_{xx} + \mathcal{D} C_{zz} + \sigma C(1 - C). \quad (5.15)$$

We solve (5.15) on the two-dimensional spatial domain $-50 \leq x \leq 50$ in the horizontal direction and $0 \leq z \leq 10$ in the vertical direction. The initial condition for the chemical concentration is considered to have the form

$$C_0(x, z) = C(x, z, 0) = e^{-a^2 x^2} e^{-b^2 (z - z_1)^2}. \quad (5.16)$$

We choose b and z_1 such that C_0 can be approximated by zero at $z = 0$. The boundary conditions are that $C \rightarrow 0$ as $x \rightarrow \pm\infty$ and $z \rightarrow \pm\infty$. This is represented on the computational domain by requiring that C remain zero at $x = \pm 50$, $z = 0$ and $z = 10$.

In Chapter 3, we considered initial condition for the chemical that has the form of a travelling-wave solution. In that chapter, we used finite differences approximations in both directions. However, in this chapter as well as in Chapter 6, we consider initial condition of the Gaussian form. This form of initial condition as well as the boundary conditions given above allow us to use the spectral method. From now on, we use the spectral method to solve (5.15). The spectral method is an effective method that is commonly used in fluid applications involving oscillatory solutions. In this section, we give an illustration of using the spectral method. We use the spectral method to solve (5.15) only in the horizontal direction. In

the vertical direction, we use the same finite difference method that is used for the gravity-wave computations in Chapters 4 and 6. As discussed in Section 4.1, since C is smooth and continuously differentiable and is absolutely integrable due to the form of boundary condition, we then could define C in terms of the Fourier transform by

$$\hat{C}(k, z, t) = \mathcal{F}[C(x, z, t)] = \frac{1}{2\pi} \int_{-\infty}^{\infty} C(x, z, t) e^{-ikx} dx, \quad (5.17)$$

and the inverse Fourier Transform by

$$C(x, z, t) = \int_{-\infty}^{\infty} \hat{C}(k, z, t) e^{ikx} dk. \quad (5.18)$$

Taking the Fourier transform of equation (5.15), we obtain

$$\hat{C}_t + \mathcal{F}[U(x, z, t) C_x] + \mathcal{F}[W(x, z, t) C_z] = -\delta k^2 \mathcal{D} \hat{C} + \mathcal{D} \hat{C}_{zz} + \mathcal{F}[C(1-C)]. \quad (5.19)$$

We solve (5.19) using the fourth-order Adams Bashforth method for the time discretization. We use the second-order central finite difference approximation to discretize the vertical advection and diffusion terms. The presence of the vertical diffusion which is larger than the horizontal diffusion makes the scheme more stable. Also, these methods are chosen here because they were found to be suitable for computations with gravity wave done in Chapter 4.

We define k as $k_m = k_0 + m\Delta k$ for $m = 0 \dots N-1$ and x is defined as $x = x_0 + j\Delta x$ for $j = 0 \dots N-1$. The Fourier integral (5.17) is computed numerically in a form of summation as

$$\hat{C}(k, z, t) = \frac{\Delta x}{2\pi} e^{-ikx_0} \sum_{j=0}^{N-1} C(x, z, t) e^{-ik_0 j \Delta x} e^{-imj \Delta k \Delta x}. \quad (5.20)$$

The Fourier transform of the nonlinear terms is approximated using the pseudo-spectral method. At each time step, the second and third terms on the left-side of (5.19) are computed in physical space by applying the inverse Fourier transform. After completing the multiplication in the physical space, we compute the Fourier transform of the resulting product. Similarly, the Fourier of the nonlinear term $\mathcal{F}[C(1 - C)]$ is computed using the pseudo-spectral method. At time step $n + 1$, we find C^n from $\hat{C}^n$ by applying inverse Fourier transform. Once we obtain C^n , we then find $C^n(1 - C^n)$, then apply the Fourier transform on the resulting product to obtain $\mathcal{F}[C(1 - C)]$.

As before, grid size is chosen based on grid sensitivity analysis. In the vertical direction, we eventually used $\Delta z = 0.0251$, which compared with $2\Delta z$ gives maximum error of 6.2×10^{-3} . As already discussed in Section 4.3, the grid sizes Δx and Δk are chosen such that $\Delta k \Delta x = \frac{2\pi}{N}$ in order to use the FFT. Based on grid sensitivity analysis, we decided to choose $N = 1024$ which gives $\Delta k = 0.0625$, where the maximum difference of solutions computed with this Δk compared with the corresponding ones computed with $2\Delta k$ corresponding to $N = 512$ was found to be 5×10^{-5} . With this choice of Δk , we have $\Delta x = 0.09$ which compared with $2\Delta x$ gives maximum error of 1.46×10^{-4} .

The initial condition for the chemical concentration (5.16) is shown in Figure 5.2, and it is considered an initial condition for the chemical concentration in all figures in this chapter. In this initial form for the chemical concentration, we consider large a and b taken as $a^2 = 5$, $b^2 = 5$ in order to start with a form of the chemical concentration that does not reach the computational boundary too fast. The reason for this is because we want to examine the behaviour of the chemical distribution by studying the effect of the diffusion and nonlinear parameters on the advection speed of the chemical. We start by showing results for (5.15) with

Figure 5.2: The initial chemical concentration $C_0(x, z) = e^{-a^2 x^2} e^{-b^2 (z-z_1)^2}$ given in (5.16) with $a^2 = 5$, $b^2 = 5$ and $z_1 = 5$.

zero advection speeds $U = 0$ and $W = 0$. The comparison of the exact solution (3.30), with $\theta = 0$, obtained in Chapter 3 and the numerical Gaussian solution of (5.15) is shown in Figure 5.3. Although the exact solution is for the case with one wave front only, we note that the advection of the horizontal wavefronts of the Gaussian solutions is very close to that of the exact solution. Figure 5.4 shows the exact solution (3.30), with $\theta = \frac{\pi}{4}$, where it compares two different values of $\mathcal{D}$ and a fixed value of σ , the coefficient of the nonlinear term, and shows that the solution evolves faster with larger diffusion. This is consistent with the wave speed $c = \frac{5\sqrt{\sigma\delta\mathcal{D}}}{\sqrt{6}}$ given in (3.30).

Figure 5.5 shows the evolution of the chemical concentration with initial Gaussian form where the solution is shown at several time steps. It compares the solution with two different values of diffusion $\mathcal{D}$ and a fixed value of σ . Similarly, Figure 5.6 shows the solution for the same configuration as Figure 5.5 but with a different value of σ . These two figures show that, although there is no advection, the solution is travelling horizontally and vertically and this speed evolution is

proportional to the parameters $\mathcal{D}$ and σ . We observe that the larger the value of σ , the faster the solution travels. Similarly we note that the larger the value of $\mathcal{D}$, the faster the solution. These observations are consistent with the definition of c in the exact solution corresponding to a travelling-wave solution.

Figures 5.7 and 5.8 shows the numerical solution $C(x, z, t)$ for (5.15) with zero advection speeds $U = 0$ and $W = 0$, at several times for two fixed vertical levels. The two vertical levels are $z = 5$, where the initial Gaussian is centred (Figure 5.2), and a lower level $z = 4$. In terms of the choice of the parameters $\mathcal{D}$ and σ , Figure 5.7 corresponds to the contours of Figure 5.5 whereas Figure 5.8 corresponds to the contours of Figure 5.6. Figures 5.7 (c) and 5.7(d), as well as Figures 5.8 (c) and 5.8(d), correspond to the vertical level $z = 4$. In all of these figures, we note that the initial amplitude is less than one, but it eventually grows with time. This is because the solutions advect vertically due to the effect of $\mathcal{D}$ and σ . This can be seen from the contour figures we already discussed. For example, we note from the initial contour in Figure 5.5 (b) that, at the vertical level $z = 4$, the amplitude is small and almost zero. However, the solutions spread as they advect vertically with time and reach this vertical level as seen in Figure 5.5 (d) and Figure 5.5 (f).

At the centre $z = 5$, however, we note that, as the solutions advect with time, the amplitude remains at one, as can be seen in Figures 5.7 (a) and 5.7 (b), and changes to lower values as can be seen in Figures 5.8 (a) and 5.8 (b). To understand this behaviour, we compare these figures with the corresponding exact solution (3.30) (with $\theta = 0$) of Fisher's equation (5.15). In the case where the parameter σ is large, we observe from Figures 5.9 (a) and 5.9 (b) that the right wave front of the initial Gaussian (dashed line) and the wave front of the initial exact solution (solid line) have comparable slopes. In this case, we note from the corresponding figures shown in Figures 5.7 (a) and 5.7 (b) that the amplitude

remains at one for the given solutions at several times. When the parameter σ is small, however, we note from Figures 5.9 (c) and 5.9 (d) that the right wave front of the initial Gaussian (dashed line) and the wave front of the initial exact solution (solid line) have totally different slopes. Comparing Figures 5.9 (c) and 5.9 (d) and the corresponding Figures 5.8 (a) and 5.8 (b), we note that the larger the difference between the slopes of the two wave fronts, the more the amplitude of the Gaussian decreases with time.

Figure 5.10 shows the evolution of the chemical concentration with the background advection $\bar{u} = \tanh(z - 5)$ and $\bar{w} = 0$, where the solution is illustrated at several time steps. It compares the solution with two different values of the diffusion coefficient $\mathcal{D}$ and a fixed value of σ . A similar comparison is shown in Figure 5.11 with different value of σ . These two figures show that the solution is dependent on the value of $\bar{u}$ as well as on the parameters $\mathcal{D}$ and σ . We observe that, with larger σ , the solution travels faster. A similar observation can be seen with larger values of the diffusion.

From the behaviour of the solution of the chemical transport equation without interaction with gravity waves, with and without advection, we note that the parameters $\mathcal{D}$ and σ affect the advection speed of the solution. In Section 5.3, we solve this equation along with the gravity-wave equations to determine the effect of the gravity-wave-induced flow on the chemical transport. Based on the experiments shown here, we choose appropriate values for $\mathcal{D}$ and σ so that the solution of the chemical does not travel too fast to ensure that, within the time frame of the computations, the wave front does not reach the upper and lower or side boundaries. In the results shown in Chapter 4, we see that the wave-induced mean flow resulting from gravity waves reaches its peak around the critical level and increases with time as shown in Figure 4.6. We should choose small enough

Figure 5.3: Contour plots of the solution of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.5$ and $\mathcal{D} = 0.001$, where we have the exact travelling-wave solution (3.30) with $\theta = 0$ on left and the numerical Gaussian solutions on right. The plots (a) and (b) are at $t = 10$; the plots (c) and (d) are at $t = 20$ and the the plots (e) and (f) are at $t = 30$.

Figure 5.4: The exact solution (3.30) of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.5$ and $\theta = \frac{\pi}{4}$. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. The plots (a) and (b) are at $t = 10$; the plots (c) and (d) are at $t = 20$ and the the plots (e) and (f) are at $t = 30$.

Figure 5.5: Contour plots of the concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.5$. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. The plots (a) and (b) are at $t = 0$; the plots (c) and (d) are at $t = 10$ and the plots (e) and (f) are at $t = 30$. Figures (b), (d) and (f) are the same as in Figure 5.3 (b), (d) and (f) (with different times).

Figure 5.6: Contour plots of the concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.005$. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. The plots (a) and (b) are at $t = 0$; the plots (c) and (d) are at $t = 10$ and the the plots (e) and (f) are at $t = 30$.

Figure 5.7: The concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.5$ plotted for two vertical levels $z = 5$ and $z = 4$ as a function of x at several times. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. Figures (a) and (b) are at the vertical level $z = 5$ and Figures (c) and (d) are at the vertical level $z = 4$. This Figure corresponds to Figure 5.5.

Figure 5.8: The concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = 0$, $W = 0$, $\sigma = 0.005$ plotted for two vertical levels $z = 5$ and $z = 4$ as a function of x at several times. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. Figures (a) and (b) are at the vertical level $z = 5$ and Figures (c) and (d) are at the vertical level $z = 4$. This Figure corresponds to Figure 5.6.

Figure 5.9: Comparison between the Gaussian initial condition (shown in figure 5.2) at $z = 5$ and the initial condition (with $\theta = 0$) of the exact travelling-wave solution (3.30) of Fisher's equation (5.15) with $U = 0$, $W = 0$ and at $z = 5$. Left figures are with $\mathcal{D} = 0.01$, and right figures are with $\mathcal{D} = 0.001$. Figures (a) and (b) are with $\sigma = 0.5$ and Figures (c) and (d) are with $\sigma = 0.005$.

Figure 5.10: Contour plots of the concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = \tanh(z - 5)$, $W = 0$ and $\sigma = 0.5$. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. The plots (a) and (b) are at $t = 0$; the plots (c) and (d) are at $t = 10$ and the plots (e) and (f) are at $t = 30$.

Figure 5.11: Contour plots of the concentration $C(x, z, t)$ of the two-dimensional Fisher's equation (5.15) with $U = \tanh(z - 5)$, $W = 0$ and $\sigma = 0.005$. Left figures are computed with $\mathcal{D} = 0.01$, and right figures are computed with $\mathcal{D} = 0.001$. The plots (a) and (b) are at $t = 0$; the plots (c) and (d) are at $t = 10$ and the plots (e) and (f) are at $t = 30$.

values for $\mathcal{D}$ and σ to allow the chemical to interact with gravity waves within the vicinity of critical layer. From several simulations with different values $\mathcal{D}$ and σ , we found that, for the computations with gravity waves we consider $\mathcal{D} = 0.001$ and $\sigma = 0.005$, which are an appropriate choice to illustrate the behaviour of the solution over a time interval from $t = 0$ to $t = 30$. This choice of small parameters is also consistent with the corresponding values for the specified chemicals in Chapter 6.

5.3 Gravity waves' effect on the chemical equation

In the absence of gravity waves, the advection of the chemical concentration in the atmosphere can be represented by a background mean flow corresponding to the wind speed. However, in the presence of the gravity waves, the background mean flow is perturbed. This perturbation corresponds to the wave-induced mean flow resulting from gravity waves' nonlinear interactions. The advection speed of the chemical concentration is expressed in terms of a background mean flow and a perturbation to the mean flow represented by the gravity-wave-velocity perturbations.

The model we consider in this chapter representing the effect of gravity waves on the chemical concentration consists of the gravity wave equations (4.82), (4.83) and (4.84) along with the chemical transport equation (5.15) given as

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\rho}\rho_x, \quad (5.21)$$

$$\zeta = \nabla^2\psi, \quad (5.22)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_z + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = 0, \quad (5.23)$$

$$C_t + (\bar{u} + \varepsilon u)C_x + \varepsilon wC_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + \sigma C(1 - C). \quad (5.24)$$

$$u = -\psi_z \quad \text{and} \quad w = \psi_x. \quad (5.25)$$

As discussed before (Section 4.1), the functions ζ , ψ , ρ and C are smooth and L_1 . The perturbation to the advection u and w in (5.24) are obtained from ψ . Thus u and w are also smooth and continuously differentiable and L_1 . We solve equations (5.21)–(5.25) on the two-dimensional spatial domain $-50 \leq x \leq 50$ in the horizontal direction and $0 \leq z \leq 10$ in the vertical direction. The equations are solved numerically using the spectral method in the horizontal direction and a finite difference method in the vertical direction and the fourth-order Adams Bashforth method for the time discretization. The description of the numerical methods is given in Section 4.3 for gravity-wave equations and in Section 5.1 for the chemical-transport equation. At each time step, the gravity wave vorticity ζ , streamfunction ψ , density ρ as well as the chemical concentration C are all computed at the same time where the perturbation to the advection u and w in the chemical equation are computed from previous time step.

5.3.1 Choice of parameters

The results shown in this section are obtained with the same choice of parameters considered in Section 4.3. The parameter δ is set to 0.2, and the background density is $\bar{\rho} = \rho_0 e^{-z/h}$, where $\rho_0 = 1$ and $h = 4.9$. We show numerical results with the amplitude parameter ε chosen as $\varepsilon = 0.05$ and show other results with $\varepsilon = 0.1$. The background flow velocity is $\bar{u} = \tanh(z - 5)$. In the boundary condition (4.85), we set $\mu = 0.2$ and $k_0 = 2$. In the initial condition for the chemical equation (5.16), we set $a^2 = 5$, $b^2 = 5$ and $z_1 = 5$, as in Section 5.2.

Figure 5.12 shows the horizontal velocity perturbation with $\varepsilon = 0.1$ at two different times. We note, as in the corresponding plots with $\varepsilon = 0.05$ shown in Figure 4.3, that the waves are entirely absorbed at the critical level at early time. However, at later time, as the nonlinearity effect increases, we note that the waves are reflected. The wave-induced mean flow, resulting from the nonlinear interaction of gravity waves, is shown in Figure 5.13. Comparing with Figure 4.6, which corresponds to the smaller ε , we note that the wave-induced mean flow is much larger with $\varepsilon = 0.1$. This leads to a greater effect on the advection speed of the concentration of chemicals in the atmosphere as a result of the effect of the wave-induced mean flow.

The significant effect of gravity waves on the chemical concentration around the critical level $z = 5$ is due to the behaviour of the wave-induced mean flow. As shown in Figures 4.6 and 5.13, we note that the wave-induced mean flow reaches its maximum at the critical level. This reflects the significant effect of the nonlinearity around the critical level.

Figure 5.14 shows the effect of the gravity waves on the chemical concentration. The figures in the first column correspond to the chemical concentration with no effect of gravity waves, whereas the figures in the second and third columns represent the chemical concentration with the effect of gravity waves. The comparison of the two cases is illustrated at several times. We see that the effect of the gravity waves on the chemical concentration is more obvious within the vicinity of critical level of the gravity waves as shown in Figure 5.15. In the horizontal direction, we note that the effect is mainly bounded within $-10 \leq x \leq 10$, which is the active domain of the gravity wave packet as we note in Figure 4.3.

We note from Figures 5.14 and 5.15, that the effect of gravity waves on the chemical concentration has oscillatory behaviour. This effect has a form similar to

that of the gravity-wave-velocity perturbation shown in Figures 4.3 and 5.12. This is consistent with the analytical asymptotic approximations obtained in Subsection 3.2.2. These asymptotic observations were also confirmed with the numerical results obtained in Chapter 3 where the chemical concentration considered to have a travelling-wave solution.

The comparison of the effect with two different values of ε is shown in Figure 5.14 where we note that the effect of gravity waves on chemical concentration in the atmosphere is more significant with $\varepsilon = 0.1$ compared with the effect with $\varepsilon = 0.05$. This effect is mainly located around the critical level in the vertical direction and within $-10 \leq x \leq 10$ in the horizontal direction, as can be seen in Figure 5.15.

Figure 5.16 shows the Fourier spectrum of the streamfunction perturbation at two different times. We note that, at early time, the zero wavenumber component is comparable with the forced wavenumbers $k = \pm 2$. At later time and as a result of nonlinearity, the zero wavenumber component grows and exceeds the forced wavenumbers $k = \pm 2$. The Fourier spectrum of the chemical concentration with and without the effect of gravity waves is shown in Figure 5.17 at two different times. Figures 5.17(a) and 5.17 (b) are the same as in Figure 5.16 but scaled with smaller vertical scale to be compared with Fourier spectrum of the chemical concentration shown in Figures 5.17 (c) and 5.17 (d). We note from Figures 5.17 (c) and 5.17 (d) that, in the absence of gravity waves, the Fourier spectrum for the chemical (dashed line) has a Gaussian form centred around the zero wavenumber at both early and late time. However, when gravity waves are present (solid line) and affect the advection of the chemical distribution, we observe that the Fourier spectrum for the chemical is modified around the zero wavenumber, around the gravity wave forced wavenumbers $k = \pm 2$, as well as around other larger

wavenumbers.

Figure 5.18 shows the solution $C(x, z, t)$ around the critical level in the case where the advection of the chemical is given by $\bar{u} = \tanh(z - 5)$ (dashed line), as well as in the case where the advection speed of the chemical is modified by gravity-wave perturbations and given by $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$ (solid line). The effect of gravity-wave perturbation can be seen especially at later time (Figure 5.18 (b)), where we note that these gravity-wave perturbations are causing the chemical distribution to have an oscillatory form in the areas where gravity waves are present.

The stronger effect with the larger ε implies that the nonlinearity of gravity waves has a significant influence on the chemical concentration. Garcia and Solomon (1983) and Xu et al. (2000) considered linear equations for gravity waves, and hence the effect of gravity waves on the chemical concentration is not as significant as in our results. In their configurations, they considered an oscillatory representation for both the waves and the chemical concentration. In our case, we consider an oscillatory representation for gravity waves, as explained in Chapter 4. This is a common representation for gravity waves. However, we are considering a more realistic Gaussian representation for the chemical concentration following observational studies as shown for example by Gille and Lyjak (1986), as discussed before.

Figure 5.12: The horizontal velocity perturbation $u(x, z, t)$ with $\varepsilon = 0.1$ at (a) $t = 10$ and (b) $t = 40$.

Figure 5.13: The wave-induced mean flow $\bar{u}_0(z, t)$ with $\varepsilon = 0.1$ at different times.

Figure 5.14: Contour plots of the chemical concentration $C(x, z, t)$ of the two-dimensional equation with $\sigma = 0.005$ and $\mathcal{D} = 0.001$, where we have $u = \tanh(z - 5)$ on the first column, $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$ with $\varepsilon = 0.05$ on second column and $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$ with $\varepsilon = 0.1$ on third column. The plots at time $t = 10$, $t = 20$, and $t = 40$ where the plots (a), (b) and (c) are at $t = 10$; the plots (d), (e) and (f) are at $t = 20$ and the the plots (g), (h) and (i) are at $t = 40$. The plots (a), (d) and (g) are the same configuration shown in Figure 5.11 (b), (d), (f) with different scaling and times.

Figure 5.15: Contour plots of the chemical concentration $C(x, z, t)$ of the two-dimensional equation. These contour plots are the same as in Figure 5.14 (c), (f) and (i) but with smaller horizontal scale.

Figure 5.16: The Fourier spectrum of the perturbation streamfunction $\hat{\psi}(k, z, t)$ at the critical level for gravity waves with $\varepsilon = 0.1$ at (a) $t = 10$ and (b) $t = 40$.

Figure 5.17: Figures (a) and (b) are the same as in Figure 5.16 but scaled with smaller vertical scale to be compared with (c) and (d). Figures (c) and (d) represent the Fourier spectrum for the chemical concentration $\hat{C}(k, z, t)$ at the critical level at $t = 10$ and $t = 40$, respectively. The dashed line represents the Fourier spectrum of the chemical concentration without the effect of gravity waves perturbation ($\varepsilon = 0$ in (5.24)) whereas the solid line represents the Fourier spectrum of the chemical concentration where its advection is affected by gravity waves perturbation with $\varepsilon = 0.1$.

Figure 5.18: The chemical concentration $C(x, z, t)$ at the critical level. The dashed line represents C without the effect of gravity waves perturbation ($\varepsilon = 0$ in (5.24)) whereas the solid line represents the chemical concentration C where its advection is affected by gravity waves perturbation with $\varepsilon = 0.1$. The plots are at times (a) $t = 10$ and (b) $t = 40$.

Chapter 6

Nonlinear Gravity-Wave Interaction Coupled with Chemical Heating

In Chapter 5, we considered a configuration where the concentration of a chemical is modelled by a nonlinear advection diffusion equation and the advection speed is modified leading to effects on the distribution of the chemical. The modification of the background mean flow corresponded to the perturbations that result from nonlinear gravity-wave interactions. In that configuration, it was assumed that the presence of the chemical did not have any influence on the gravity-wave structure. However, in reality, chemical changes in the atmosphere result in heat release, which in turn may affect the energy profile of gravity-wave perturbations. Therefore, as a more realistic model, we consider a coupled system of gravity-wave equations where the energy equation is forced by chemical heating effects and a chemical transport equation where the advection velocity is modified by the nonlinear gravity-wave interactions.

We start with Section 6.1 by considering the interaction of gravity waves with

ozone. Prior to showing results for the coupled system representing the interaction of gravity waves with ozone, we first discuss the case where gravity waves are affected by a steady-state chemical. The interaction of gravity waves with water vapour is considered in Section 6.2. The interaction of gravity waves with chlorine monoxide, which has a continuity equation that is quite similar to the form of Fisher's equation, is discussed in Section 6.3.

6.1 Gravity waves' interactions with ozone in the atmosphere

Ozone, denoted as O_3 , is a chemical gas that exists in the lower and middle atmosphere. The bulk of natural ozone is present in the stratosphere, whereas a small portion of natural ozone, as well as pollution-related ozone, is present in the troposphere. Stratospheric ozone is mostly produced in the tropical stratosphere through chemical reactions in the presence of sunlight. Natural stratospheric ozone, although poisonous, is very important to humans and life in general since it absorbs the harmful ultraviolet radiation from the Sun [Carpenter et al. (2014)].

Ozone is a source of heating in the middle atmosphere due to its absorption of ultraviolet radiation. The heating released in the atmosphere due to ozone was investigated by several studies, as discussed in Chapter 1. Early studies, such as Murgatroyd and Goody (1958) and Leovy (1964) concerned the radiative equilibrium of the mesosphere. The distributions of the heating rates due to the absorption of solar radiation by ozone was calculated by Park and London (1974) where they observed that most of heating in the middle atmosphere is due the absorption of solar radiation by ozone. The radiative heating rates of water vapour and ozone as well as the thermal cooling rates of carbon dioxide were computed for

the global atmosphere by Dopplack (1972) and Dopplack (1979). Gille and Lyjak (1986) computed solar heating due to water vapour, ozone and other chemicals in the middle atmosphere by considering more accurate data taken from the Limb Infrared Monitor of the Stratosphere LIMS. Lacis and Hansen (1974) introduced a parameterization method for the computation of the absorption of solar radiation. The method is based on multiple-scattering computations and is used in some global atmospheric circulation models. An analytical computation of heating due to ozone was introduced by Lindzen and Will (1973), which was then parametrized by Strobel (1978). This analytical parameterization was used by Hartmann (1978) to compute the heating released by ozone due to the absorption of solar radiation. Hartmann (1978) examined the relation between the heating released by ozone and the photodissociation of ozone, which corresponds to the reaction of ozone and ultraviolet radiation, and found that they are quite proportional to each other.

Following Brasseur and Solomon (1984), the continuity equation for ozone O_3 (Eq (5.24))

$$\frac{\mathbf{D}(\mathbf{O}_3)}{\mathbf{Dt}} + (\mathbf{J}_3 + \mathbf{J}_3^*)(\mathbf{O}_3) + k_3(O)(O_3) + k_5(O(^1D))(O_3) = k_2(M)(O_2)(O) \quad (6.1)$$

In our configuration, we consider gravity waves coupled with only one chemical. Therefore, we consider only terms in boldface which depend solely on ozone and terms in grey are neglected. Thus, the non-dimensional continuity equation for ozone, written in terms of mixing ratio and with the diffusion being considered, can be expressed as

$$\frac{\partial C(O_3)}{\partial t} + U \frac{\partial C(O_3)}{\partial x} + W \frac{\partial C(O_3)}{\partial z} = -\sigma_{O_3} C(O_3) + \mathcal{D} \nabla^2 C(O_3), \quad (6.2)$$

where $C(O_3)$ is the mixing ratio of ozone; U and W are the horizontal and vertical

velocities; $\sigma_{o_3} = \tau R_{O_3}$ where τ is a reference timescale as shown in Chapter 2 and $R_{O_3} = J_3 + J_3^*$ is the photolysis rate. The photolysis rate R_{O_3} can be averaged as $R_{O_3} = 4 \times 10^{-3} \text{ s}^{-1}$, as shown by Park and London (1974). The term $-\sigma_{o_3} C(O_3)$ describes the process of photodissociation of ozone.

The heating released by ozone is mainly due to the absorption of ultraviolet radiation. This absorption occurs in a range of wavelengths of ultraviolet radiation. These wavelengths are classified as the Hartley band (ranging between 200–310 nm), the Huggins bands (ranging between 310–350 nm) and the Chappuis bands (ranging between 400–850 nm) [Andrews (2010)]. Following Andrews (2010), the heating rate per unit mass due to ozone can be computed as

$$J_{O_3} = \frac{1}{\rho} \left(C(O_3) \int_{\nu} \kappa_{\nu} F_{s,\nu} d\nu \right), \quad (6.3)$$

where ρ is the density of air; κ_{ν} is the absorption coefficient; $F_{s,\nu}$ is the incident solar radiation which is given as

$$F_{s,\nu} = F_{s,\nu}(\infty) \exp \left(-\kappa_{\nu} \int_z^{\infty} \bar{C}(O_3) dz' \right). \quad (6.4)$$

Equation (6.3) was simplified and expressed in terms of an analytical formula by Lindzen and Will (1973), which was parametrized by Strobel (1978). Following Strobel (1978), the heating rate due to ozone can be expressed as

$$J_{O_3} = C_p C(O_3) \left[A_{Ha} \exp(-B_{Ha} N_3) + \frac{1}{N_3} \left(A_{Hu} - B_{Hu} \exp(-C_{Hu} N_3) - D_{Hu} \exp(-H_{Hu} N_3) \right) + A_C \exp(-B_C N_3) \right], \quad (6.5)$$

where C_p is constant representing the specific heat at constant pressure, and $A_{Ha}, B_{Ha}, A_{Hu}, B_{Hu}, C_{Hu}, D_{Hu}, H_{Hu}, A_C$ and B_C are positive constants correspond-

ing to Hartley, Huggins and Chappuis bands, respectively. The quantity N_3 represents the column mixing ratio of ozone and is a function of the altitude z .

We note that the formula for the heating rate due to ozone given in (6.5) is proportional to a function of z multiplied by the mixing ratio $C(O_3)$. From (6.2), we note that the first term in the right-hand side is proportional to $C(O_3)$. As was found by Hartmann (1978), we note that the heating due to ozone is related to the photodissociation of ozone represented by the first term in the right-hand side of (6.2). In the absence of diffusion in the continuity equation (6.2), we note that $\left(-\frac{D C(O_3)}{Dt}\right)$ is proportional to $C(O_3)$. The heating rate due to ozone can then be expressed as $\left(-\frac{D C(O_3)}{Dt}\right)$, which is consistent with (6.5). In Section 6.2, where we consider water vapour, we shall see that a similar representation for the heating is considered following Holton (2004). We consider a configuration where diffusion is not neglected, so the heating due to ozone is $J_{O_3} = -\gamma_{o_3} \frac{D C(O_3)}{Dt}$, where γ_{o_3} is heating coefficient and $\frac{D C(O_3)}{Dt}$ is given by (6.2).

The model that represents the interaction of gravity waves with ozone consists of the gravity waves' equations (2.41)–(2.43), with the density equation being modified, as well as the continuity equation for ozone (6.2) expressed in analogous form of (2.44). This model is represented by the following system of equations:

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\bar{\rho}}\rho_x, \quad (6.6)$$

$$\zeta = \nabla^2\psi, \quad (6.7)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = \gamma_{o_3} \frac{D C(O_3)}{Dt}, \quad (6.8)$$

$$\frac{D C(O_3)}{Dt} = \frac{\partial C(O_3)}{\partial t} + (\bar{u} + \varepsilon u) \frac{\partial C(O_3)}{\partial x} + \varepsilon w \frac{\partial C(O_3)}{\partial z} = -\sigma_{o_3} C(O_3) + \mathcal{D} \nabla^2 C(O_3), \quad (6.9)$$

$$u = -\psi_z \quad \text{and} \quad w = \psi_x. \quad (6.10)$$

The initial profile of ozone concentration is specified based on the distribution of ozone observed by measurement studies; for example, Figure 1(b) of Gille and Lyjak (1986), which shows the ozone concentration that attains peak values around 30 km altitude and around the equator in latitude and decays away from this central location. We consider a situation where a gravity-wave packet forced at low levels in the troposphere propagates upward to a critical level (zero wind line) at an altitude around 30 km.

We consider ozone between 0 and 60 km on the vertical direction and consider the dimensional horizontal direction to be $-670 \text{ km} \leq x^* \leq 670 \text{ km}$. We solve equations (6.6)–(6.10) in the non-dimensional spatial domain $-50 \leq x \leq 50$ in the horizontal direction, and $0 \leq z \leq 10$ in the vertical direction. Following the scaling discussion in Chapter 2, this choice of the non-dimensional domain corresponds to the scaling references $L_z = 6$, $L_x = 13.4$ and hence $\delta = 0.2$.

The ozone distribution shown in Figure 1(b) of Gille and Lyjak (1986) then suggests that we can consider an ozone profile in the form of a Gaussian function of both x and z centred at the critical level $z = 5$. This can be specified in a nondimensional Gaussian form as

$$C(O_3)(x, z, 0) = e^{-a^2 x^2} e^{-b^2 (z - z_1)^2}, \quad (6.11)$$

where the altitude of the maximum concentration z_1 is at the gravity-wave critical level $z = 5$.

The boundary and initial conditions for the gravity-wave equations are the same as the ones considered in Chapter 4. As before, the streamfunction boundary condition is given as

$$\psi(x, 0, t) = \frac{e^{-\mu^2 x^2}}{2} (e^{ik_0 x} + e^{-ik_0 x}). \quad (6.12)$$

The model is solved numerically using the pseudo-spectral method in the horizontal direction and a finite-difference method in the vertical direction. The description of the numerical methods is given in Chapter 5. At each time step, the gravity-wave vorticity ζ , the streamfunction ψ and the density ρ , as well as the chemical concentration C , are all computed simultaneously based on information from the previous time step. The advection terms in the chemical equation contain the effect of gravity-wave perturbations u and w , which are obtained from the previous time step. Similarly, the chemical heating term $\frac{DC}{Dt}$ (in the density equation) is a term that depends on the chemical and it is computed at each time step based on information from the previous time step.

The simulation of the solutions in this section is obtained with the following choice of parameters. The background velocity is $\bar{u} = \tanh(z - 5)$, so the critical level at $z = 5$. The factor δ is set to 0.2; and the background density $\bar{\rho} = \rho_0 e^{-z/h}$, where $\rho_0 = 1$, and $h = 4.9$. The parameter ε is set to 0.05, and $\gamma_{o_3} = 0.5$. In the boundary wave packet condition (6.12), we set $\mu = 0.2$ and $k_0 = 2$. To approximately match the horizontal and vertical width of the contours for ozone given by Gille and Lyjak (1986), we set $a^2 = 0.1$, $b^2 = 0.5$ and $z_1 = 5$ in the initial condition for the chemical equation (6.11). For the parameters in (6.9), we set $\mathcal{D} = 0.001$ and $\sigma_{o_3} = 0.1$.

Before showing the numerical results for the interaction of the time-dependent ozone and gravity waves, we show numerical results corresponding to nonlinear gravity waves affected by a steady-state chemical distribution. This configuration corresponds to the case where gravity waves are affected by the presence of the chemical but the chemical distribution is not affected by nonlinear gravity-wave evolution. Numerical results for these steady-state simulations are shown in Section 6.1.1.

6.1.1 Simulations with a steady-state chemical

In this section, we consider the case where the spatial distribution of the mixing ratio C of the chemical is given by a steady-state expression of the form (6.11) and it does not change with time, so for all time C takes the form $C(x, z) = e^{-a^2 x^2} e^{-b^2 (z-z_1)^2}$ with $a^2 = 0.05$, $b^2 = 0.5$ and $z_1 = 5$, as shown in Figure 6.1. The model is given by equations (6.6), (6.7) and (6.8). Since C is steady, $\frac{\partial C}{\partial t} = 0$, and so $\frac{DC}{Dt}$ in (6.8) takes the form

$$\frac{DC}{Dt} = (\bar{u} + \varepsilon u) \frac{\partial C}{\partial x} + \varepsilon w \frac{\partial C}{\partial z},$$

with $C(x, z) = e^{-a^2 x^2} e^{-b^2 (z-z_1)^2}$.

The steady-state mixing ratio $C(x, z)$ of the chemical is shown in Figure 6.1. The contour plots of the horizontal perturbation velocity at two different times are shown in Figure 6.2. Figure 6.3 shows the contour plots for the perturbation density at two different times. In all of these four figures, we see the effect of the steady-state chemical on the gravity waves, especially around the critical level ($z = 5$). The chemical is continuously affecting the gravity waves at all times as it is in a steady-state form.

The remaining figures in this section concern the Fourier spectrum of the streamfunction and density perturbations. At the level ($z = 2.5$), we note from Figures 6.4, 6.5, 6.8 and 6.9 that, in the absence of the chemical effect, the dominant contribution comes from the forced wavenumbers $k = \pm 2$ but in the case of the chemical effect (solid line), the contribution coming from the vicinity of the zero wavenumber is dominant at all times. At the critical level ($z = 5$), we note from Figures 6.6, 6.7, 6.10 and 6.11 that, in the absence of the chemical effect (dashed-circled line), the contribution of the zero wavenumber increases with time

Figure 6.1: The mixing ratio $C(x, z)$ of the steady-state chemical, which takes the form (6.11) with $a^2 = 0.05$, $b^2 = 0.5$ and $z_1 = 5$.

and eventually dominates the contribution coming from the forcing wavenumbers $k = \pm 2$, which become very small at later times compared with the zero wavenumber. This behaviour of gravity-wave spectrum in the absence of chemical was already shown in Campbell and Maslowe (2003). However, we note from the same aforementioned figures that, in the case of chemical effect (solid lines), the contribution from the vicinity of the zero wavenumber dominates both at early and late time, and we note that the chemical effect damps the gravity-waves at the forced wavenumbers $k = \pm 2$, especially at later times.

Figure 6.2: The horizontal velocity perturbation of gravity waves $u(x, z, t)$, where (a) and (c) represents u with no chemical effect at time $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents u with the effect of the steady-state chemical at time $t = 10$ and $t = 30$, respectively.

Figure 6.3: The density perturbation of gravity waves $\rho(x, z, t)$ where (a) and (c) represents ρ with no chemical effect at time $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents ρ with the effect of the steady-state chemical at time $t = 10$ and $t = 30$, respectively.

Figure 6.4: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves affected by the steady-state chemical (solid line) and gravity waves without the chemical effect (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.5: Same as in Figure 6.4 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves affected by the steady-state chemical and the dashed-circled line represents the gravity waves without the chemical effect.

Figure 6.6: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves affected by the steady-state chemical (solid line) and gravity waves without the chemical effect (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.7: Same as in Figure 6.6 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves affected by the steady-state chemical and the dashed-circled line represents the gravity waves without the chemical effect.

Figure 6.8: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves affected by the steady-state chemical (solid line) and gravity waves without the chemical effect (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.9: Same as in Figure 6.8 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves affected by the steady-state chemical and the dashed-circled line represents the gravity waves without the chemical effect.

Figure 6.10: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves affected by the steady-state chemical (solid line) and gravity waves without the chemical effect (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

Figure 6.11: Same as in Figure 6.10 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves affected by the steady-state chemical and the dashed-circled line represents the gravity waves without the chemical effect.

6.1.2 Time-dependent simulations

The simulations of the gravity-wave propagation and mean-flow interaction coupled with time-dependent ozone transport are described in this section. The concentration of ozone is considered to be evolving with time, so in addition to equations (6.6), (6.7) and (6.8), we also consider equations (6.9) and (6.10). That is, the full system is now considered where $\frac{DC(O_3)}{Dt}$ in (6.8) is given as

$$\frac{DC(O_3)}{Dt} = \frac{\partial C(O_3)}{\partial t} + (\bar{u} + \varepsilon u) \frac{\partial C(O_3)}{\partial x} + \varepsilon w \frac{\partial C(O_3)}{\partial z},$$

which represents the left-hand side of equation (6.9).

As discussed before, the initial profile of ozone concentration is specified based on the distribution of ozone observed by measurement studies by Gille and Lyjak (1986). As before, the gravity-wave packet forcing is $\psi(x, 0, t) = e^{ik_0 x} e^{-\mu^2 x^2} + \text{c.c.}$, where $k_0 = 2$. We consider a situation where a gravity-wave packet forced at low levels in the troposphere propagates upward to a critical level (zero wind line) at an altitude around 30 km. The ozone distribution shown in Figure 1(b) of Gille and Lyjak (1986) then suggests that we can consider an ozone profile in the form of a Gaussian function of both x and z centred at the critical level $z = 5$. This is shown in Figure 6.12.

Figure 6.13 shows the evolution of ozone concentration where we see the effect of gravity waves around the critical level. Comparing the evolution at different times in Figure 6.13 and also in Figure 6.14, we note that ozone is damping with time. This is not surprising, since the first term in the right-hand side of equation (6.9) is negative and hence, as found in Chapter 3, the evolution of ozone is proportional to $e^{-\sigma_{o_3} t}$ which is decaying with time. Figures 6.15 and 6.16 show the effect of ozone on the horizontal velocity as well as the density of

gravity waves at early and late time. In both figures, we note that the evolution around the critical level is modified when compared to the case where there is no interaction with ozone. This modification is proportional to the evolution of ozone as can also be seen from later time solutions in Figures 6.15 and 6.16.

The Fourier spectrum of streamfunction at $z = 2.5$ is shown in Figures 6.17 and 6.18. We note that the gravity waves are affected by the ozone around the zero wavenumber as well as around the forcing wavenumbers $k = \pm 2$, which are being damped as can also be seen from Figures 6.19 and 6.20 at the critical level ($z = 5$). Figure 6.21 shows the Fourier spectrum of density at different times around $z = 2.5$. We note that, although the density is affected by ozone around the zero wavenumber, this effect is not dominant at later time as in the steady-state case. At the critical level ($z = 5$), however, the effect around the zero wavenumber is dominant at early and later times as shown in Figures 6.22 and 6.23. From the density figures 6.21, 6.22 and 6.23, we note that gravity waves are damped around the forcing wavenumber at early and later times at $z = 2.5$, whereas at the critical level, this is true only at early time.

Comparing the Fourier spectrum of the streamfunction to that of the density at the zero wavenumber $k = 0$ at the critical level, we note from Figures 6.19 and 6.22 that although ozone affects the vicinity of the zero wavenumber, no effect is obvious at $k = 0$ in the streamfunction spectrum for both early and later times, whereas in the density case, the $k = 0$ component is affected, and it represents the peak at all times as can be seen in Figure 6.22. These results are consistent with the analytical equations for the wave-induced mean streamfunction and the wave-induced mean density, which we derived in Section 4.2. The analytical equation for the wave-induced mean streamfunction derived in Subsection 4.2.1 is given by

(4.73) and has the form

$$\frac{\partial}{\partial t} \hat{\psi}_z(0, z, t) = -\varepsilon \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right), \quad (6.13)$$

and the wave-induced mean density equation (4.81) derived in Subsection 4.2.2 and has the form

$$\frac{\partial}{\partial t} \hat{\rho}(0, z, t) = -\varepsilon \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_x \rho dx \right) + \gamma \int_{-\infty}^{\infty} \left(\frac{\partial C}{\partial t} + \varepsilon w \frac{\partial C}{\partial z} \right) dx. \quad (6.14)$$

Equations (6.13) and (6.14) can be used in a parameterization scheme. These equations include the effect of the chemical, ozone in this case, and hence can be used to compute gravity-wave drag in a situation where gravity waves are coupled with ozone. We note that, although in our configuration waves are modified by a chemical forcing, the effect of the chemical forcing does not appear in (6.13), and hence no direct effect of the chemical on the zero wavenumber component of the streamfunction spectrum. In wave-induced mean density equation (6.14), however, we note that the wave-induced mean density is affected by the chemical forcing, as can be seen from the second term on the right-hand side of (6.14). Thus, the zero wavenumber component of the density spectrum is affected.

Comparing with the steady-state simulations at the critical level, we find that, from the Fourier spectrum of the density for the time-dependent case, the zero wavenumber component reaches its maximum, as can be seen in Figure 6.22, whereas this was not true for the corresponding steady-state spectrum shown in Figure 6.10. This can be understood from the analytical equation of wave-induced mean density (6.14). In the steady-state case, the dominant term $\frac{\partial C}{\partial t} = 0$, so the zero wavenumber component in Fourier spectrum of density is small, whereas in the time-dependent simulations $\frac{\partial C}{\partial t} \neq 0$, so the zero wavenumber component in

Fourier spectrum of density is large.

Figure 6.12: The initial mixing ratio of ozone $C(O_3)(x, z, 0)$ based on the profile shown in Figure 1(b) of Gille and Lyjak (1986).

Figure 6.13: The mixing ratio of ozone $C(O_3)(x, z, t)$ at time (a) $t = 10$ and (b) $t = 30$. The maximum amplitude in (a) is 0.3, whereas the maximum amplitude in (b) is 0.024 as shown in the side bars. This shows that the ozone is damping with time.

Figure 6.14: The mixing ratio of ozone $C(O_3)(x, z, t)$ at $z = 4$ at different times.

Figure 6.15: The horizontal velocity perturbation $u(x, z, t)$ of the gravity-wave packet, where (a) and (c) represents u with no chemical effect at time $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents u with the effect of ozone at time $t = 10$ and $t = 30$, respectively.

Figure 6.16: The density perturbation $\rho(x, z, t)$ of the gravity-wave packet, where (a) and (c) represents ρ with no chemical effect at time $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents ρ with the effect of ozone at time $t = 10$ and $t = 30$, respectively.

Figure 6.17: The Fourier spectrum of streamfunction $\hat{\psi}(k, z, t)$ for the gravity-wave packet interacting with the time-dependent ozone (solid line) and the gravity-wave packet without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.18: Same as in Figure 6.17 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity-wave packet interacting with the time-dependent ozone and the dashed-circled line represents the gravity-wave packet without any interaction.

Figure 6.19: The Fourier spectrum of streamfunction $\hat{\psi}(k, z, t)$ for the gravity-wave packet interacting with the time-dependent ozone (solid line) and the gravity-wave packet without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.20: Same as in Figure 6.19 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity-wave packet interacting with the time-dependent ozone and the dashed-circled line represents the gravity-wave packet without any interaction.

Figure 6.21: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity-wave packet interacting with the time-dependent ozone (solid line) and the gravity-wave packet without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.22: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity-wave packet interacting with the time-dependent ozone (solid line) and the gravity-wave packet without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

Figure 6.23: Same as in Figure 6.22 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity-wave packet interacting with the time-dependent ozone and the dashed-circled line represents the gravity-wave packet without any interaction.

6.2 Gravity waves' interactions with water vapour in the atmosphere

In the form of liquid, vapour or solid, water is present in our atmosphere, and it changes from one state to another according to the surrounding temperature. When changing from one state to another, latent heat is released [Wallace and Hobbs (2006)]. All of the three states of water release and absorb long-wave and solar radiation; thus water is considered to be an important factor in the radiation balance of our planet. Water is also present in various chemical reactions in the atmosphere. The value of latent heat of evaporation of water is the largest among all substances excluding NH_3 [Curry and Webster (1998)]. Therefore, water and its transformation between the three states have an important effect on the atmosphere and the climate.

Among the three states of water, our focus will be on water vapour. Water vapour is considered to be the most important greenhouse gas in the atmosphere [Wallace and Hobbs (2006)]. Recent studies show that the influence of heating released by water vapour in the atmosphere could double the climate warming caused primarily by CO_2 [Hansen (2008)].

Following Brasseur and Solomon (1984), the continuity equation for water vapour H_2O (Eq (5.105)) is

$$\begin{aligned} \frac{D(\text{H}_2\text{O})}{Dt} + [\mathbf{J}_{\text{H}_2\text{O}} + a_1^*(O^1D)](\text{H}_2\text{O}) \\ = a_{16}(OH)^2 + a_{17}(OH)(HO_2) + a_{19}(OH)(H_2) + a_{23c}(H)(HO_2) \end{aligned} \quad (6.15)$$

Since in our model we are considering only water vapour coupled with gravity waves, the continuity equation for water vapour can be expressed in terms of

mixing ratio as

$$\frac{\partial C(H_2O)}{\partial t} + U \frac{\partial C(H_2O)}{\partial x} + W \frac{\partial C(H_2O)}{\partial z} = -\sigma_{h_2o} C(H_2O) + \mathcal{D} \nabla^2 C(H_2O), \quad (6.16)$$

where $C(H_2O)$ is the mixing ratio of water vapour; U and W are the dimensional horizontal and vertical velocities; and $\sigma_{h_2o} = \tau R_{H_2O}$ where R_{H_2O} is the photolysis rate. Following London and Park (1974), the photolysis rate R_{H_2O} can be approximated as $R_{H_2O} = 8.7 \times 10^{-6} \text{s}^{-1}$.

The heating rate due the absorption of solar radiation by water vapour can be computed using a form that is similar to the form obtained in Section 6.1 for ozone. According to Holton (2004), the total heat rate released by water vapour is given as

$$J_{H_2O} = -L_c \frac{D C(H_2O)}{Dt}, \quad (6.17)$$

where L_c is the latent heat of condensation, which is released during the process of changing from vapour to liquid.

The model that represents the development of gravity waves in the presence of water vapour consists of the gravity waves' equations (6.6)–(6.8) coupled with the continuity equation for water vapour (6.16), where the density equation (6.8) is replaced by

$$\rho_t + \bar{u} \rho_x + \bar{\rho}' \psi_x + \varepsilon(\psi_x \rho_z - \psi_z \rho_x) = \gamma_{h_2o} \frac{D C(H_2O)}{Dt}, \quad (6.18)$$

and the chemical-transport equation (6.16) is considered with the advection velocity being represented in a perturbation form as in (6.9) with components $U(x, z, t) = \bar{u}(z) + \varepsilon u(x, z, t)$ and $W(x, z, t) = \varepsilon w(x, z, t)$. We solve the model on the two-dimensional spatial domain $-50 \leq x \leq 50$ in the horizontal direction and $0 \leq z \leq 10$ in the vertical direction. The model is solved with the same initial

conditions and boundary condition (6.12) as in Section 6.1.

To specify the initial distribution of the water vapour concentration, we refer to distribution shown in observational studies. For example, Figure 1(c) of Gille and Lyjak (1986) shows a water-vapour distribution that could be approximated by a Gaussian function in both the horizontal and the vertical directions, but, unlike ozone which has a peak around 30 km, the water vapour distribution is greater in the lower atmosphere with a peak around 10 km altitude and around the equator in the latitude. Based on this, the initial profile for water vapour in our nondimensional configuration is represented as

$$C(H_2O)(x, z, 0) = e^{-a^2 x^2} e^{-b^2 (z-z_1)^2}, \quad (6.19)$$

where the altitude of the maximum concentration z_1 is below the gravity-wave critical level z_c . The simulation of the solutions in this section are obtained with the following choice of parameters. In the continuity equation for the chemical, we set $\mathcal{D} = 0.001$ and $\sigma_{h_2o} = 0.01$; and we set $a^2 = 0.1$, $b^2 = 0.5$ and $z_1 = 1.5$ in the initial condition for the chemical equation (6.19). The remaining parameters are the same as in Section 6.1.

Figure 6.24: The initial mixing ratio of water vapour $C(H_2O)(x, z, 0)$ based on the profile shown in Figure 1(c) of Gille and Lyjak (1986) is shown in (a). The other two subfigures show the mixing ratio of water vapour $C(H_2O)(x, z, t)$ at times (b) $t = 10$ and (c) $t = 30$.

Figure 6.25: The horizontal velocity perturbation of gravity waves $u(x, z, t)$, where (a) and (c) represents u with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents u with the effect of water vapour at times $t = 10$ and $t = 30$, respectively.

Figure 6.26: The density perturbation of gravity waves $\rho(x, z, t)$, where (a) and (c) represents ρ with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents ρ with the effect of water vapour at times $t = 10$ and $t = 30$, respectively.

Based on the profile shown in Figure 1(c) of Gille and Lyjak (1986), as discussed earlier, water vapour is present mostly in the lower atmosphere, so the initial form of water-vapour concentration is centred at the level $z = 1.5$ as shown in Figure 6.24 (a). Figure 6.24 shows the evolution of water-vapour concentration at different times. As already discussed, the velocity components are $U(x, z, t) = \bar{u}(z) + \varepsilon u(x, z, t)$ and $W(x, z, t) = \varepsilon w(x, z, t)$. At the lower part of the domain, where water vapour concentration is centred, the mean flow $\bar{u} = \tanh(z - 5)$ is approximately $\bar{u} \approx -1$. The advection due to the mean flow in the lower domain dominates the advection due to the perturbation from gravity waves, which is of order $O(\varepsilon)$. This is shown in Figure 6.24, where we observe that the concentration is advecting to the left and leaving the effective domain of gravity waves. This was not the case for ozone which is centred at the critical level and hence advects to the left below the critical level and to the right above the critical level as shown in Figure 6.13. This means that ozone remains centred around the critical level and hence has an effect on gravity waves where the effect is proportional to the distribution of ozone as shown in Figure OZU10. Figures 6.25 and 6.26 shows the effect of water vapour on the horizontal velocity, as well as the density of gravity waves at early and late time. In both figures, we note less effect on gravity waves compared to ozone and the steady-state cases where the chemical is centred at the critical level. In the steady-state case, the chemical was centred at the critical level of gravity waves and hence was affecting the gravity waves. In the ozone case the chemical was moving but centred at the critical level, so around the critical level where the background mean flow $\bar{u} \approx 0$, the advection of the chemical was only of order $O(\varepsilon)$. This small advection around the critical level allows the chemical to interact with gravity waves and not leave the area of interaction as in the water-vapour case.

From Figures 6.27 and 6.28, we note that, away from the zero wavenumber, the Fourier spectrum of streamfunction corresponding to the case of interaction is almost identical to that corresponding to the case with no interaction. Similarly, we note from the Fourier spectrum of density that, at $z = 2.5$, the effect is mainly around the zero wavenumber and there almost no effect at the critical level, as can be seen in Figures 6.29 and 6.30. We therefore conclude that the effect of water vapour on gravity waves is mainly in the neighbourhood of the zero wavenumber of the spectrum of streamfunction and density, and this effect around the zero wavenumber is larger at $z = 2.5$ compared with that at the critical level $z = 5$. This is consistent with the analytical equation of the wave-induced mean density (4.81) derived in Section 4.2.2 and shown in (6.14), where we note that the chemical forcing is affecting the wave-induced mean density. Since the water vapour distribution is centred at lower level $z = 1.5$, then the distribution of water vapour is larger at $z = 2.5$ than at $z = 5$. Thus the effect of the chemical shown on the right-hand side of (6.14) is much larger at the level $z = 2.5$ compared with that at the critical level $z = 5$.

Figure 6.27: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent water vapour (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.28: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent water vapour (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.29: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent water vapour (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.30: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent water vapour (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

6.3 Simulations with a chemical-transport equation possessing a nonlinear source term

Water vapour and ozone were studied in previous sections and were modelled by advection-diffusion equations having a linear source term. In this section, we study the interaction of gravity waves with a chemical that has a nonlinear source term in its continuity equation. We first investigate the case where the source term is in the form of the nonlinear term in Fisher's equation (3.12), where $f(C) = \sigma C(1 - C)$. A continuity equation of this form may represent some chemical constituent in the atmosphere.

As a second example, we consider a configuration where chlorine monoxide (ClO) is present in a localized region with gravity-wave interactions. Brasseur and Solomon (1984) suggest that the transport of ClO can be modelled by a nonlinear advection-diffusion-reaction equation with a nonlinear term of the form $f(C) = -\sigma_{clo}C(ClO) - k_{clo}C(ClO)^2$, as shall be seen in Subsection 6.3.2. The interaction of ClO with gravity waves will be studied after studying gravity-wave interaction with Fisher's equation.

6.3.1 Simulations with Fisher's equation

The coupled system of gravity-wave equations with Fisher's equation is considered in this section. The model representing the interaction of internal gravity waves with Fisher's equation is given as

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x + \varepsilon(\psi_x\zeta_z - \psi_z\zeta_x) = -\frac{g}{\bar{\rho}}\rho_x, \quad (6.20)$$

$$\zeta = \nabla^2\psi, \quad (6.21)$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x + \varepsilon(\psi_x\rho_z - \psi_z\rho_x) = \gamma\frac{DC}{Dt}, \quad (6.22)$$

$$\frac{\partial C}{\partial t} + (\bar{u} + \varepsilon u)\frac{\partial C}{\partial x} + \varepsilon w\frac{\partial C}{\partial z} = \sigma C(1 - C) + \mathcal{D}\nabla^2 C, \quad (6.23)$$

$$u = -\psi_z \quad \text{and} \quad w = \psi_x. \quad (6.24)$$

We solve the model with the same domain, parameters, boundary and initial conditions considered for gravity waves in Section 6.1. We start by setting the parameters in the chemical equation to $\sigma = 0.1$ and $\mathcal{D} = 0.001$ and show results for this choice. We then show results with all parameters fixed but with larger σ chosen as $\sigma = 0.5$. The reason for these two experiments is to show the effect of this parameter in Fisher's equation. With the linear source term discussion in Section 6.1 and Section 6.2, we found that the mixing ratio of the chemical C is proportional to $e^{-\sigma t}$ and thus it is damped with time, and larger σ leads to even more damping.

The initial condition of the chemical is taken as

$$C(x, z, 0) = e^{-0.1x^2} e^{-0.5(z-5)^2}. \quad (6.25)$$

The initial profile is shown in Figure 6.31. Figures 6.32 and 6.33 show the evolution of Fisher's equation at several times. We observe from these figures that the mixing ratio is not damping as in the case with the linear source term in the previous two sections. The effect of the chemical modelled by Fisher's equation on the gravity-wave-perturbation velocity and density is shown in Figures 6.34 and 6.35 at early and late times. We note from these figures that gravity waves are greatly affected especially at later times. From the late time effects shown in Figures 6.34 and 6.35, we note that, around the critical level, gravity waves' perturbations are taking the form of the chemical concentration. This effect

Figure 6.31: The initial mixing ratio $C(x, z, 0)$ for Fisher's equation.

extends to a larger vicinity around the critical level compared to the effect of the linear equations for ozone and water vapour in previous sections.

The Fourier spectrum of streamfunction of gravity waves at $z = 2.5$ and $z = 5$ is shown in Figures 6.36, 6.37 and 6.38. We note that, in addition to the significant effect around the zero wavenumber, the effect spreads and reaches to the forcing wavenumber $k = \pm 2$. Figures 6.39, 6.40 and 6.41 show the Fourier density of gravity waves, where we find that solid line corresponding to the interaction of gravity-wave equations with Fisher's equation is dominant around the zero wavenumber as well as the forcing wavenumbers $k = \pm 2$.

The remaining results in this section are computed with $\sigma = 0.5$. Figure 6.42 shows the mixing ratio at the level $z = 4$ at several times. We note that the mixing ratio $C(x, 4, t)$ is not damped with time as in the case of ozone in Section 6.1 or the case of chlorine monoxide ClO, which shall be discussed in the next section. The evolution of the solution of Fisher's equation at several times is shown in

Figure 6.32: The mixing ratio $C(x, z, t)$ of Fisher's equation at the level $z = 4$ at several times.

Figure 6.43. Comparing this figure to Figure 6.33, which was computed with a smaller σ , we find that σ has a great influence on the advection of the solution of Fisher's equation. This is consistent with the numerical results in Chapter 5 and the analytical results in Chapter 3, where we found that the speed of the waves is proportional to σ . The perturbation velocity and density of gravity waves interacting with Fisher's equation with $\sigma = 0.5$ is shown in Figures 6.44 and 6.45 at several times. It can be seen from these figures that there is significant effect compared with the corresponding results with $\sigma = 0.1$.

The Fourier spectrum of streamfunction at $z = 2.5$ and $z = 5$ at several times is shown in Figures 6.46–6.49. We note that the maximum amplitude in these figures is much higher than those with the smaller σ . Figures 6.50–6.53 concern the Fourier spectrum of density, which also show much higher amplitude compared with the corresponding figures obtained with $\sigma = 0.1$. In all of these Fourier

Figure 6.33: The mixing ratio $C(x, z, t)$ of Fisher's equation at times (a) $t = 10$ and (b) $t = 30$.

Figure 6.34: The horizontal velocity perturbation of gravity waves $u(x, z, t)$, where (a) and (c) represents u with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents u in the case of interaction of gravity waves with Fisher's equation at times $t = 10$ and $t = 30$, respectively.

Figure 6.35: The density perturbation of gravity waves $\rho(x, z, t)$, where (a) and (c) represents ρ with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents ρ in the case of interaction of gravity waves with Fisher's equation at times $t = 10$ and $t = 30$, respectively.

Figure 6.36: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.37: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.38: Same as in Figure 6.37 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation and the dashed-circled line represents the gravity waves without any interaction.

Figure 6.39: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.40: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

Figure 6.41: Same as in Figure 6.40 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation and the dashed-circled line represents the gravity waves without any interaction.

spectrum figures of streamfunction and density, we note that the effect is not only around the zero wavenumber. The effect can be seen in a much wider spectrum, which even exceeds the forcing wavenumbers, especially at later times. We note that the effect on the Fourier spectrum of the gravity waves coupled with Fisher's equation is much stronger with the larger σ . In general, we note that the effect on the Fourier spectrum of the gravity waves coupled with Fisher's equation is much stronger than the corresponding effect from ozone, water vapour or ClO. This is consistent with the analytical observation we can conclude from the analytical equation of the wave-induced mean density (4.81), which is derived in Subsection 4.2.2 and shown in (6.14). In this equation, we note that the chemical forcing is affecting the wave-induced mean density. As discussed before, the mixing ratio of Fisher's equation is found to be growing with time, whereas in the case of ozone, water vapour or ClO, the mixing ratio is damped with time. Therefore, from the right-hand side of (6.14), we observe that the effect of the chemical is stronger in the case of Fisher's equation compared to other cases corresponding to ozone, water vapour or ClO.

Figure 6.42: The mixing ratio $C(x, z, t)$ of Fisher's equation with $\sigma = 0.5$ at the level $z = 4$ at several times.

Figure 6.43: The mixing ratio $C(x, z, t)$ for Fisher's equation with $\sigma = 0.5$ at time (a) $t = 10$ and (b) $t = 20$.

Figure 6.44: The horizontal velocity perturbation of gravity waves $u(x, z, t)$, where (a) and (c) represents u with no chemical effect at times $t = 10$ and $t = 20$, respectively. Figures (b) and (d) represents u in the case of interaction of gravity waves with Fisher's equation with $\sigma = 0.5$ at times $t = 10$ and $t = 20$, respectively.

Figure 6.45: The density perturbation of gravity waves $\rho(x, z, t)$, where (a) and (c) represents ρ with no chemical effect at times $t = 10$ and $t = 20$, respectively. Figures (b) and (d) represents ρ in the case of interaction of gravity waves with Fisher's equation with $\sigma = 0.5$ at times $t = 10$ and $t = 20$, respectively.

Figure 6.46: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.47: Same as in Figure 6.46 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ and the dashed-circled line represents the gravity waves without any interaction.

Figure 6.48: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.49: Same as in Figure 6.48 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ and the dashed-circled line represents the gravity waves without any interaction.

Figure 6.50: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.51: Same as in Figure 6.50 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ and the dashed-circled line represents the gravity waves without any interaction.

Figure 6.52: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

Figure 6.53: Same as in Figure 6.52 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent Fisher's equation with $\sigma = 0.5$ and the dashed-circled line represents the gravity waves without any interaction.

6.3.2 Simulations with chlorine monoxide

Chlorine monoxide (ClO) is one of the most reactive gases associated with ozone destruction in the stratosphere. It is produced from the reaction of ozone and chlorine in the chlorine catalytic cycle leading to ozone depletion [Carpenter et al. (2014)].

As can be seen in Brasseur and Solomon (1984), the continuity equation for ClO (Eq (5.241)) is

$$\begin{aligned} \frac{D(\text{ClO})}{Dt} + (\text{ClO})[d_3(O) + d_4(NO) + \mathbf{J}_{\text{ClO}} + (d_8 + d_{46})(OH) + d_{31}(M)(NO_2) + 2d_{60}(M)(ClO) \\ + 2(\mathbf{d}_{47} + \mathbf{d}_{48} + \mathbf{d}_{49})(\text{ClO}) + (e_{5a} + e_{5b} + e_{5c})(BrO)] = d_2(O_3)(Cl) + [J_{ClONO_2}^b \\ + d_{32}(O)](ClONO_2) + 2d_{61}(M)(Cl_2O_2) + J_{OClO}(OClO) \end{aligned}$$

However, since we are considering only ClO to be present in our model, the continuity equation for ClO can then be expressed in non-dimensional form as

$$\frac{\partial C(ClO)}{\partial t} + U \frac{\partial C(ClO)}{\partial x} + W \frac{\partial C(ClO)}{\partial z} = -\sigma_{clo} C(ClO) - k_{clo} C(ClO)^2 + \mathcal{D} \nabla^2 C(ClO), \quad (6.26)$$

where the parameter σ_{clo} is a non-dimensional photolysis rate and k_{clo} is a non-dimensional reaction rate.

The model representing the interaction of internal gravity waves with chlorine monoxide (ClO) is represented by equations (6.20)–(6.24) except that equation (6.23) is replaced by (6.26) with $U = \bar{u} + \varepsilon u(x, z, t)$ and $W = \varepsilon w(x, z, t)$. The model is solved with the same domain, parameters, boundary and initial conditions considered for gravity waves in Section 6.1. The parameters in the chemical equation are given as $\sigma_{clo} = 0.1 = k_{clo}$ and $\mathcal{D} = 0.001$, where we considered the same parameters in order to compare with the case of Fisher's equation in the last section. The initial condition of ClO is also considered to be the same as the initial condition given in (6.25), which is centred at the critical level as in the ozone case.

We consider this initial from since ClO is associated with the destruction of ozone, and hence we consider the initial distribution of ClO to be centred at the same level as that of ozone.

The difference between the ClO equation in this section and Fisher's equation in Subsection 6.3.1 is that the source term in Fisher's equation is composed of two terms that have opposite sign, whereas these same terms have the same negative sign for ClO. This negative sign suggests that the mixing ratio will be damping as in the ozone case.

Figure 6.54 shows the initial condition of ClO. The distribution of ClO at two different times is shown in Figure 6.56, and the influence of gravity waves is seen in the interaction vicinity. Figure 6.55 shows the mixing ratio at the level $z = 4$ at several times. Figures 6.56 and 6.55 show that the chemical is damping with time. Figure 6.57 shows the effect of ClO on the horizontal perturbation velocity of gravity waves. This effect is qualitatively proportional to the distribution of ClO. A similar effect can be seen in Figure 6.58, which represents the density perturbation at two different times. A lesser effect is seen at later times, as shown in Figures 6.57 and 6.58, since the chemical is damping with time.

Comparing the early time effect in Figures 6.57 and 6.58 with the corresponding figures in Fisher's equation, in Figures 6.34 and 6.35, we note that the effect is much apparent in ClO case. However, at later times we note that the effect on gravity-wave perturbation velocity and density shown in Figures 6.34 and 6.35 corresponding to Fisher's equation is much greater than that corresponding to the ClO effect. This is because ClO is damped as shown in Figure 6.55 whereas the chemical is not damped in the case of Fisher's equation as shown in the corresponding Figure 6.32.

The Fourier spectrum of streamfunction at two different times is shown in Fig-

Figure 6.54: The initial mixing ratio $C(ClO)(x, z, 0)$ for ClO.

ures 6.60 and 6.59. Figures 6.63 and 6.62 show the Fourier spectrum of density perturbation at two different times. In these Figures, we note that the effect of ClO on gravity waves is mainly around the zero wavenumber component. Comparing with Fisher's equation, we note that the density spectrum at critical level at later time shown in Figure 6.63 has a smaller amplitude compared with the corresponding density spectrum at the critical level in the case of Fisher's equation shown in Figure 6.40.

Figure 6.55: The mixing ratio $C(ClO)(x, z, t)$ of ClO at $z = 4$ at several times.

Figure 6.56: The mixing ratio $C(\text{ClO})(x, z, t)$ of ClO at times (a) $t = 10$ and (b) $t = 30$.

Figure 6.57: The horizontal velocity perturbation of gravity waves $u(x, z, t)$, where (a) and (c) represents u with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents u with the effect of chlorine monoxide ClO at times $t = 10$ and $t = 30$, respectively.

Figure 6.58: The density perturbation of gravity waves $\rho(x, z, t)$, where (a) and (c) represents ρ with no chemical effect at times $t = 10$ and $t = 30$, respectively. Figures (b) and (d) represents ρ with the effect of chlorine monoxide ClO at times $t = 10$ and $t = 30$, respectively.

Figure 6.59: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent CIO (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 2.5, 10)|$ and (b) $|\hat{\psi}(k, 2.5, 30)|$.

Figure 6.60: The Fourier spectrum of the streamfunction $\hat{\psi}(k, z, t)$ for the gravity waves interacting with the time-dependent CIO (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\psi}(k, 5, 10)|$ and (b) $|\hat{\psi}(k, 5, 30)|$.

Figure 6.61: Same as in Figure 6.60 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent CIO and the dashed-circled line represents the gravity waves without any interaction.

Figure 6.62: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent CIO (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 2.5, 10)|$ and (b) $|\hat{\rho}(k, 2.5, 30)|$.

Figure 6.63: The Fourier spectrum of density $\hat{\rho}(k, z, t)$ for the gravity waves interacting with the time-dependent CIO (solid line) and gravity waves without any interaction (dashed-circled line), where we have (a) $|\hat{\rho}(k, 5, 10)|$ and (b) $|\hat{\rho}(k, 5, 30)|$.

Figure 6.64: Same as in Figure 6.63 (a) and (b) but with smaller vertical scale, where the solid line represents the gravity waves interacting with the time-dependent CIO and the dashed-circled line represents the gravity waves without any interaction.

Chapter 7

Conclusions

7.1 Summary

The interaction of internal gravity waves with chemical constituents in the atmosphere was studied in this thesis. Internal gravity waves were represented by a system of equations obtained by applying the Boussinesq approximation, which is commonly used in the field of fluid dynamics. Applying this approximation allowed us to obtain analytical solutions for the gravity waves in addition to the computational approximate solutions.

The equations for internal gravity waves under the Boussinesq approximation were introduced in Chapter 2. The transport equation representing the chemical in the atmosphere was also presented. The gravity-wave equations as well as the transport equation were all scaled to have nondimensional form.

The analytical and numerical solution of the chemical equation representing a chemical constituent in the atmosphere, with different forms of reaction terms, was discussed in Chapter 3. Whenever it was possible, we derived analytical exact solutions and used approximate asymptotic methods for the more complicated cases. For the case where the source term was only linear, exact solutions are obtained

readily using the method of characteristics. For the case with nonlinear source term represented by Fisher's equation, we found that the well-known travelling-wave solution of Fisher's equation can be generalized for the two-dimensional case as long as the advection is constant.

When the advection speed of the chemical is not constant, as occurs when the chemical is affected by gravity waves, there is no exact solution in closed form. For this case, we used a perturbation method to study the behaviour of the travelling-wave solution. The non-constant advection was represented as a constant plus a small perturbation with amplitude of order $O(\epsilon)$ and in the form of a function of z . The solution to the perturbed equation can then be represented as perturbation series in powers of ϵ . The leading-order term satisfies the unperturbed Fisher's equation with the well-known travelling-wave solution. The solution corresponding to the leading order was found exactly. The first-order solution was approximated asymptotically by the WKB approximation. We concluded that the first-order solution is proportional to the qualitative behaviour of the perturbation of the mean flow. This suggests that the modification in the total solution of the perturbed Fisher's equation is proportional to the behaviour of the perturbed mean flow. This was found to be consistent with the numerical results obtained in Chapter 5 where we observed that the effect of gravity waves on the chemical-mixing ratio is proportional to velocity perturbations of the gravity waves.

The description of the numerical method to solve the chemical-transport equation, as well as numerical results, were given in Chapter 3. The numerical results for Fisher's equation with constant advection were compared with the exact ones and found to be accurate. Numerical results for non-constant advection were given. The numerical form of the first-order approximation $C^{(1)}(x, z)$ was found to satisfy $C^{(1)}(x, z) \rightarrow 0$ as $x \rightarrow \pm\infty$ and is proportional to a Gaussian in the

vertical direction, in agreement with the WKB approximations of $C^{(1)}$. It was also found that, in agreement with the analytical approximations, that the qualitative behaviour of the total solution in the vertical direction follows that of the first-order approximations $C^{(1)}(x, z)$, which takes a form that is similar to the shape of the perturbed wind speed.

Analytical linear and weakly-nonlinear investigations of gravity-wave equations affected by a chemical were carried out in Chapter 4. We started by studying the linearized equations with constant mean flow, then discussed the case where the mean flow is not constant. In both configurations, it was found that the chemical has a considerable effect on gravity waves. This effect was seen to be proportional to the qualitative behaviour of the chemical. In the case of the mean flow with vertical shear, we found that gravity waves have a critical level at which the linearized equation is singular. We observed that the waves are entirely absorbed as they approach the critical level.

The streamfunction mean flow and density mean flow were discussed in Section 4.2. The wave-induced mean flow equation derived in Subsection 4.2.1 implies that the change of the wave-induced mean flow with time is proportional to the change in the momentum flux with respect to the vertical direction. The density mean flow equation is derived in Subsection 4.2.2, and it indicates that heating due to the chemical interacting with gravity waves has a direct impact on the density mean flow. This is consistent with the numerical results obtained in Chapter 6 for different chemicals, where we observed that the zero component of the Fourier spectrum of the density when interacting with the chemical has the greatest effect compared with the corresponding Fourier spectrum of the streamfunction.

The numerical description of the method, as well as numerical solutions of the gravity-wave equations with no chemical, were presented in Section 4.3. The

linear numerical results were found to be consistent with the analytical approximations where the waves were found to be entirely absorbed at the critical level. Nonlinear numerical results showed that propagating waves are reflected at later time, in agreement with nonlinear critical theory. The numerical results of the wave-induced mean flow indicated that it reaches its maximum at the critical level.

Chapter 5 started a description of the numerical method as well as numerical results of the chemical equation with a Gaussian initial condition. We first considered the chemical equation without interaction with gravity waves and studied the effect of the diffusion and the source term where the background wind speed is zero. It was found that the solution advects faster with larger values of diffusion and source term parameters. This kind of behaviour was also confirmed by the travelling-wave-solution case, for which we obtained exact solutions in Chapter 3. To see the effect of gravity waves, we decided to consider small enough values of the diffusion and source term parameters. This was found to agree with the more realistic models that we studied later in Chapter 6.

The effect of gravity waves on the distribution of the chemical was also studied in Chapter 5. In this case we considered nonlinear gravity-wave interactions that generate a gravity-wave perturbation, which then affects the advection and the distribution of the chemical. However, it was assumed that chemical heating effects on the waves could be ignored. The initial background mean flow is considered to be with vertical shear thus leading to a critical level configuration. We found that gravity waves caused a considerable modification of the evolution of the chemical, especially around the critical level. This is due to the effect of the wave-induced mean flow which is maximum at the critical level. The effect of gravity waves on the chemical-mixing ratio was even greater when the parameter ε was considered to

be larger. The modification in the mixing ratio of the chemical due to the effect of gravity waves corresponds to the evolution of the velocity perturbations of gravity waves, as suggested by the analytical approximation in Chapter 3. The effect of wave-induced mean flow was not obtained in the work of Xu et al. (2000), since they considered linear equations for gravity waves. Although our results of the effect of gravity waves on the chemical concentration are in general agreement with the work of Garcia and Solomon (1983) and Xu et al. (2003), we emphasize that our results reflect the effect of the wave-induced mean flow due to the presence of the critical level because of the non-constant mean flow, whereas the aforementioned studies considered constant mean flow, so no critical level was present in their investigations.

The fully coupled model representing the interaction of gravity waves with specific chemical constituents was considered in Chapter 6. The chemicals studied were ozone, water vapour and chlorine monoxide. The initial distribution of these chemicals was specified following the observational study by Gille and Lyjak (1986), where the initial profile of each of these chemical is shown in Figure 1 of Gille and Lyjak (1986) and is determined based on observational data. Before we study the interaction of these chemicals with gravity waves, we started by considering the effect of a steady-state chemical on gravity waves. This corresponds to a configuration where gravity waves are affected by the chemical heating of a chemical that does not change with time. Comparing the solutions of gravity waves with and without the effect of the steady-state chemical, we found that gravity waves are greatly influenced. Fourier spectrum figures of the streamfunction and density shows that most of the effect is around the zero wavenumber components.

As a fully coupled model, we studied the interaction between time-dependent ozone and gravity waves. The evolution of ozone was found to be affected by grav-

ity waves as we already concluded from Chapter 5. The effect of gravity waves on the mixing ratio of ozone was found to be proportional to the velocity perturbation of gravity waves as suggested by the analytical investigation in Chapter 3. Gravity waves, on the other hand, are greatly affected by the time-dependent ozone especially around the critical level where it is centred. The effect of ozone on gravity waves was observed to be corresponding with the mixing ratio of ozone as it evolves with time. This is consistent with the analytical observations obtained in Chapter 4. In addition to the effect around the zero wavenumber component, ozone was found to be affecting the forcing wavenumbers

Comparing with the steady-state simulations, we found from the Fourier spectrum of the density for the time-dependent case that the zero wavenumber component reaches its maximum, whereas this was not true for the corresponding steady-state spectrum. This is consistent with the analytical equation of the wave-induced mean density (4.81) derived in Subsection 4.2.2. From (4.81), we find that, in the steady-state case, the dominant term $\frac{\partial C}{\partial t} = 0$, so the zero wavenumber component in Fourier spectrum of density is small, whereas in the time-dependent case $\frac{\partial C}{\partial t} \neq 0$, so the zero-wavenumber component reaches its maximum. We also found that the zero wavenumber component of the streamfunction spectrum is not affected by the chemical as in the corresponding case of the zero wavenumber component of the density. This is in agreement with the analytical equation of the wave-induced mean streamfunction (4.73), derived in Subsection 4.2.1, where we note that the effect of the chemical forcing does not appear in (4.73), and hence no direct effect of the chemical on the zero wavenumber component of the streamfunction spectrum.

The interaction of gravity waves with the time-dependent water vapour was discussed in Section 6.2. The mixing ratio of water vapour was centred at a lower

level, and its evolution was found to be dominated by the background mean flow. The effect of water vapour on gravity waves was observed to be less compared with the case of ozone. This suggests that the chemical has a greater influence when it interacts with gravity waves at its critical level. This also indicates that a configuration of gravity waves with a critical level has a significant effect compared with that without a critical level.

The interaction of gravity-wave equations with a chemical modelled by a nonlinear continuity equation was discussed in Section 6.3. The nonlinear equation representing the chemical was represented by Fisher's equation as well as a similar equation representing chlorine monoxide. It was found that the evolution of the chemical modelled by Fisher's equation is not damping with time as in the case of ozone, water vapour and chlorine monoxide. The effect of Fisher's equation on gravity waves was found to be much greater compared with the other chemicals. This effect was even more significant with a larger reaction parameter, which would lead to less effect in the case of other chemicals as a result of the greater damping.

The numerical simulations for the interaction of gravity waves with chlorine monoxide, which has a continuity equation that is similar to Fisher's equation, show that more effect on gravity waves can be seen at early time results compared to later time ones. Comparing the early time effect of chlorine monoxide on gravity waves with that corresponding to the effect of Fisher's equation on gravity waves, we noted that the effect is much apparent in chlorine monoxide simulations. However, at later time, we find that the effect resulting from the interaction of gravity waves with Fisher's equation is much greater than that resulting from the interaction of chlorine monoxide with gravity waves. This due to the fact that chlorine monoxide is damping with time.

Overall, with all of these simulations corresponding to the interaction of gravity waves with different chemicals, we found that gravity waves are always affected when they interact with chemicals. This effect is significant when the chemical interacts with gravity waves at the critical level. In addition, chemical concentration modelled by an equation that has a nonlinear source term, as in the case of Fisher’s equation, has a greater effect on gravity waves compared to that with a linear source term.

7.2 Discussion

The effects of chemical concentrations on the gravity waves were already observed by Leovy (1966), Zhu and Holton (1986) and Xu (1999). However, these investigations considered different types of waves and were based on linear representations of the wave equations. Also, they considered constant background mean flow; thus there was no critical level in their configuration. In our simulations, we considered the full nonlinear equations and considered mean flow with vertical shear and thus a configuration with critical level. We found that the nonlinearity of gravity waves and the presence of a critical level has a great influence on the wave-induced mean flow, leading to more effect on the chemical as the waves propagate and the effect of the nonlinearity increased. The larger effect of the nonlinearity leads to a larger effect on the distribution of the chemical. This ultimately leads to more effects on gravity waves due to the chemical heating. Therefore, the nonlinearity as well as the configuration with non-constant mean flow play vital role in the investigation of gravity waves with chemicals in the atmosphere.

As discussed in Chapter 1, it is important to represent gravity waves correctly in atmospheric climate- and weather-prediction models, but, because they are of relatively small scale, it is numerically expensive to model them accurately using

the grid spacing and time steps sizes that models use. Hence we need parameterization schemes. Parameterization schemes are based on analytical expressions for the wave drag based on weakly-nonlinear theories and analysis, as shown in Section 4.2. Here we have taken into account the effects of different chemicals present in localized areas of the atmosphere and examined how the presence of the chemicals affects the gravity-wave structure. We also investigated how the gravity-wave interactions with the background flow affect the chemical transport. We studied the coupling between dynamics (represented by the gravity-wave equations) and chemistry (represented by the chemical-transport equation) and examined the differences in the effects of different chemicals. The information obtained could be taken into account in a parameterization scheme.

Gravity-wave drag obtained in parameterization schemes follows from the weakly-nonlinear analysis. From the weakly-nonlinear analysis discussion in Section 4.2, we obtained the wave-induced mean flow equation (4.74) which has the form

$$\frac{\partial}{\partial t} \bar{u}_0 = \frac{\varepsilon^2}{L} \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right) = X(z, t). \quad (7.1)$$

Gravity-wave drag $X(z, t)$ affects the mean flow velocity. In our model, $X(z, t)$ includes the effect of localized chemical heating. Gravity-wave drag force $X(z, t)$ can be obtained by substituting for the functions ψ_z and ψ_x and then evaluating the integral. The streamfunction $\psi(x, z)$ was already approximated in Section 4.1 and it is given by (4.41) for the configuration where the background mean flow is constant, and by (4.58) for the case where the mean flow is with a vertical shear. This form of gravity-wave drag which includes the effect of chemical heating can help to resolve some of the issues associated with the Climate Chemistry Models (CCMs) and Climate Transport Models (CTMs) and eventually improve CCMs and CTMs.

7.3 Future work

In this section we discuss some of the possible future projects that can be considered in relation to what we have done in the thesis. These include, for example:

More than one chemical:

In this thesis we considered a configuration where only one chemical is present and followed Brasseur and Solomon (1984) to obtain continuity equations for the chemicals we considered. As a second step, we could consider chemical transport equations with more than one chemical. This can be either in uncoupled form, where chemicals do not interact with each other, but present in the same region of the atmosphere, or in a coupled form where chemicals are present in the same region and interact with each other. From the equations shown by Brasseur and Solomon (1984), we could consider chemicals that can be considered together to give a reasonable mathematical model. For example, we could consider a set of chemicals that absorb solar radiation and hence release heating that could have an impact on gravity waves.

More realistic chemical profile:

In this thesis, Gaussian profiles were used for easier comparison with analyses. We could consider a more realistic profile for the chemical distribution based on observations studies such as Gille and Lyjak (1986). With the more realistic initial profile, we could then repeat the simulations in Chapter 6 to see the difference compared to the current results.

More realistic profile for the background temperature (density) and velocity:

We considered background mean flow that has the form $\bar{u} = \tanh(z - 5)$. This corresponds to a configuration where the wind advects to the left (south) near the ground and to the right (north) at higher levels and changes direction at the critical level. Based on observations, there could be more realistic profiles for the background temperature (density) and velocity. We could then repeat numerics with these new profile to see the changes. Also, in our simulations, we considered $c = 0$ for the gravity-wave packet. Instead, we could have a lower boundary condition of the form $e^{ik(x-ct)}$ with nonzero c . Then the critical level would be at $\bar{u} = c$ and could consider the more realistic $\bar{u}$ with c chosen so that we still have a critical level at some level.

More realistic model for the gravity waves:

Instead of Boussinesq approximation that we used in the thesis, where $\bar{\rho}$ is treated like a constant except in the terms involving the gravitational force “g”, we could use the anelastic approximation. Illustration of the anelastic approximation can be found, for example in Sutherland (2010). Sayed and Campbell (2018) derived gravity-wave equations under the anelastic approximation. Under the anelastic approximation, $\bar{\rho}$ is written as a function of z everywhere. This gives a better approximation where the gravity-wave amplitude increases with altitude as a result of the density decrease with altitude. We can then study wave breaking and other effects that are included in the parameterization schemes.

Gravity-wave drag parameterization:

Parameterization schemes are based on (4.74) and (4.81) with different analytical expressions used for the forcing terms on the right hand-side of these equations. In our model, these terms include the effect of the chemical. We could take a well-known parameterization scheme like some of the ones mentioned in Campbell and Shepherd (2005a,b) and add in the effect of a localized chemical. The terms to add would depend on the chemical, e.g. in the troposphere we add H_2O , in the stratosphere add O_3 , and so on.

More accurate numerical schemes:

In this thesis, we used many well-known schemes for gravity-wave equations as well as the chemical-transport equation and we obtained good results. However, we could explore more accurate numerical methods which are more accurate but not computationally expensive. This could be considering methods that deal with the spatial discretization more accurately. This also include considering more accurate methods with respect to time discretization. We could consider more accurate methods where the source term is computed with implicit or semi-implicit schemes, especially if the source term represents several chemicals. In this case, we could also consider the operator splitting approach which is commonly used in atmospheric chemistry. As illustrated by Brasseur and Jacob (2017), the idea behind the approach is to split the chemical-transport equation into two operators: the advection diffusion operator and the source term operator as

$$\begin{aligned}\frac{\partial C^*}{\partial t} &= A_{dv} C^* + D_f C^* \quad \text{with } C^*(0) = C(0), \\ \frac{\partial C^{**}}{\partial t} &= S(C^{**}) \quad \text{with } C^{**}(0) = C^*(\Delta t),\end{aligned}\tag{7.2}$$

on the interval $[0, \Delta t]$, where A_{dv} and D_f are the differential operators of advection and diffusion. Then the results obtained for C^{**} represent the solution C at the time step Δt . The process is repeated over each time step until the maximum desired time is reached.

Appendix A

Conservation laws

The equations for conservation of mass, momentum and energy are considered to be the fundamental equations in fluid dynamics. In this section, both the integral and the differential forms of these equations are derived based on the conservation laws of mass, momentum and energy following Anderson Jr (2010).

A.1 Conservation of mass

Consider a two-dimensional region, A , within a three-dimensional flow field flowing through A , and consider velocity component u_n normal to A . In time dt , the fluid going through A is $u_n dt$, which is the distance travelled by a fluid particle. The volume of fluid passing through A , in time dt is $u_n dt$ multiplied by the area A given as

$$\text{Volume} = (u_n dt)A.$$

The mass inside this volume is

$$\text{Mass} = \rho(\mathbf{x}, t)(u_n dt)A,$$

where $\rho(\mathbf{x}, t)$ is the density of the fluid. The mass flow is then given as

$$m = \frac{\rho(\mathbf{x}, t)(u_n dt)A}{dt} = \rho(\mathbf{x}, t)u_n A.$$

The mass flow per unit area gives the so-called *mass flux*, so we have

$$\text{Mass flux} = \frac{m}{A} = \rho(\mathbf{x}, t) u_n,$$

provided that A is perpendicular to the direction of flow velocity $\mathbf{u}$.

Consider now a fixed control volume V and a control surface S . Based on the physical principle that says mass can neither be created nor destroyed, we find that the net mass that flows out of the control volume through the surface equals the time rate of decrease of mass inside the control volume. Based on the previous discussion of mass flow, we note that the elemental mass flow throughout the area dS is $\rho u_n dS = \rho \mathbf{u} \cdot \mathbf{dS}$, where $\mathbf{dS}$ is the vector elemental surface area. The net mass flow out of the whole control surface S is then given as

$$\iint_S \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{dS}.$$

From the definition of mass, we find that mass inside the elemental volume dV is given as ρdV , the overall mass within the control volume V is given as

$$\iiint_V \rho(\mathbf{x}, t) dV,$$

and a decrease of mass over time within the control volume V is expressed as

$$-\frac{\partial}{\partial t} \iiint_V \rho dV.$$

Therefore, we have

$$\iint_S \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{dS} = -\frac{\partial}{\partial t} \iiint_V \rho(\mathbf{x}, t) dV,$$

which is called the continuity equation in integral form (for a fixed control volume).

Now, since the control volume is fixed, then so are the end limits of the volume integral. Thus, the time derivative can be brought inside the volume integral

$$\iint_S \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{dS} + \iiint_V \frac{\partial}{\partial t} \rho(\mathbf{x}, t) dV = 0. \quad (\text{A.1})$$

To derive the differential form of the continuity equation, the divergence theorem is applied to yield

$$\iint_S \rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t) \cdot \mathbf{dS} = \iiint_V \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) dV.$$

Substituting this into equation (A.1) yields

$$\iiint_V [\nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) + \frac{\partial}{\partial t} \rho(\mathbf{x}, t)] dV = 0. \quad (\text{A.2})$$

Assuming ρ and $\mathbf{u}$ are continuous functions of $\mathbf{x}$ everywhere in the volume V , equation (A.2) equals zero only if the integrand equals zero, so we get

$$\frac{\partial}{\partial t} \rho(\mathbf{x}, t) + \nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) = 0, \quad (\text{A.3})$$

which is the continuity equation in differential form. This can be written in terms of total derivative or Lagrangian derivative, which is defined by Kundu et al. (2012) as

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla). \quad (\text{A.4})$$

Thus the total derivative of the fluid density is given as

$$\frac{D\rho(\mathbf{x}, t)}{Dt} = \frac{\partial\rho(\mathbf{x}, t)}{\partial t} + \mathbf{u}(\mathbf{x}, t) \cdot \nabla\rho. \quad (\text{A.5})$$

Since ρ is a scalar function and $\mathbf{u}(\mathbf{x}, t)$ is a vector, then, based on vector identities, the second term in the left-hand side of (A.3), the divergence term, can be rewritten as

$$\nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) = \mathbf{u}(\mathbf{x}, t) \cdot \nabla\rho(\mathbf{x}, t) + \rho(\mathbf{x}, t) (\nabla \cdot \mathbf{u}(\mathbf{x}, t)). \quad (\text{A.6})$$

Based on equations (A.5), and (A.6), the continuity equation (A.3) can be rewritten as

$$\frac{1}{\rho(\mathbf{x}, t)} \frac{D\rho(\mathbf{x}, t)}{Dt} + \nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0. \quad (\text{A.7})$$

If the density of the fluid is constant, the total derivative $\frac{D\rho}{Dt}$ is zero, so equation (A.7) reduces to

$$\nabla \cdot \mathbf{u}(\mathbf{x}, t) = 0, \quad (\text{A.8})$$

which is the continuity equation for incompressible flow, whether steady or not. In the case of steady flow, however, equation (A.3) will then have the form

$$\nabla \cdot (\rho(\mathbf{x}, t) \mathbf{u}(\mathbf{x}, t)) = 0.$$

A.2 Conservation of momentum

Newton's second law can be expressed as $F = m\mathbf{a}$, where F is the force applied on a body, m is the mass of the body and $\mathbf{a}$ is its acceleration. In terms of the momentum of a body with a mass m and a velocity $\mathbf{u}$, the force can be expressed

as

$$F = \frac{d}{dt}(m\mathbf{u}). \quad (\text{A.9})$$

Before proceeding with the derivation of momentum equation, we first explore the left-hand side of (A.9), the force F applied on the fluid. Such force can be a result of:

- Body forces: Defined as a force that acts on every part of the volume of the body. Examples include gravity and electromagnetic forces.
- Surface forces: Defined as a force that acts directly on the boundary of the body. Examples are pressure and shear-stress forces.

Denoting a body force per unit mass applied on the fluid within the control volume V as $\mathbf{g}$, the body force acting on the elemental volume dV is then given as $\rho\mathbf{g}dV$. The body force applied on the fluid within the control volume is then given as

$$\text{Body force} = \iiint_V \rho\mathbf{g} dV.$$

For the surface force, consider first the pressure p acting on an elemental area dS , so the elemental pressure force is given as $(-p\mathbf{dS})$, where the negative sign occurs because the force has opposite direction to $\mathbf{dS}$. The total pressure force acting across the control surface is then given as

$$\text{Pressure force} = - \iint_S p \mathbf{dS}.$$

Pressure is not the only surface force that should be considered. Shear stress and other types of viscous stresses should also be considered in the case of viscous flow. Denoting such viscous forces as $\mathbf{F}_{\text{visc}}$, the total forces F given in the left-hand side

of equation (A.9) can be expressed as

$$F = \text{Body force} + \text{Pressure force} + \mathbf{F}_{\text{visc}} = \iiint_V \rho \mathbf{g} dV - \iint_S p \mathbf{dS} + \mathbf{F}_{\text{visc}}. \quad (\text{A.10})$$

Now we discuss the right-hand side of equation (A.9), the change in momentum with respect to time. A change in momentum of the fluid can be thought of as the total of the net flow of momentum out the fixed control volume through the surface S , denoted as M_s , and the change in momentum with respect to time inside the fixed control volume, denoted as M_{in} . Since the mass flow through the elemental area dS is given as $(\rho \mathbf{u} \cdot \mathbf{dS})$, the flow of momentum through dS is then $(\rho \mathbf{u} \cdot \mathbf{dS})\mathbf{u}$, and hence the net flow of momentum (M_s) is

$$M_s = \iint_S (\rho \mathbf{u} \cdot \mathbf{dS})\mathbf{u}.$$

For the momentum within the control volume V , since the momentum of the fluid in terms of the elemental volume is $(\rho dV)\mathbf{u}$, the change in momentum with respect to time inside the control volume is

$$M_{in} = \frac{\partial}{\partial t} \iiint_V \rho \mathbf{u} dV.$$

Adding M_s and M_{in} , we obtain the right side of equation (A.9), so

$$\frac{d}{dt}(m\mathbf{u}) = M_s + M_{in} = \iint_S (\rho \mathbf{u} \cdot \mathbf{dS})\mathbf{u} + \frac{\partial}{\partial t} \iiint_V \rho \mathbf{u} dV. \quad (\text{A.11})$$

Combining equations (A.10) and (A.11) in terms of equation (A.9), we obtain

$$\iint_S (\rho \mathbf{u} \cdot dS)\mathbf{u} + \frac{\partial}{\partial t} \iiint_V \rho \mathbf{u} dV = \iiint_V \rho \mathbf{g} dV - \iint_S p \mathbf{dS} + \mathbf{F}_{\text{visc}}, \quad (\text{A.12})$$

which is the equation of conservation of momentum of the fluid in integral form. Taking into account that the control volume is fixed, the derivative with respect to time in the previous equation can be brought inside the integral, so we have

$$\iint_S (\rho \mathbf{u} \cdot d\mathbf{S}) \mathbf{u} + \iiint_V \frac{\partial}{\partial t} (\rho \mathbf{u}) dV = \iiint_V \rho \mathbf{g} dV - \iint_S p d\mathbf{S} + \mathbf{F}_{\text{visc}}. \quad (\text{A.13})$$

Equation (A.13) can be expressed in terms of scalar equations. Provided that the velocity vector given as $\mathbf{u} = \mathcal{U}\mathbf{i} + \mathcal{V}\mathbf{j} + \mathcal{W}\mathbf{k}$, the x component of equation (A.13) is

$$\iint_S (\rho \mathbf{u} \cdot d\mathbf{S}) \mathcal{U} + \iiint_V \frac{\partial}{\partial t} (\rho \mathcal{U}) dV = \iiint_V \rho g_x dV - \iint_S p d\mathbf{S} + (F_x)_{\text{visc}}. \quad (\text{A.14})$$

To obtain the differential form of the momentum equation, we apply the divergence theorem to the terms with surface integrals, so we have

$$\iint_S p d\mathbf{S} = \iiint_V \nabla p dV,$$

and

$$\iint_S (\rho \mathbf{u} \cdot d\mathbf{S}) \mathcal{U} = \iiint_V \nabla \cdot (\rho \mathbf{u} \mathcal{U}) dV.$$

Substituting that into equation (A.14), we obtain

$$\iiint_V \left[\nabla \cdot (\rho \mathbf{u} \mathcal{U}) + \frac{\partial}{\partial t} (\rho \mathcal{U}) - \rho g_x + \frac{\partial p}{\partial x} - (\mathcal{F}_x)_{\text{visc}} \right] dV = 0,$$

where $(\mathcal{F}_x)_{\text{visc}}$ is a suitable form of $(F_x)_{\text{visc}}$ to be placed inside the integral. Assuming that all fluid properties ρ , $\mathbf{u}$, $\mathbf{g}$, p , $(\mathcal{F}_x)_{\text{visc}}$ are continuous functions of $\mathbf{x}$ everywhere in the volume V , this leads to

$$\frac{\partial}{\partial t} (\rho \mathcal{U}) + \nabla \cdot (\rho \mathbf{u} \mathcal{U}) = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{\text{visc}}. \quad (\text{A.15})$$

Similarly, for the y and z components of the velocity, we have

$$\frac{\partial}{\partial t}(\rho \mathcal{V}) + \nabla \cdot (\rho \mathbf{u} \mathcal{V}) = \rho g_y - \frac{\partial p}{\partial y} + (\mathcal{F}_y)_{visc}, \quad (\text{A.16})$$

and

$$\frac{\partial}{\partial t}(\rho \mathcal{W}) + \nabla \cdot (\rho \mathbf{u} \mathcal{W}) = \rho g_z - \frac{\partial p}{\partial z} + (\mathcal{F}_z)_{visc}. \quad (\text{A.17})$$

Equations (A.15), (A.16) and (A.17) are the scalar equations of the conservation of momentum of the fluid in differential form. These equations are usually referred to as the *Navier–Stokes equations*. Equations (A.15), (A.16) and (A.17) can be expressed in terms of the total derivative notation. Considering the x -component, equation (A.15), we note that the first term on the left-hand side of equation (A.15) can be written as

$$\frac{\partial}{\partial t}(\rho \mathcal{U}) = \rho \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \frac{\partial \rho}{\partial t},$$

whereas the second term on left side of equation (A.15) can be expressed as

$$\nabla \cdot (\rho \mathbf{u} \mathcal{U}) = \mathcal{U} \nabla \cdot (\rho \mathbf{u}) + \nabla \mathcal{U} \cdot (\rho \mathbf{u}).$$

Substituting theses two expressions into equation (A.15), we get

$$\rho \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \frac{\partial \rho}{\partial t} + \mathcal{U} \nabla \cdot (\rho \mathbf{u}) + \nabla \mathcal{U} \cdot (\rho \mathbf{u}) = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (\text{A.18})$$

Rearranging, we obtain

$$\rho \frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \right) + \nabla \mathcal{U} \cdot (\rho \mathbf{u}) = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (\text{A.19})$$

We then note that, in the second term of the left side of the previous equation, we have the continuity equation multiplied by the scalar function $\mathcal{U}$, so this term will vanish, and we are left with

$$\rho \frac{\partial \mathcal{U}}{\partial t} + \nabla \mathcal{U} \cdot (\rho \mathbf{u}) = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (\text{A.20})$$

Rearranging, we obtain

$$\rho \left(\frac{\partial \mathcal{U}}{\partial t} + \nabla \mathcal{U} \cdot \mathbf{u} \right) = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (\text{A.21})$$

From the definition of total derivative, we have

$$\frac{D\mathcal{U}}{Dt} = \frac{\partial \mathcal{U}}{\partial t} + \mathbf{u} \cdot \nabla \mathcal{U},$$

so equation (A.21) is simplified to

$$\rho \frac{D\mathcal{U}}{Dt} = \rho g_x - \frac{\partial p}{\partial x} + (\mathcal{F}_x)_{visc}. \quad (\text{A.22})$$

Similarly, for the y and z components, we have

$$\rho \frac{D\mathcal{V}}{Dt} = \rho g_y - \frac{\partial p}{\partial y} + (\mathcal{F}_y)_{visc}, \quad (\text{A.23})$$

$$\rho \frac{D\mathcal{W}}{Dt} = \rho g_z - \frac{\partial p}{\partial z} + (\mathcal{F}_z)_{visc}. \quad (\text{A.24})$$

A.3 Conservation of energy

The energy equation is mainly important for compressible flow since, for incompressible flow, ρ is constant, and hence the continuity and momentum equations

will be in terms of two variables. Therefore, for incompressible flow, the continuity and momentum equations represent a system of two equations in two unknowns, p and $\mathbf{u}$, so it is sufficient to work with such system.

Following the same approach in the previous two sections, we start with a physical principle that says: “Energy can neither be destroyed or created; it can only change in form.”

Consider a system defined as a determined amount of matter filling a closed boundary. Based on the physical principle, the first law of thermodynamics is given as

$$\partial q + \partial w = d e . \quad (\text{A.25})$$

where ∂q measures how much heat is added to the system from the surroundings, ∂w is the work done on the system by the surroundings, and $d e$ is the change in the internal energy of the system. Applying this law to a fixed control volume with fluid passing by, we have

$$A_1 + A_2 = A_3 , \quad (\text{A.26})$$

where A_1 measures the average of the heat added to the fluid in the control volume from the surroundings, A_2 is the average of the work done on the fluid within the control volume and A_3 is rate of change of energy of the fluid flowing within the control volume.

Let $\mathbf{q}$ represent the heat flux vector added to the control volume per unit area. The rate of heat outflow is represented as $\mathbf{q} \cdot \mathbf{dS}$, and we have

$$A_1 = - \iint_S \mathbf{q} \cdot \mathbf{dS} + Q_{chemical} + Q_{visc}, \quad (\text{A.27})$$

where the negative sign is present because the direction of $\mathbf{dS}$. The quantity

$Q_{chemical}$ represents the rate of heat added to the flow within the control volume due to the effect of a chemical, and the quantity Q_{visc} represents the rate of heat added to the flow within the control volume by the effect of viscosity.

The work done on a fluid within a control volume is composed of the sum of the pressure force, the body force and the viscous force. Starting with the pressure force, since the rate of work done on a moving object is represented by the product of the velocity of the object $\mathbf{u}$ and its parallel force component, we then have

$$F_1 = - \iint_S (p \mathbf{dS}) \cdot \mathbf{u} ,$$

where F_1 is the rate of work done on the fluid due to the pressure force on the control surface S and $(-p \mathbf{dS})$ represents the pressure force on the elemental area dS .

For the work done on a fluid due to a body force, let $\mathbf{g}$ represent a body force per unit mass; the rate of work done on dV (the elemental volume) as a result of the body force is then $(\rho \mathbf{g} dV) \cdot \mathbf{u}$. It follows that, on the whole control volume, we have

$$F_2 = \iiint_V (\rho \mathbf{g} dV) \cdot \mathbf{u} ,$$

where F_2 is the rate of work done on the fluid due to the body forces. Finally, let W_{visc} represent the rate of work done on fluid due to viscosity effects. Then the rate of total work done on fluid within the control volume, A_2 , is given as

$$A_2 = \iiint_V \rho (\mathbf{g} \cdot \mathbf{u}) dV - \iint_S p \mathbf{u} \cdot \mathbf{dS} + W_{visc} . \quad (\text{A.28})$$

Since the total energy per unit mass for the fluid moving within the control volume

is given as $e + \frac{|\mathbf{u}|^2}{2}$, we have

$$E_1 = \iint_S (\rho \mathbf{u} \cdot \mathbf{dS}) \left(e + \frac{|\mathbf{u}|^2}{2} \right),$$

where E_1 is the net rate of flow of total energy across the control surface S and $(\rho \mathbf{u} \cdot \mathbf{dS})$ is the elemental mass flow across dS . Since the total energy within an elemental volume dV is $\rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) dV$, the total energy inside the whole control volume is then given as

$$\iiint_V \rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) dV.$$

We then have

$$E_2 = \frac{\partial}{\partial t} \iiint_V \rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) dV,$$

where E_2 is the time rate of change of total energy inside the control volume V . Therefore the rate of change of energy of fluid flowing within the control volume, A_3 , is given as

$$A_3 = \iint_S (\rho \mathbf{u} \cdot \mathbf{dS}) \left(e + \frac{|\mathbf{u}|^2}{2} \right) + \frac{\partial}{\partial t} \iiint_V \rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) dV. \quad (\text{A.29})$$

Substituting the expressions for A_1 , A_2 and A_3 into equation (A.26), we obtain the energy equation in integral form. Applying the divergence theorem, we obtain

$$\begin{aligned} \frac{\partial}{\partial t} \left(\rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) \right) + \nabla \cdot \left(\rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) \mathbf{u} \right) &= \nabla \cdot \mathbf{q} - \nabla \cdot (p\mathbf{u}) + \rho(\mathbf{g} \cdot \mathbf{u}) + \mathcal{W}_{visc} \\ &\quad + \mathcal{Q}_{chemical} + \mathcal{Q}_{visc}, \end{aligned} \quad (\text{A.30})$$

which is the energy equation in differential form. In terms of the total derivative,

equation (A.30) can be written, ignoring viscous effect, as

$$\rho \frac{D}{Dt} \left(e + \frac{|\mathbf{u}|^2}{2} \right) = \nabla \cdot \mathbf{q} - \nabla \cdot (p\mathbf{u}) + \rho(\mathbf{g} \cdot \mathbf{u}) + \mathcal{Q}_{chemical}. \quad (\text{A.31})$$

In the case of steady-inviscid flow with no heat addition and in the absence of body forces, equation (A.30) simplifies to

$$\nabla \cdot \left(\rho \left(e + \frac{|\mathbf{u}|^2}{2} \right) \mathbf{u} \right) = -\nabla \cdot (p\mathbf{u}) . \quad (\text{A.32})$$

Appendix B

Boussinesq approximation

The Boussinesq approximation is often applied in compressible fluid applications in order to simplify the basic equations. This approximation is considered appropriate under certain conditions as discussed by Spiegel and Veronis (1960). Boussinesq (1903) proposed that the perturbation density is very small and thus can be ignored in the fluid equations except if it is combined with gravity. He also suggested that the change in density with respect to pressure is negligible compared to the change in density with respect to temperature. In this section, we apply the Boussinesq approximation to the continuity equation (A.3), the momentum equations (A.22) and (A.24) and the energy equation (A.31), following Kundu et al. (2012). The density and pressure are often expressed in atmospheric applications involving waves as

$$\rho(\mathbf{x}, t) = \rho_0 + \tilde{\rho}(\mathbf{x}, t), \text{ and } p(\mathbf{x}, t) = p_0 + \tilde{p}(\mathbf{x}, t), \quad (\text{B.1})$$

where ρ_0 is the background density and p_0 is the background pressure; $\tilde{\rho}$ and $\tilde{p}$ are the perturbation density and pressure, respectively. The perturbation quantities represent the waves, which are considered to be small amplitude fluctuations in

the background fluid flow. Taking this into account, the continuity equation (A.3) becomes

$$\frac{\partial}{\partial t} (\rho_0 + \tilde{\rho}(\mathbf{x}, t)) + \nabla \cdot ((\rho_0 + \tilde{\rho}(\mathbf{x}, t)) \mathbf{u}(\mathbf{x}, t)) = 0, \quad (\text{B.2})$$

and the vector form of momentum equations (A.22) and (A.24) become

$$(\rho_0 + \tilde{\rho}) \frac{D\mathbf{u}}{Dt} = -\nabla \tilde{p} + \tilde{\rho} \mathbf{g} + \mu \nabla^2 \mathbf{u}, \quad (\text{B.3})$$

where the body force in the atmosphere is considered to be the gravitational force $\mathbf{g} = (0, 0, -g)$; and $\nabla p_0 = \rho_0 \mathbf{g}$.

We consider a two-dimensional configuration in terms of the horizontal x and the vertical direction z . Under the Boussinesq approximation, the continuity equation is reduced to

$$\nabla \cdot \mathbf{u} = 0, \quad (\text{B.4})$$

and the momentum equation (B.3), in terms of two dimensions x and z , becomes

$$\rho_0 \frac{D\mathcal{U}}{Dt} = -\frac{\partial \tilde{p}}{\partial x} + \mu \nabla^2 \mathcal{U} \quad (\text{B.5})$$

$$\rho_0 \frac{D\mathcal{W}}{Dt} = -\tilde{\rho} g - \frac{\partial \tilde{p}}{\partial z} + \mu \nabla^2 \mathcal{W}. \quad (\text{B.6})$$

Dividing by ρ_0 , we obtain

$$\frac{\partial \mathcal{U}}{\partial t} + \mathcal{U} \frac{\partial \mathcal{U}}{\partial x} + \mathcal{W} \frac{\partial \mathcal{U}}{\partial z} = -\frac{1}{\rho_0} \frac{\partial \tilde{p}}{\partial x} + \nu \nabla^2 \mathcal{U} \quad (\text{B.7})$$

$$\frac{\partial \mathcal{W}}{\partial t} + \mathcal{U} \frac{\partial \mathcal{W}}{\partial x} + \mathcal{W} \frac{\partial \mathcal{W}}{\partial z} = -\frac{1}{\rho_0} \tilde{\rho} g - \frac{1}{\rho_0} \frac{\partial \tilde{p}}{\partial z} + \nu \nabla^2 \mathcal{W}, \quad (\text{B.8})$$

where $\nu = \frac{\mu}{\rho_0}$ is the kinematic viscosity. To write the previous two equations in

terms of one equation, we define the streamfunction $\Psi(x, z, t)$ such that

$$\mathcal{U} = -\Psi_z \text{ and } \mathcal{W} = \Psi_x, \quad (\text{B.9})$$

where the subscripts denote the partial derivatives. Equations (B.7) and (B.8) can then be rewritten as

$$-\Psi_{zt} + \Psi_z \Psi_{zx} - \Psi_x \Psi_{zz} = -\frac{1}{\rho_0} \frac{\partial \tilde{p}}{\partial x} - \nu \nabla^2 \Psi_z \quad (\text{B.10})$$

$$\Psi_{xt} - \Psi_z \Psi_{xx} + \Psi_x \Psi_{xz} = -\frac{1}{\rho_0} \tilde{\rho} g - \frac{1}{\rho_0} \frac{\partial \tilde{p}}{\partial z} + \nu \nabla^2 \Psi_x. \quad (\text{B.11})$$

In order to cancel the pressure term as we combine the previous two equations, we differentiate the first one with respect to z and the second one with respect to x to get

$$-\Psi_{zzt} + \Psi_{zz} \Psi_{zx} + \Psi_{zzx} \Psi_z - (\Psi_x \Psi_{zzz} + \Psi_{xz} \Psi_{zz}) = -\frac{1}{\rho_0} \left(\frac{\partial^2 \tilde{p}}{\partial x \partial z} \right) - \nu \nabla^2 \Psi_{zz} \quad (\text{B.12})$$

$$\Psi_{xxt} - (\Psi_{zx} \Psi_{xx} + \Psi_z \Psi_{xxx}) + \Psi_{xx} \Psi_{xz} + \Psi_x \Psi_{xxz} = -\frac{g}{\rho_0} \tilde{\rho}_x - \frac{1}{\rho_0} \left(\frac{\partial^2 \tilde{p}}{\partial z \partial x} \right) + \nu \nabla^2 \Psi_{xx}. \quad (\text{B.13})$$

Subtracting equation (B.12) from equation (B.13), we obtain

$$\Psi_{xxt} + \Psi_{zzt} - \Psi_z (\Psi_{zzx} + \Psi_{xxx}) + \Psi_x (\Psi_{zzz} + \Psi_{xxz}) = -\frac{g}{\rho_0} \tilde{\rho}_x + \nu (\nabla^2 \Psi_{zz} + \nabla^2 \Psi_{xx}), \quad (\text{B.14})$$

which can be written in terms of $\nabla^2 \Psi = \Psi_{xx} + \Psi_{zz}$ as

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \tilde{\rho}_x + \nu \nabla^2 (\nabla^2 \Psi). \quad (\text{B.15})$$

From the definition of vorticity, we have

$$\xi = \nabla \times \mathbf{u} = w_x - u_z = \Psi_{xx} + \Psi_{zz} = \nabla^2 \Psi, \quad (\text{B.16})$$

so equation (B.15) can then be written as

$$\xi_t - \Psi_z \xi_x + \Psi_x \xi_z = -\frac{g}{\rho_0} \tilde{\rho}_x + \nu \nabla^2 \xi. \quad (\text{B.17})$$

Now we study the effect of applying the Boussinesq approximation on the energy equation (A.31). From equation (A.6), equation (A.31) then takes the form

$$\rho \frac{De}{Dt} + \rho \frac{D}{Dt} \left(\frac{|\mathbf{u}|^2}{2} \right) = -\nabla \cdot \mathbf{q} - \mathbf{u} \cdot \nabla p - p \nabla \cdot \mathbf{u} - \rho g w + \rho J, \quad (\text{B.18})$$

where $(\mathbf{g} \cdot \mathbf{u})$ is represented by $-gw$, the gravitational force in the atmosphere. From the momentum equations (A.22), (A.23) and (A.24) we have (ignoring friction)

$$\rho \frac{D\mathbf{u}}{Dt} = \rho \mathbf{g} - \nabla p. \quad (\text{B.19})$$

Multiplying (B.19) by $\mathbf{u}$, we obtain

$$\rho \frac{D}{Dt} \left(\frac{|\mathbf{u}|^2}{2} \right) = -\rho g w - \mathbf{u} \cdot \nabla p. \quad (\text{B.20})$$

Substituting (B.20) into the equation (B.18), we get

$$\rho \frac{De}{Dt} = -p(\nabla \cdot \mathbf{u}) - \nabla \cdot \mathbf{q} + \rho J. \quad (\text{B.21})$$

Although we stated above that, under Boussinesq approximation, the continuity equation reduces to $\nabla \cdot \mathbf{u} = 0$, this should not be applied for the first term in the

right-hand side because otherwise all the effects of the pressure force would be neglected. Instead, from the continuity equation (A.7), we find that

$$-p(\nabla \cdot \mathbf{u}) = \frac{p}{\rho} \frac{D\rho}{Dt}. \quad (\text{B.22})$$

Considering a perfect gas, the density is $\rho = \frac{p}{RT}$, where T is the temperature; $R = C_p - C_v$; and C_p, C_v are the specific heat capacities of constant pressure and volume, respectively. Under Boussinesq approximation, the density is changing slightly with respect to pressure, so the corresponding partial derivative is then ignored, and we have

$$\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial T} \frac{DT}{Dt}. \quad (\text{B.23})$$

Thus equation (B.22) can be rewritten as

$$-p(\nabla \cdot \mathbf{u}) = \frac{p}{\rho} \frac{\partial \rho}{\partial T} \frac{DT}{Dt} = -\frac{p}{\rho} \frac{1}{T^2} \frac{p}{R} \frac{DT}{Dt} = -p \frac{1}{T} \frac{DT}{Dt} = -\rho R \frac{DT}{Dt}. \quad (\text{B.24})$$

Substituting this into equation (B.21), we obtain

$$\rho \frac{De}{Dt} = -\rho R \frac{DT}{Dt} - \nabla \cdot \mathbf{q} + \rho J. \quad (\text{B.25})$$

For a perfect gas, we have $e = C_v T$, so the previous equation becomes

$$\rho C_v \frac{DT}{Dt} = -\rho (C_p - C_v) \frac{DT}{Dt} - \nabla \cdot \mathbf{q} + \rho J, \quad (\text{B.26})$$

which then reduces to

$$\rho C_p \frac{DT}{Dt} = -\nabla \cdot \mathbf{q} + \rho J. \quad (\text{B.27})$$

Applying Fourier's law, which is stated as

$$\mathbf{q} = -k\nabla T , \quad (\text{B.28})$$

on equation (B.27), we get

$$\frac{DT}{Dt} = -\frac{1}{\rho C_p} \nabla \cdot (-k\nabla T) + \frac{J}{C_p} = \kappa \nabla^2 T + \frac{J}{C_p}, \quad (\text{B.29})$$

where $\kappa = \frac{k}{\rho C_p}$ is the thermal diffusivity coefficient. Because of the relation between density and temperature in the perfect gas law, the previous equation can be expressed in terms of the density. In addition to equation (B.1), we also write the temperature in terms of background and perturbation functions, $T = T_0 + \tilde{T}$, where the perturbation quantities $\tilde{\rho}$, $\tilde{p}$ and $\tilde{T}$ are assumed to be much smaller than their corresponding background quantities. From the perfect gas law, we have

$$(p_0 + \tilde{p}) = R(T_0 + \tilde{T})(\rho_0 + \tilde{\rho}). \quad (\text{B.30})$$

Under the Boussinesq approximation, the pressure is almost constant and can be approximated by its background quantity p_0 . From the perfect gas law, we have $p_0 = RT_0\rho_0$, so equation (B.30) becomes

$$RT_0\rho_0 = R(T_0 + \tilde{T})(\rho_0 + \tilde{\rho}), \quad (\text{B.31})$$

which reduces to

$$T_0\rho_0 = T_0\rho_0 + T_0\tilde{\rho} + \tilde{T}\rho_0, \quad (\text{B.32})$$

where the perturbations product term is very small and thus can be neglected.

Rearranging, we get

$$\rho_0 \tilde{T} = -T_0 \tilde{\rho} \quad (\text{B.33})$$

and since $\tilde{T} = T - T_0$, then B.33 is given as

$$T = T_0 \left(1 - \frac{\tilde{\rho}}{\rho_0} \right) = T_0 \left(1 - \frac{\rho}{\rho_0} + 1 \right) = T_0 \left(2 - \frac{\rho}{\rho_0} \right). \quad (\text{B.34})$$

Substituting this into equation (B.29), we obtain

$$-\frac{T_0}{\rho_0} \frac{D\rho}{Dt} = -\kappa \frac{T_0}{\rho_0} \nabla^2 \rho + \frac{J}{C_p}, \quad (\text{B.35})$$

so we have

$$\frac{D\rho}{Dt} = \kappa \nabla^2 \rho - \alpha J. \quad (\text{B.36})$$

where $\alpha = \frac{\rho_0}{T_0 C_p}$. Equation (B.36) can be written as

$$\frac{\partial \rho}{\partial t} + \mathbf{u}(\mathbf{x}, t) \cdot \nabla \rho(\mathbf{x}, t) + \rho \left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right) = \kappa \nabla^2 \rho - \alpha J. \quad (\text{B.37})$$

Under the Boussinesq approximation, $\left(\frac{\partial u}{\partial x} + \frac{\partial w}{\partial z} \right)$ equals zero. In terms of the streamfunction (B.9), equation (B.37) becomes

$$\frac{\partial \rho}{\partial t} - \Psi_z \frac{\partial \rho}{\partial x} + \Psi_x \frac{\partial \rho}{\partial z} = \kappa \nabla^2 \rho - \alpha J. \quad (\text{B.38})$$

Therefore the system of equations under the Boussinesq approximation are given as

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + \nu \nabla^2 (\nabla^2 \Psi) \quad (\text{B.39})$$

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = \kappa \nabla^2 \rho - \alpha J. \quad (\text{B.40})$$

These equations are used as the basis for the gravity waves model derived in Chapter 2.

Appendix C

The WKB approximations

Consider an equation of the form

$$\epsilon^2 Q''(\xi) - P(\xi)Q(\xi) = 0, \quad (\text{C.1})$$

where ϵ is small positive parameter. We derive the Wentzel, Kramers and Brillouin (WKB) approximation following Bender and Orszag (1999). We make use of the WKB approximation in Section 3.2.2.

Equation (C.1) can have a dissipative and/or dispersive behaviour and in both cases, the solution is characterized in exponential form. Thus it is reasonable to represent the solution $Q(\xi)$ as

$$Q(\xi) \sim A(\xi)e^{S(\xi)/\delta}, \quad \delta \rightarrow 0, \quad (\text{C.2})$$

where $A(\xi)$ is the amplitude and $S(\xi)$ is nonconstant function. The approximation (C.2) is commonly referred to as the WKB approximation. According to Bender and Orszag (1999), the form (C.2) is not in an appropriate form to derive asymptotic approximation since the functions $A(\xi)$ and $S(\xi)$ in (C.2) depend implicitly

on δ , so it is more suitable to represent the functions $A(\xi)$ and $S(\xi)$ in a form where the dependence on δ is explicit. This can be done by expanding these functions as asymptotic series in power of δ . These series then can be merged in one exponential power series of the form

$$Q(\xi) \sim \exp \left[\frac{1}{\delta} \sum_{n=0}^{\infty} \delta^n S_n(\xi) \right], \quad \delta \rightarrow 0, \quad (\text{C.3})$$

and we have

$$\begin{aligned} Q' &\sim \left(\frac{1}{\delta} S'_0 + S'_1 + \dots \right) e^{\left(\frac{1}{\delta} S_0 + S_1 + \dots \right)}, \\ Q'' &\sim \left(\frac{1}{\delta} S'_0 + S'_1 + \dots \right)^2 e^{\left(\frac{1}{\delta} S_0 + S_1 + \dots \right)} + \left(\frac{1}{\delta} S''_0 + S''_1 + \dots \right) e^{\left(\frac{1}{\delta} S_0 + S_1 + \dots \right)}. \end{aligned} \quad (\text{C.4})$$

Equation (C.1) can be written in terms of (C.3) and (C.4) as

$$\frac{\epsilon^2}{\delta^2} (S'_0)^2 + 2 \frac{\epsilon^2}{\delta} S'_0 S'_1 + \frac{\epsilon^2}{\delta} S''_0 + \dots = P(\xi). \quad (\text{C.5})$$

The first term $\frac{\epsilon^2}{\delta^2} (S'_0)^2$ is the largest term on the left side of (C.5). Based on the method of dominant balance, the term $\frac{\epsilon^2}{\delta^2} (S'_0)^2$ should have the same magnitude as that of $P(\xi)$ on the right hand side. This implies that δ is proportional to ϵ , so we choose $\delta = \epsilon$. Substituting for $\delta = \epsilon$ in (C.5) and comparing the powers of ϵ , we then obtain

$$(S'_0)^2 = P(\xi), \quad (\text{C.6})$$

and

$$2S'_0 S'_1 = -S''_0. \quad (\text{C.7})$$

Equation (C.6) implies that

$$S_0 = \pm \int \sqrt{P(\xi)} d\xi, \quad (\text{C.8})$$

so equation (C.7) is given as

$$2S'_0S'_1 = \mp \frac{d}{d\xi} \left(\sqrt{P(\xi)} \right), \quad (\text{C.9})$$

which simplifies to

$$S'_1 = \frac{\mp \frac{d}{d\xi} \left(\sqrt{P(\xi)} \right)}{\pm 2\sqrt{P(\xi)}}, \quad (\text{C.10})$$

so that

$$S_1 = -\frac{1}{2} \ln \sqrt{P(\xi)}. \quad (\text{C.11})$$

The approximation $Q(\xi)$ is then given as

$$Q(\xi) \sim e^{(\pm \frac{1}{\epsilon} \int \sqrt{P(\xi)} d\xi - \frac{1}{2} \ln \sqrt{P(\xi)})}, \quad (\text{C.12})$$

which simplifies to

$$Q(\xi) \sim \frac{e^{\pm \frac{1}{\epsilon} \int \sqrt{P(\xi)} d\xi}}{P(\xi)^{\frac{1}{4}}}. \quad (\text{C.13})$$

Thus, if $P(\xi) > 0$ then we have

$$Q(\xi) \sim \frac{e^{\pm \frac{1}{\epsilon} \int \sqrt{P(\xi)} d\xi}}{P(\xi)^{\frac{1}{4}}}, \quad (\text{C.14})$$

on the other hand, if $P(\xi) < 0$ then

$$Q(\xi) \sim \frac{e^{\pm i \frac{1}{\epsilon} \int \sqrt{-P(\xi)} d\xi}}{(-P(\xi))^{\frac{1}{4}}}. \quad (\text{C.15})$$

If $P(\xi) = 0$ for some value of ξ , we then have a turning point at that value of ξ .

When equation (C.1) is not multiplied by a small parameter ε , we then have

$$Q''(\xi) - P(\xi)Q(\xi) = 0. \quad (\text{C.16})$$

In this case, we can still follow the same approach of the WKP method provided that the first term $(S'_0)^2$, in the analogous equation of (C.5) corresponding to (C.16), is larger than the other two terms (S''_0 and $2S'_0S'_1$). Based on the method of dominant balance, this holds if

$$S''_0 \ll (S'_0)^2 \quad (\text{C.17})$$

$$\frac{d}{d\xi} \left(\sqrt{P(\xi)} \right) \ll P \quad (\text{C.18})$$

$$P' \ll P^{\frac{3}{2}} \quad (\text{C.19})$$

and

$$2S'_0S'_1 \ll (S'_0)^2 \quad (\text{C.20})$$

$$-\frac{\frac{d}{d\xi} \left(\sqrt{P} \right)}{\sqrt{P}} \sqrt{P} \ll P \quad (\text{C.21})$$

$$P' \ll P^{\frac{3}{2}} \quad (\text{C.22})$$

which is the same condition given in (C.19). Therefore, the WKB method is valid and can be used to approximate the solution of (C.16) as long as

$$P(\xi)' \ll P(\xi)^{\frac{3}{2}},$$

which holds if

$$\lim_{\xi \rightarrow \xi_0} \frac{P(\xi)'}{P(\xi)^{\frac{3}{2}}} = 0,$$

which means that $P(\xi)$ is a slowly varying function.

Once the condition $P' \ll P^{\frac{3}{2}}$ is satisfied and $P(\xi)$ is slowly varying then, as shown by Nayfeh (2011), we can introduce the slowly varying variable $\nu = \epsilon\xi$ and define $Y(\nu) = Q(\xi)$ and $H(\nu) = P(\xi)$ so that equation (C.16) is rewritten in a

form similar to equation (C.1) as

$$\epsilon^2 Y''(\nu) - H(\nu)Y(\nu) = 0, \quad (\text{C.23})$$

The coefficient $H(\nu)$ determines the form of the asymptotic solution obtained and we have different cases:

if $H(\nu) > 0$ then

$$Y(\nu) \sim \frac{e^{\pm \frac{1}{\epsilon} \int \sqrt{H} d\nu}}{H^{\frac{1}{4}}}. \quad (\text{C.24})$$

If $H(\nu) < 0$ then

$$Y(\nu) \sim \frac{e^{\pm \frac{1}{\epsilon} i \int \sqrt{-H} d\nu}}{(-H)^{\frac{1}{4}}}, \quad (\text{C.25})$$

If $H(\nu) = 0$ at some point $\nu = \nu_0$, then there is a turning point at $\nu = \nu_0$ and in that case we approximate the solution within a small layer around ν_0 and outside this layer the solution takes the form of either (C.25) or (C.24) depending on the sign of $H(\nu)$.

Appendix D

Taylor–Goldstein Equation

In this appendix, we present derivation of the Taylor–Goldstein equation for steady amplitude for linear gravity waves, and present solutions of the equation and discuss the direction of propagation of the solutions using the concept of group velocity.

The linear forms of equations (2.38), (2.39) and (2.40) are given as

$$\zeta_t + \bar{u}\zeta_x - \bar{u}''\psi_x = -\frac{g}{\bar{\rho}}\rho_x, \quad (\text{D.1})$$

$$\zeta = \nabla^2\psi, \quad (\text{D.2})$$

$$\rho_t + \bar{u}\rho_x + \bar{\rho}'\psi_x = 0. \quad (\text{D.3})$$

The functions ψ and ρ can be represented in terms of normal modes given as

$$\psi(x, z, t) = \phi(z)e^{i(kx - \omega t)} + \text{c.c.}, \quad (\text{D.4})$$

$$\rho(x, z, t) = \varrho(z)e^{i(kx - \omega t)} + \text{c.c.}, \quad (\text{D.5})$$

where c.c. denotes the complex conjugate. The amplitude functions $\phi(z)$ and $\varrho(z)$

are complex, and the functions $\psi(x, z, t)$ and $\rho(x, z, t)$ are real. The constant k is the horizontal wavenumber and the constant ω is the frequency. The horizontal phase speed of the waves is $c = \frac{\omega}{k}$. Plugging (D.4) and (D.5) into equations (D.1), (D.2) and (D.3), we have

$$-\omega\zeta + k\bar{u}\zeta - k\bar{u}''\phi + k\frac{g}{\bar{\rho}}\varrho = 0, \quad (\text{D.6})$$

$$\zeta = \nabla^2\psi = (\phi'' - \delta k^2\phi)e^{i(kx - \omega t)}, \quad (\text{D.7})$$

$$(k\bar{u} - \omega)\varrho + k\bar{\rho}'\phi = 0. \quad (\text{D.8})$$

Combining the first two equations, we get

$$(k\bar{u} - \omega)\phi'' - (k\bar{u} - \omega)\delta k^2\phi - k\bar{u}''\phi + k\frac{g}{\bar{\rho}}\varrho = 0. \quad (\text{D.9})$$

Solving (D.8) for ϱ then substituting that into equation (D.9), we obtain

$$(k\bar{u} - \omega)\phi'' - (k\bar{u} - \omega)\delta k^2\phi - k\bar{u}''\phi - k^2\frac{g\bar{\rho}'}{\bar{\rho}(k\bar{u} - \omega)}\phi = 0. \quad (\text{D.10})$$

Dividing by $(k\bar{u} - \omega)$ and rearranging, we get

$$\frac{d^2\phi}{dz^2} + \left\{ \frac{N^2}{(\bar{u} - c)^2} - \frac{\bar{u}''}{(\bar{u} - c)} - \delta k^2 \right\} \phi = 0, \quad (\text{D.11})$$

where $c = \frac{\omega}{k}$ and the buoyancy frequency is $N^2 = \frac{-g\bar{\rho}'}{\bar{\rho}}$. This equation is known as the Taylor–Goldstein equation. In general, the background flow speed $\bar{u}$ is considered to be a function of z . In that case, the background flow is said to be a shear flow. If there is a value $z = z_c$ for which $\bar{u}(z_c) = c$, then equation (D.11) is singular at $z = z_c$. This singular point is called a critical level. We only consider the situation where $\bar{u}$ is an infinitely differentiable (non-singular) function of z

everywhere in the domain and in particular at $z = z_c$, so $\bar{u}$ can be expanded as a Taylor series around z_c . In that case, equation (D.11) can be solved using Frobenius series. We write ϕ in terms of a Frobenius series as

$$\phi(z) = \sum_{n=0}^{\infty} a_n (z - z_c)^{n+\alpha}, \quad (\text{D.12})$$

where z_c is the critical level. Substituting this series into equation (D.11), approximating $\bar{u}$ and $\bar{u}''$ by their Taylor expansions and assuming N is constant, we obtain

$$\begin{aligned} & a_0((\alpha^2 - \alpha)\bar{u}_c'^2 + N^2)(z - z_c)^\alpha + \left(a_1((\alpha^2 + \alpha)\bar{u}_c'^2 + N^2) + a_0\bar{u}_c'\bar{u}_c''((\alpha^2 - \alpha - 1)) \right)(z - z_c)^{\alpha+1} \\ & + \left(a_2((\alpha^2 + 3\alpha + 2)\bar{u}_c' + N^2) + a_1\bar{u}_c'\bar{u}_c''(\alpha^2 + \alpha - 1) - a_0\gamma_1 \right)(z - z_c)^{\alpha+2} \\ & + \sum_{n=0}^{\infty} \left(a_{n+3}((n+3+\alpha)(n+\alpha+2)\bar{u}_c'^2 + N^2) + a_{n+2}\bar{u}_c'\bar{u}_c''((n+2+\alpha)(n+\alpha+1) - 1) \right. \\ & \left. - a_{n+1}\gamma_1 - a_n\gamma_2 \right)(z - z_c)^{n+\alpha+3} = 0, \end{aligned} \quad (\text{D.13})$$

where $\gamma_1 = \frac{\bar{u}_c''^2}{2} + \bar{u}_c'\bar{u}_c''' + \delta k^2\bar{u}_c'^2$, $\gamma_2 = \frac{\bar{u}_c''\bar{u}_c'''}{2} + \delta k^2\bar{u}_c'\bar{u}_c''$ and the subscript c denotes evaluating at z_c . From the coefficient of $(z - z_c)^\alpha$, $a_0 \neq 0$, so we have

$$\alpha = \frac{1}{2} \pm \frac{1}{2}(1 - 4Ri_c)^{\frac{1}{2}}, \quad (\text{D.14})$$

where $Ri_c = \frac{N^2}{\bar{u}_c'^2}$. The Richardson number is defined as $Ri(z) = \frac{N^2}{(\bar{u}'(z))^2}$ so $Ri_c = Ri(z_c)$ is the Richardson number at the critical level. According to Miles (1961), $Ri > \frac{1}{4}$ is a condition for stability. If $Ri < \frac{1}{4}$, then α is always real and the leading-order solution takes the form

$$\phi(z) \sim a_0 e^{\alpha \log(z - z_c)}, \quad (\text{D.15})$$

which is a decay/growth solution. We consider the case where $Ri > \frac{1}{4}$ and find that the first two terms of the series are

$$\phi(z) \sim a_0(z - z_c)^{\frac{1}{2} \pm i\beta} + a_1(z - z_c)^{\frac{1}{2} \pm i\beta + 1}, \quad (\text{D.16})$$

where $\beta = (Ri_c - \frac{1}{4})^{\frac{1}{2}}$, a_0 is arbitrary constant and $a_1 = a_0 \frac{(1+Ri)\bar{u}_c''}{2\alpha\bar{u}_c'}$, which can be found from the coefficient of $(z - z_c)^{\alpha+1}$ in (D.13). This solution can be written in terms of exponential functions as

$$\phi(z) \sim (z - z_c)^{\frac{1}{2}} (A_1 e^{i\beta \log(z - z_c)} + A_2 e^{-i\beta \log(z - z_c)} + O(z - z_c)), \quad (\text{D.17})$$

where $\log(z - z_c)$ is defined as

$$\log(z - z_c) = \begin{cases} \log(z - z_c), & \text{for } z > z_c \\ \log\{(-1)|z - z_c|\}, & \text{for } z < z_c, \end{cases} \quad (\text{D.18})$$

and since $e^{\pm i\pi} = -1$, we then have

$$\log(z - z_c) = \begin{cases} \log(z - z_c), & \text{for } z > z_c \\ \log|z - z_c| \pm i\pi, & \text{for } z < z_c. \end{cases} \quad (\text{D.19})$$

The sign of the complex exponents in (D.17) determines the direction of the wave propagation, which is discussed below. To determine the sign of the branch in (D.19), we have to consider the case with time-dependent amplitude $\phi(z, t)e^{ikx}$. By taking the Laplace transform we find that the sign of the phase change is $(-)$, as shown by Miles (1961), so we choose the $(-i\pi)$ branch. The leading-order term

of (D.17) can then be written as

$$\phi(z) \sim \begin{cases} |z - z_c|^{\frac{1}{2}} (A_1 e^{i\beta \log(z - z_c)} + A_2 e^{-i\beta \log(z - z_c)}), & \text{for } z > z_c \\ -i|z - z_c|^{\frac{1}{2}} (A_1 e^{i\beta \log|z - z_c| + \beta\pi} + A_2 e^{-i\beta \log|z - z_c| - \beta\pi}), & \text{for } z < z_c. \end{cases} \quad (\text{D.20})$$

The solution (D.20) shows that the wave amplitude is reduced by a factor of $e^{-\beta\pi}$ across the discontinuity from $z < z_c$ to $z > z_c$. Plugging the solution (D.20) into a time-independent form of (D.4), we obtain the time-independent streamfunction solution for the linear equations. This solution is shown in Figure D.1 in the domain $0 < x < 2\pi$, $0 < z < 10$. The background wind speed is $\bar{u} = \tanh(z - 5)$, so we have a discontinuity at $z = 5$ as shown in Figure D.1. The background density is $\bar{\rho} = e^{-z/h}$, where $h = 4.9$, so $N^2 = \frac{g}{h} = 2$, and the Richardson number at the critical level is $Ri_c = 2$. Since $Ri_c > \frac{1}{4}$ the solution is stable. The wave amplitude is reduced by a factor of $e^{-\frac{\sqrt{7}}{2}\pi}$ as it moves from $z < 5$ to $z > 5$. There are no visible contours in the upper half of the domain, since the solution is so close to zero.

Figure D.1: The time-independent streamfunction $\psi(x, z)$ (D.4) with amplitude given by (D.20). Parameters are $Ri_c = 2$, $k = 2$ and $\delta = 0.2$.

Upward and downward travelling waves

To discuss the direction of wave propagation, let us consider the Taylor–Goldstein equation with a constant wind speed $\bar{u}$ and a constant N , of the form

$$\frac{d^2\phi}{dz^2} + \left\{ \frac{N^2}{(\bar{u} - c)^2} - \delta k^2 \right\} \phi = 0. \quad (\text{D.21})$$

This equation is defined on a semi-infinite domain $z_1 < z < \infty$, where $z_1 > 0$ corresponds to some altitude near the ground. We are interested in the situation where the waves are generated by an oscillatory boundary condition given at $z = z_1$, and they propagate upwards as $z \rightarrow \infty$. From the equation (D.21), we note that if we have $\frac{N^2}{(\bar{u}-c)^2} < \delta k^2$, then the solution takes the form

$$\phi(z) = Ae^{-\gamma z} + Be^{\gamma z},$$

where $\gamma = \left(\frac{N^2}{(\bar{u}-c)^2} - \delta k^2 \right)^{\frac{1}{2}}$. In order for the solution to be bounded as $z \rightarrow \infty$, we must have $B = 0$. This gives an exponentially decaying solution, which represents a disturbance trapped near the ground. Thus, in order to have wave solutions, we consider $\frac{N^2}{(\bar{u}-c)^2} > \delta k^2$, and the general solution will then have the form

$$\phi(z) = Ae^{imz} + Be^{-imz}, \quad (\text{D.22})$$

where m is defined as

$$m = \left(\frac{N^2}{(\bar{u}-c)^2} - \delta k^2 \right)^{\frac{1}{2}}, \quad (\text{D.23})$$

and it represents the wavenumber in the vertical direction. We define m such that it has the same sign as $(\bar{u} - c)$.

The time-independent streamfunction solution is given as

$$\psi(x, z) = Ae^{i(kx+mz)} + Be^{i(kx-mz)} + \text{c.c.}, \quad (\text{D.24})$$

where k is assumed to be positive. This solution can be expressed in terms of $\cos(kx \pm mz)$ and $\sin(kx \pm mz)$, with a phase front $\Phi = kx \pm mz = \text{constant}$. The phase lines are then defined by $\frac{dz}{dx} = \left(\frac{-k}{\pm m} \right)$, so with the choice of $(-m)$ the slope is positive, and with the choice of $+m$ the slope is negative.

The direction of wave propagation can be determined by examining the group velocity of the waves as discussed by Booker and Bretherton (1967). The group velocity in two dimensions is defined as the vector

$$c_g = \left(\frac{\partial \omega}{\partial k}, \frac{\partial \omega}{\partial m} \right).$$

From (D.23), we find

$$(\bar{u} - c)^2 = \frac{N^2}{(m^2 + \delta k^2)}. \quad (\text{D.25})$$

Taking the square root and solving for c , we find

$$c = \bar{u} \mp \frac{N}{(m^2 + \delta k^2)^{\frac{1}{2}}}. \quad (\text{D.26})$$

Therefore the frequency is given as

$$\omega = kc = k\bar{u} \mp \frac{kN}{(m^2 + \delta k^2)^{\frac{1}{2}}} \quad (\text{D.27})$$

This is the dispersion relation for gravity waves. The vertical component of the group velocity for the first solution in (D.22), with $(+m)$, is given as

$$\frac{\partial \omega}{\partial m} = \pm \frac{kmN}{(m^2 + \delta k^2)^{\frac{3}{2}}}. \quad (\text{D.28})$$

From (D.26), we find that

$$\bar{u} - c = \pm \frac{N}{(m^2 + \delta k^2)^{\frac{1}{2}}}, \quad (\text{D.29})$$

so (D.28) becomes

$$\frac{\partial \omega}{\partial m} = \frac{km\bar{u}}{(m^2 + \delta k^2)}. \quad (\text{D.30})$$

Since we have defined $k > 0$ and specified that m and $\bar{u} - c$ have the same sign, we find that equation (D.30) is positive. This means that the vertical component of group velocity is positive, and hence the waves are travelling upward for the solution corresponding to $(+m)$ in (D.22). Similarly, we find that, for the second solution where we have the vertical wavenumber $(-m)$, the vertical component of

group velocity is

$$\frac{\partial \omega}{\partial(-m)} = -\frac{km\bar{u}}{(m^2 + \delta k^2)}, \quad (\text{D.31})$$

which is negative, so the second solution e^{-imz} is a downward-travelling wave. So, in order to have an upward propagating wave, we must set $B = 0$ in (D.24).

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