

Article

Nonlinear Gravity-Wave Effects on the Distribution of Chemical Constituents in a Vertically-Sheared Atmospheric Flow

Ahmed S. Almohaimeed ¹ and Lucy J. Campbell ^{2,*} ¹ Department of Mathematics, College of Science, Qassim University, Buraydah 51452, Saudi Arabia; ahs.almohaimeed@qu.edu.sa² School of Mathematics and Statistics, Carleton University, Ottawa, ON K1S 5B6, Canada

* Correspondence: campbell@math.carleton.ca

Abstract

The dynamical processes in the atmosphere are coupled with the chemistry of the atmosphere. Internal gravity waves influence the distribution of chemical constituents in the atmosphere through their effects on the background wind or mean flow. We examine a coupled system of equations comprising a nonlinear transport equation of Fisher type for the distribution of the chemical species, along with nonlinear Boussinesq equations for internal gravity waves in a vertically stratified and vertically sheared fluid flow in a two-dimensional region. In our model, a horizontally localized gravity-wave packet is generated and propagates upward into a localized region where the chemical species is present. Numerical solutions show that the wave-induced mean flow resulting from nonlinear gravity-wave interactions in the vicinity of a critical level leads to modifications in the distribution of the chemical. An asymptotic analysis of a related qualitatively similar problem gives us information on the dominant behaviour of the chemical concentration perturbation. We conclude that nonlinearity and vertical shear play a vital role in the interplay between gravity-wave dynamics and chemical distributions in the atmosphere.

Keywords: internal gravity waves; nonlinear waves; partial differential equations; transport equations; asymptotic solution; WKB method; numerical solution; atmospheric modelling; heating

MSC: 35Q35; 35Q49; 76B15; 76B55; 76M45

1. Introduction

Atmospheric waves play a significant role in the transport of momentum and energy in the middle atmosphere. The stratosphere is dynamically stable, but waves propagating up from the troposphere affect the dynamical balance. The breaking of planetary-scale and synoptic-scale Rossby waves in the stratosphere leads to horizontal mixing. On smaller scales, mesoscale and microscale internal gravity waves are generated by the buoyancy-restoring force resulting from the stable stratification of the atmosphere, coupled with the gravitational force. Internal gravity waves also propagate from the troposphere and may break down, leading to turbulence. They are the primary cause of vertical mixing in the middle atmosphere [1]. The importance of gravity-wave effects increases with altitude as their amplitudes increase exponentially with altitude.

The atmosphere contains major chemical constituents such as nitrogen N_2 , oxygen O_2 , argon Ar, and water vapour H_2O , as well as trace gases that are present in smaller concentrations, such as carbon dioxide CO_2 , methane CH_4 , and ozone O_3 . Although these trace



Academic Editor: Xudan Luo

Received: 24 November 2025

Revised: 8 January 2026

Accepted: 13 January 2026

Published: 17 January 2026

Copyright: © 2026 by the authors.

Licensee MDPI, Basel, Switzerland.

This article is an open access article

distributed under the terms and

conditions of the [Creative Commons](https://creativecommons.org/licenses/by/4.0/)[Attribution \(CC BY\)](https://creativecommons.org/licenses/by/4.0/) license.

gases are not present in high concentrations, they play an important role in atmospheric reactivity and hence can affect the temperature of the Earth's surface. Free radicals, such as hydroxyl OH and chlorine monoxide ClO, are highly reactive to other species and regulate the concentrations of some trace gases through processes such as oxidation [2]. In general, the concentrations of chemicals in the atmosphere are influenced by four kinds of activities: chemistry, emissions, deposition, and transport [3,4].

Dynamical–chemical coupling occurs in the atmosphere as planetary Rossby waves and internal gravity waves undergo multi-scale interactions which modify the background wind and thus affect the distribution of chemical species. Planetary Rossby waves influence the composition of some long-lived chemical species in the Northern Hemisphere stratosphere, notably in the late summer [5].

Internal gravity waves are affected by the presence of chemical constituents in the atmosphere but also impact their distribution. Chemical processes, such as photochemical heating of chemical constituents in the atmosphere, lead to damping or enhancement of gravity waves [6–8]. Gravity waves, on the other hand, impact the distribution of chemical species in the atmosphere through their effects on the background wind or mean flow. Wave–mean-flow interactions result from a mechanism known as the critical-level interaction that can occur in a mean flow with vertical shear. When the mean flow speed is equal to the phase speed of the wave at some altitude, there is a critical level, which corresponds to a singularity in the linearized equations for internal gravity waves [3,9]. The speed of the wind in the atmosphere can be perturbed as a result of interactions between different wave modes and between the waves and the mean flow, especially in the vicinity of the critical level [10]. The wave-induced mean flow may affect the speed of transport and hence the distribution of chemical constituents [11].

General circulation models (GCMs) must correctly represent all of these gravity-wave interactions in order to accurately predict weather and climate. However, because of their relatively small scale, compared with the planetary scale, gravity-wave effects are not completely resolved and predicted by large-scale GCMs [11,12]. Analytical and numerical studies based on simpler models, which have fewer degrees of freedom than a GCM, provide insights into the interactions and quantify their effects. Similarly, mathematical models based on advection–diffusion–reaction equations give important insights into the spatial and temporal evolution of the chemical concentrations in different regions of the atmosphere.

The objective of our investigation is to describe and quantify the effects of a gravity-wave perturbation and wave-induced mean flow on the propagation of chemical species in the atmosphere. The novel aspects of our formulation are the consideration of a background flow with vertical shear and a critical level, nonlinear wave–mean-flow interactions, and the development of a wave-induced mean flow in the vicinity of the critical level.

Previous researchers have investigated gravity-wave development in the presence of different chemical species by means of numerical modelling, but without the specific focus on the wave-induced mean flow. Hickey and Plane [13] studied linear internal gravity waves in the presence of sodium species in the mesopause region of the atmosphere and showed that the presence of the gravity waves leads to sodium fluctuations at specific altitudes around the sodium layer. Xu et al. [14] studied the influence of linear inertia-gravity waves on the distribution of some chemical species. The chemical concentrations are modelled by advection–diffusion transport equations including terms representing the production and loss of the chemicals, which are coupled with the gravity-wave equations. In their formulation, there is no wave-induced mean flow since the gravity waves are linear. For each of the chemicals considered, a monochromatic gravity-wave oscillation leads to sinusoidal perturbations in the chemical concentration. In some cases, this causes the

spurious effect of negative values of the chemical concentration, which is dealt with by adjusting the model to reset the negative values to zero. This suggests that a nonlinear gravity-wave model could give a more physically realistic representation.

Xu et al. [15] presented a model comprising nonlinear gravity-wave equations along with transport equations for the chemical species. A gravity-wave packet is introduced into the model by an initial condition for the gravity-wave temperature equation with a vertically localized and horizontally and vertically oscillatory initial function. The model takes into account the variation in density with altitude in a non-Boussinesq formulation. This means that the gravity-wave amplitude increases with altitude and there could potentially be wave breaking at some level. To avoid this, the amplitude of the initial perturbation is kept small, and thus, the propagation of the wave packet, according to the numerical solution, agrees with linear theory. Numerical solutions are carried out for cases with realistic background temperature profiles. There are no breaking levels or critical levels. The gravity-wave packet propagates through the region under consideration and affects the chemical distribution and these effects persist for some time after it has propagated out of the region. Although the gravity-wave model is nonlinear, the variations in the gravity-wave profile with altitude appear to be the result of the temperature profile, not due to a wave-induced mean flow. The results show that a nonbreaking propagating gravity wave can induce significant changes in the mean distribution of atmospheric chemical species, especially at nighttime.

Liu et al. [16], on the other hand, investigated gravity-wave breaking and the resulting impact on chemical distributions. Their model comprises three interacting components: a dynamical model with nonlinear gravity-wave equations, a turbulence model that parameterizes the effects that occur beyond wave breaking, and a chemistry model derived by modifying and simplifying a component from a GCM. The formulation allows gravity waves to propagate upwards and break; this causes a divergence of momentum flux which generates a wave-induced mean flow acceleration and, in some cases, turbulence. In the experiments involving the chemical model, an upward-propagating gravity-wave packet breaks and causes a downward transport of atomic oxygen and other chemical species.

The above-mentioned studies examined situations where the gravity waves propagate upwards and either reach a breaking level or propagate out of the domain. This motivates us to consider a configuration in which there is a critical level in the domain. In our investigation, we examine the effects of a gravity-wave-induced mean flow acceleration on chemical transport, but focus on the wave-induced effects that occur at a critical level.

We present a model comprising nonlinear gravity-wave equations, derived by applying the Boussinesq approximation to the fundamental equations of fluid dynamics [17], coupled with a nonlinear continuity equation of Fisher type to represent the distribution of the chemical species. Under the Boussinesq approximation, the background density and temperature do not vary significantly with altitude and there is no density-weighted increase in the wave amplitude with altitude and, hence, no wave breaking level in the domain. Making this approximation thus allows us to focus on critical-level interactions.

In our formulation, the background wind is a vertically sheared horizontal mean flow with a horizontal speed that depends on altitude. The gravity waves are defined as perturbations to the background flow which are generated by a specified oscillatory lower boundary condition. This is a representation for gravity wave generated by flow over topography in the lower atmosphere that propagate up into the middle atmosphere. The chemical transport equation includes terms that represent chemical reaction and diffusion processes, and an advection term which initially transports the chemical with the speed of the specified background flow. We solve this problem numerically using a Fourier

pseudo-spectral representation, combined with a high-resolution spatial approximation and time-marching.

In the gravity-wave model, wave-mean-flow interactions occur in the vicinity of the critical level, leading to a wave-induced mean flow that appears as a perturbation to the advection speed in the chemical transport equation. This results in modifications to the chemical distribution, which are most significant in the vicinity of the critical level, where the wave-induced mean flow is maximum.

We seek to determine the dependence of the profile of the chemical distribution on the gravity-wave structure. We obtain further insights into the numerical results by carrying out a perturbation and asymptotic analysis of the chemical transport problem to obtain approximate asymptotic solutions for the chemical concentration. In the analysis, we examine the chemical transport equation by imposing a vertically varying advection speed, which is of the form that results when an initially constant background mean flow is modified by the gravity-wave-induced mean flow in the vicinity of a critical level. In the absence of the gravity-wave perturbation, with the constant advection speed, an exact travelling-wave solution can be obtained for the reaction–diffusion transport equation. With the addition of the gravity-wave-induced mean flow component to the chemical advection speed, there is no exact solution in closed form for the transport equation. Instead, we use asymptotic methods to study the behaviour of the solution by considering it to be an expression in powers of a small parameter defined by the wave amplitude. The solution corresponding to the leading order is the travelling wave solution, which is found exactly. At the next order, an asymptotic solution is obtained by means of a WKB approximation and is found to be proportional to the profile of the perturbation of the mean flow.

The model, comprising the nonlinear gravity-wave equations coupled with the chemical transport equation, is presented in Section 2. The methods used for the numerical discretization of the model equations are described in Appendix A. A list of symbols for the parameters, variables and functions used in the model is given in the Nomenclature. Numerical solutions of the gravity-wave equations are shown in Section 3. From these, we obtain profiles for the wave-induced mean flow that occurs in the vicinity of the critical level. These results are verified by comparison with previous analytical and numerical studies of gravity-wave critical-level interactions. In Section 4 we present and discuss the results of numerical solutions of the coupled gravity-wave and chemical transport equations, which show the development of the wave-induced mean flow and the resulting changes in the distribution of the chemical. In Section 5 we present the asymptotic analysis of the chemical transport problem with perturbed advection speed.

2. The Model

2.1. Transport Equation for the Chemical Species

In this section, we present an equation that models the distribution of a chemical species in the atmosphere by applying the law of conservation of mass. 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 and is, in general, a nonlinear function of n . We consider a situation where the mass of chemical is advected by a background wind with velocity $\vec{U}$ and there is second-order diffusion with a constant diffusion coefficient $\mathcal{D}$. The rate of change in mass with time t 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. This conservation law is expressed in integral form as

$$\iiint_V \left[\frac{\partial n}{\partial t} + \nabla \cdot (n\vec{U}) - \mathcal{D}\nabla^2 n - s \right] dV = 0. \quad (1)$$

Considering n and $\vec{U}$ to be continuous functions of time t and of the space variables everywhere in the volume V , the integral in Equation (1) equals zero only if the integrand equals zero. This gives

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

Equation (2) 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 [6,18–21].

The concentration of the chemical may be represented by the mixing ratio C , which is a dimensionless variable defined in terms of the number density by

$$C = \frac{n}{n_a}, \quad (3)$$

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 a fluid that is incompressible or for which the effects of compressibility are so weak that the conservation of mass of the fluid can be approximated by the incompressible form of the continuity equation $\nabla \cdot \vec{U} = 0$. Equation (2) can then be written in terms of the mixing ratio C as [21]

$$C_t + U C_x + W C_z = \mathcal{D}(C_{xx} + C_{zz}) + S(C), \quad (4)$$

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 (4) 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 [20]. In general, there can be several chemicals, with each chemical modelled by an equation of the form (4) and with some chemicals reacting with each other so that the equations are coupled, e.g., [22].

In this study, the goal is to obtain some insights by mathematical analyses as well as numerical simulations; hence, we restrict the focus to a situation where there is one distinct chemical present with concentration given by (4) and with the source term S depending solely on the mixing ratio C of the chemical under investigation. We consider a chemical such as chlorine monoxide (ClO) which can be modelled by this form with a source term of Fisher type, $S(C) = \sigma C(1 - C)$ [20,23]. Chlorine monoxide (ClO) is a chlorine radical that is known to play a role in the depletion of methane CH_4 and ozone O_3 , particularly in the northern polar troposphere [24].

The nonlinear Fisher equation is a well-known equation which is classified as a reaction–diffusion partial differential equation and has solutions that describe travelling waves under certain conditions [25]. It is mostly used in biological applications such as modeling population growth and tumor growth. In addition, it can be used in chemical applications such as modeling chemical reactions with nonlinear source terms.

The nondimensional form of Equation (4) is

$$C_t + U C_x + W C_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + S(C). \quad (5)$$

where $\delta = L_z^2/L_x^2$ is the square of the vertical-to-horizontal aspect ratio, and L_x and L_z are reference values of the dimensional horizontal and vertical scales. The nondimensional value of the diffusion coefficient $\mathcal{D}$ is defined in terms of the corresponding dimensional value $\mathcal{D}^*$ by $\mathcal{D} = \tau \mathcal{D}^*/L_z^2$, where τ is a reference time scale. The nondimensional source function S is defined in terms of the corresponding dimensional function S^* by $S = \tau S^*$.

We note that, in the special case where the advection velocity components U and W are constant in (5) and the source term has the form $\sigma C(1 - C)$, then, following [26], (5) has an exact travelling-wave solution

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

where the angle θ is the tilt of the direction of travel of the wave, i.e., the angle that the direction of travel makes with the positive x -axis. The travelling wave speed is

$$c = \frac{5\sqrt{\sigma \delta \mathcal{D}}}{\sqrt{6}} + U \cos(\theta) + W \sin(\theta). \quad (7)$$

This expression shows that stronger diffusion ($\mathcal{D}$), higher chemical reaction rate (σ), and larger vertical scale (δ) all act to increase the propagation speed of the travelling wave, while the advection velocity components determine the direction of propagation.

2.2. Gravity-Wave Equations

The gravity-wave equations are based on the Boussinesq approximation [17]. This approximation is valid in situations where the layer of fluid is relatively shallow and the spatial and temporal variations in the density are small enough that they are considered only in the terms involving the gravitational force in the vertical momentum conservation equation and the continuity equation is approximated by its incompressible form. It is also considered that the change in the density with respect to pressure is negligible compared to the change in density with respect to temperature so that the equation of state is approximated by a linear relation between the density and the temperature, and thus the energy conservation equation is expressed in terms of the density.

The density is approximated by a constant ρ_0 in the continuity equation. This allows us to define a streamfunction $\Psi(x, z, t)$ in terms of the horizontal and vertical velocity components as $\mathcal{U} = -\Psi_z$ and $\mathcal{W} = \Psi_x$. The density is also approximated by ρ_0 in the momentum equations except in the gravitational term where it is taken to be a function $\rho(x, z, t)$. These momentum equations are combined to give a single equation in streamfunction-vorticity form. The energy equation is written in terms of the density function ρ . These approximations give

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + \nu \nabla^2 (\nabla^2 \Psi), \quad (8)$$

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = \kappa \nabla^2 \rho - \alpha J, \quad (9)$$

where again subscripts denote partial derivatives, ν is the kinematic viscosity coefficient, κ is the thermal diffusivity coefficient. In addition, J is the chemical heating rate and α the chemical heating coefficient is given in terms of the reference density ρ_0 , reference temperature T_0 and specific heat capacity C_p .

In nondimensional form, Equations (8) and (9) have the form

$$\nabla^2 \Psi_t - \Psi_z \nabla^2 \Psi_x + \Psi_x \nabla^2 \Psi_z = -\frac{g}{\rho_0} \rho_x + Re^{-1} \nabla^2 (\nabla^2 \Psi), \quad (10)$$

$$\rho_t - \Psi_z \rho_x + \Psi_x \rho_z = Re^{-1} Pr^{-1} \nabla^2 \rho - \frac{\tau \alpha \mathcal{A} \mathcal{H}}{D} J, \quad (11)$$

where τ , $\mathcal{A}$, $\mathcal{H}$ and D are reference values for t , α , J and ρ , respectively. The nondimensional Laplacian operator in (10) and (11) is defined as $\nabla^2 = \delta \frac{\partial^2}{\partial^2 x^2} + \frac{\partial^2}{\partial^2 z^2}$, where δ is the square of the aspect ratio, as defined in Equation (5). The Reynolds and Prandtl numbers are given as

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

where $\mathcal{W}$, L_z , $\mathcal{M}$ and κ are reference values for $\mathcal{W}$, z , ν and κ , respectively. The fluid (air) in the atmosphere has low viscosity, and thus the Reynolds number may be considered to be a large parameter. The Prandtl number for air is approximately 0.72. Thus, the viscous and heat conduction terms in (10) and (11) are neglected as a first approximation in our analyses in Section 5, but retained in the numerical solutions in Sections 3 and 4. The focus of this investigation is on the effect of gravity waves on the chemical distribution C in a situation where the effect of the chemical heating on the gravity waves is of the same order as and less significant than the heat conduction effects. Thus, the nonhomogeneous chemical heating term in (11) is also omitted. We note that retaining this term would give a fully coupled system; this is examined in [27] as a further step in this investigation.

The gravity waves are considered to be perturbations to a steady background flow, and thus, the total streamfunction and density are expressed as

$$\Psi(x, z, t) = \bar{\psi}(z) + \varepsilon \psi(x, z, t), \quad \rho(x, z, t) = \bar{\rho}(z) + \varepsilon \rho(x, z, t), \quad (12)$$

where $\varepsilon = \varphi / (UL_z) = D_p / D$ gives the magnitude of the perturbations relative to the background flow, U and L_z are reference values of the horizontal velocity and the vertical scale, respectively, D is a reference value of the density, and φ and D_p are reference values of the streamfunction and density perturbations, respectively. 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 $\bar{u}(z) = -d\bar{\psi}/dz$ and the vertical component $\bar{w}$ is zero. We substitute (12) into (10) and (11) and neglect the viscous, heat-conduction and chemical heating terms in comparison to the nonlinear terms. These considerations give the following system of equations for the perturbation streamfunction ψ , vorticity ζ and density ρ :

$$\zeta_t + \bar{u} \zeta_x - \bar{u}'' \psi_x + \varepsilon (\psi_x \zeta_z - \psi_z \zeta_x) = -\frac{g}{\bar{\rho}} \rho_x, \quad (13)$$

$$\zeta = \nabla^2 \psi = \delta \psi_{xx} + \psi_{zz}, \quad (14)$$

$$\rho_t + \bar{u} \rho_x + \bar{\rho}' \psi_x + \varepsilon (\psi_x \rho_z - \psi_z \rho_x) = 0, \quad (15)$$

In the absence of gravity waves, the advection of the chemical species in the atmosphere results from the background flow with wind velocity vector $(U, W) = (\bar{u}, 0)$. However, in the presence of the gravity waves with velocity $\varepsilon(u, w)$, the background mean flow is perturbed and the advection velocity of the chemical concentration is $(U, W) = (\bar{u} + \varepsilon u, \varepsilon w)$ in (5). This gives

$$C_t + (\bar{u} + \varepsilon u) C_x + \varepsilon w C_z = \mathcal{D}(\delta C_{xx} + C_{zz}) + \sigma C(1 - C), \quad (16)$$

with

$$u = -\psi_z \text{ and } w = \psi_x. \quad (17)$$

In Section 3, we present numerical solutions of the nonlinear gravity-wave Equations (13)–(15) and numerically compute the wave-induced mean flow that results from the nonlinear interaction. A numerical solution of the chemical Equation (16) with this numerically computed gravity-wave-induced mean flow is presented in Section 4.

We seek to obtain more information on the effects of the gravity-wave-induced mean flow on the chemical distribution by carrying out a weakly nonlinear analysis. In order to do so, we first note that in the special case where $\bar{u}$ is constant, and in the absence of the gravity-wave perturbation ($\varepsilon = 0$), the exact solution of (16) is a travelling wave that is transported in the direction of x only. It takes the form (6) with velocity components $U = \bar{u}$, $W = 0$ and $\theta = 0$. With the effects of the gravity-wave perturbation added, the velocity components are $U = \bar{u} + \varepsilon u$ and $W = \varepsilon w$, and we cannot in general obtain an exact solution for (16). We may seek a solution in the form of a perturbation series in powers of ε . In that case, the exact solution (6) gives the leading-order term in the series and we can use it to obtain expressions for the higher-order terms in the series. This analysis is presented in Section 5.

3. Numerical Computation of the Gravity-Wave-Induced Mean Flow

3.1. Gravity Wave Nonlinear Interactions

In this section, we solve the nonlinear gravity-wave Equations (13)–(15), in the absence of the chemical effect, and obtain the form of the wave-induced mean flow velocity profile which is used in the asymptotic analysis of Section 5. We consider Equations (13)–(15), for $t > 0$, in the two-dimensional rectangular domain given by $-\infty < x < \infty$ and $0 \leq z < \infty$. The initial conditions are that ζ and ρ are zero at $t = 0$. 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 $x \rightarrow \pm\infty$. 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 nonlinear Jacobian term is zero at the boundaries.

For the numerical solutions, the semi-infinite domain in two-dimensional space is approximated by a finite rectangular domain defined by $x_1 \leq x \leq x_2$ and $0 \leq z \leq z_2$, with $x_1 < 0 < x_2$ and $-x_1$ and x_2 chosen to be large enough to ensure that ψ and its derivatives are zero at $x = x_1$ and $x = x_2$. We impose the lower boundary condition

$$\psi(x, 0, t) = \frac{e^{-\mu^2 x^2}}{2} (e^{ik_0 x} + e^{-ik_0 x}), \quad (18)$$

where k_0 is a constant positive integer and μ is a real constant, $\mu \ll 1$. This generates a perturbation in the form of an upward-propagating horizontally localized wave packet in the domain, with horizontal wavenumber k_0 and zero phase speed (zero frequency) and with horizontal extent determined by the parameter μ .

We specify the background flow speed $\bar{u}$ so that $\bar{u} = 0$ at some level $z = z_c$ in the domain. This gives us the critical-level problem, which has been studied extensively in the past 60 years. The case with a monochromatic horizontally periodic wave ($\mu = 0$) was analyzed in linear [28] and nonlinear configurations [29–31], and cases with horizontally localized wave packets have been studied analytically and numerically, e.g., [32,33].

In the linear theory ($\varepsilon = 0$) for small-amplitude gravity waves [28], forced with a given horizontal wavenumber and phase speed, the vertical wavenumber is given by the

gravity-wave dispersion relation. In a case with no shear, the vertical wavenumber is constant. In a case with shear, where $d\bar{u}/dz$ is not identically zero in the vertical domain, the vertical wavenumber varies like $(\bar{u} - c)^{-1}$, according to the dispersion relation. Hence, the vertical wavelength depends on z . If there is a critical level at $z = z_c$ where $\bar{u} = c$, then the physical description of the solution is a wave which oscillates increasingly rapidly with altitude, with a vertical wavelength that decreases to zero, as it propagates upwards to the critical level. The linear steady-amplitude wave solution is not valid at the critical level as the wave amplitude is discontinuous and there is a phase change across the critical level. This singular behaviour is a consequence of the approximation of the nonlinear equations with linear steady-amplitude solutions.

The nonlinear time-dependent problem which we study here gives a more physically realistic representation of the critical level development. In this configuration, the vertical wavelength becomes shorter as the wave approaches the critical level. The wave propagating with upward group velocity transports energy and momentum upwards. At the critical level, the vertical flux of horizontal momentum is greatly reduced and this results in a wave-induced change in the horizontal mean velocity. The corresponding change in the wave energy flux results in wave-induced changes in the temperature and density of the background flow. This transfer of momentum and energy from the waves to the mean flow defines absorption of the waves by the mean flow.

Brown and Stewartson [29–31] extended the work of [28] by including the nonlinear terms in the gravity-wave equations in an “inner” critical layer around the critical level. They found asymptotic expressions for the wave-induced mean flow components. They concluded that the waves are absorbed at the critical level at early time and reflected at later time.

These effects are also seen in critical-level numerical studies (e.g., [32]) and in observational studies of the stratosphere [34] and mesosphere [35]. At late time, the wave-induced effects near the critical level may become so large that the density is no longer stably stratified. If the vertical gradient of the density becomes positive in some regions of the domain then the flow is no longer statically stable and wave breaking may occur.

Campbell and Maslowe [32] and Campbell and Nikitina [33] carried out numerical investigations of the nonlinear critical-layer evolution for cases with a horizontally localized wave packet forcing of the form (18), as well as with a monochromatic forcing ((18) with $\mu = 0$). It was seen that, at early time, the waves are absorbed as a result of momentum flux divergence in the critical layer, and at later time, as the nonlinear terms become important at the critical level, the waves can be reflected, as predicted by the nonlinear theory.

In the present investigation, we compute the wave-induced mean flow that results from the nonlinear interactions of the horizontally localized wave packet that is generated by the boundary condition (18). The boundary function in (18), with slowly varying amplitude $A(x) = e^{-\mu^2 x^2}$, comprises a continuous spectrum of horizontal wavenumbers (Fourier modes) centered around the wavenumbers $\pm k_0$. Following [32], the horizontal average is taken over the length of the packet L , which in the numerical computations is chosen to be the horizontal width L of the computational domain. We define the horizontal average of each function $q(x, z, t)$ by

$$\bar{q} = \frac{1}{L} \int_{-\infty}^{\infty} q(x, z, t) dx. \quad (19)$$

The nonlinear terms in the gravity-wave equations involve products of these Fourier modes. This means that with time, Fourier modes with wavenumbers $\pm 2k_0, \pm 3k_0, \dots$ develop, in addition to wavenumbers $k_0 + (-k_0) = 0$. These are proportional to $e^0, e^{\pm 2k_0 i x}$,

$e^{\pm 3k_0 i x}$, and so on. The zero-wavenumber component corresponds to the wave-induced mean flow.

The streamfunction $\psi(x, z, t)$ may be expressed as an inverse Fourier transform,

$$\psi(x, z, t) = \int_{-\infty}^{\infty} \hat{\psi}(k, z, t) e^{ikx} dk, \quad (20)$$

where $\hat{\psi}(k, z, t)$ is the Fourier transform of $\psi(x, z, t)$. The wave-induced mean streamfunction corresponds to the zero wavenumber component of $\hat{\psi}(k, z, t)$ and can be written as

$$\bar{\psi}_0(z, t) = \frac{\varepsilon}{L} \hat{\psi}(0, z, t) = \frac{\varepsilon}{L} \int_{-\infty}^{\infty} \psi(x, z, t) dx \quad (21)$$

and the wave-induced horizontal velocity is $\bar{u}_0 = -\bar{\psi}_{0z}(z, t)$.

The vertical flux of horizontal momentum is [36]

$$F = -\overline{uw} = -\frac{1}{L} \int_{-\infty}^{\infty} u w dx, \quad (22)$$

where $u = -\psi_z$ and $w = \psi_x$ are the horizontal and vertical velocity components of the perturbation.

The equation for the evolution of the wave-induced mean velocity can be obtained by taking the average of each term of the vorticity Equation (13) and integrating the resulting equation with respect to x , applying the zero limiting conditions at $x \rightarrow \pm\infty$. It can also be obtained more directly by taking the average of each term of the horizontal momentum equation. We obtain

$$\frac{\partial}{\partial t} \bar{u}_0(z, t) = -\frac{\varepsilon^2}{L} \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_z \psi_x dx \right) = \varepsilon^2 \frac{\partial F}{\partial z}. \quad (23)$$

This is the well-known equation that describes the wave-induced mean acceleration in terms of the gravity-wave drag force or the divergence of the wave momentum flux. The Eliassen–Palm Theorem [37] tells us that F , which is also known as the E-P flux, is constant if there is no vertical shear and no critical level. In the presence of a critical level, F varies with z across the critical level and, thus there is a nonzero gravity-wave drag force that modifies the mean flow in the critical layer. This is seen in numerical simulations [32].

Similarly, the equation for the evolution of the wave-induced mean density

$$\bar{\rho}_0(z, t) = \frac{\varepsilon}{L} \hat{\rho}(0, z, t) = \frac{\varepsilon}{L} \int_{-\infty}^{\infty} \rho(x, z, t) dx \quad (24)$$

is obtained by taking the average of each term of the density Equation (15). We obtain

$$\frac{\partial}{\partial t} \bar{\rho}_0(z, t) = -\frac{\varepsilon^2}{L} \frac{\partial}{\partial z} \left(\int_{-\infty}^{\infty} \psi_x \rho dx \right). \quad (25)$$

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).

3.2. 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 40,000 km, which means that the distance between the north and south poles is about 20,000 km. This corresponds to the dimensional horizontal coordinate x^* . 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 $\delta = (\frac{L_z}{L_x})^2$. If we define our domain to be $-50 \leq x \leq 50, 0 \leq z \leq 10$ 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 correspond to small values of δ . The long-wave limit of $\delta = 0$ gives a hydrostatic flow approximation. We maintain non-zero values of δ which give a more physically realistic and numerically stable configuration. We consider a range of δ given as $0.01 \leq \delta \leq 0.2$, which corresponds to a reasonable dimensional scale.

The parameter ε defines the amplitude of the wave perturbation relative to the magnitude of the background flow. For a perturbation with dimensional streamfunction amplitude ϕ and dimensional horizontal wind speed u^* , this is defined by the ratio $\varepsilon = \phi/UL_z = u^*/U$. We consider values for the background wind speed up to a maximum of about 20 m s^{-1} with fluctuations of up to 10%; thus, we set values of $\varepsilon \leq 0.1$. This means we can consider $\varepsilon \ll 1$, which allows the validity of the asymptotic analysis in Section 5.

Specifically, we present numerical solutions of the same configuration as [32] with background shear flow velocity $\bar{u} = \tanh(z - z_c)$ and background density $\bar{\rho} = \rho_0 e^{-z/h}$, where ρ_0 is an $O(1)$ constant and z_c , the location of the critical level, satisfies $0 < z_c < z_2$. We choose $z_c = \frac{z_2}{2}$ so that the critical level is at half the height of the domain. The wave packet propagating upwards from the lower boundary is almost completely “absorbed” at the critical level, i.e., its amplitude is greatly reduced at the critical level, as is expected from critical level theory [28]. Therefore, in the numerical computation, the wave packet amplitude remains so small at the upper boundary that it is sufficient to simply set zero upper boundary conditions for ψ , ζ and ρ . With the forcing function given in (18), the solution goes to zero as $x \rightarrow \pm\infty$; hence, we choose the computational domain to be of sufficiently great horizontal extent that the solution is zero at the left and right boundaries $x = x_1$ and $x = x_2$.

The nonlinear numerical simulations also include the viscous and heat conduction terms that are present in Equations (10) and (11). The Prandtl number is set to 0.72, a typical value for the air in the atmosphere. The Reynolds number Re is taken to be large, as appropriate for atmospheric situations with low viscosity. The addition of viscosity and heat conduction enhances the numerical stability of the computations by reducing the amplitude of small-scale high-wavenumber modes that may develop at late time. According to critical layer theory, the ratio of the nondimensional viscous parameter Re^{-1} to the value of ε^2 gives a measure of the relative importance of viscosity to nonlinearity in the critical layer. This is discussed in [32]. For the results shown in Section 3.3, we have set the viscous parameter value so that this ratio is 0.1. This value is sufficient to contribute to improving the numerical stability, but not so large as to damp the zero wavenumber and forced wave modes and it corresponds to situations in which the nonlinear effects are dominant compared with the viscous effects in the critical layer, according to the theory.

We carried out several numerical experiments exploring the parameter space for δ and ε . We found that changing the values of these parameters modifies the quantitative behaviour of the solution, but for values of the parameters within the intervals $0.01 \leq \delta \leq 0.2, \varepsilon \leq 0.1, 0.02 \leq \lambda \leq 0.1$, we were able to obtain qualitatively similar results, which are in agreement with the results obtained by [32]. Some representative results are discussed in Section 3.3.

3.3. Gravity-Wave Simulations

Figure 1 shows results obtained from the numerical solution of (13)–(15) for the horizontal velocity perturbation u with $\delta = 0.2$ and $\varepsilon = 0.05$ at two different times $t = 10$ and $t = 40$. At early time, the behaviour of the solutions is as predicted by the linear theory; 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, the solutions experience a different behaviour around the critical level. The incident waves are reflected and the reflected waves are superimposed on the incident ones below the critical level, as found by [32].

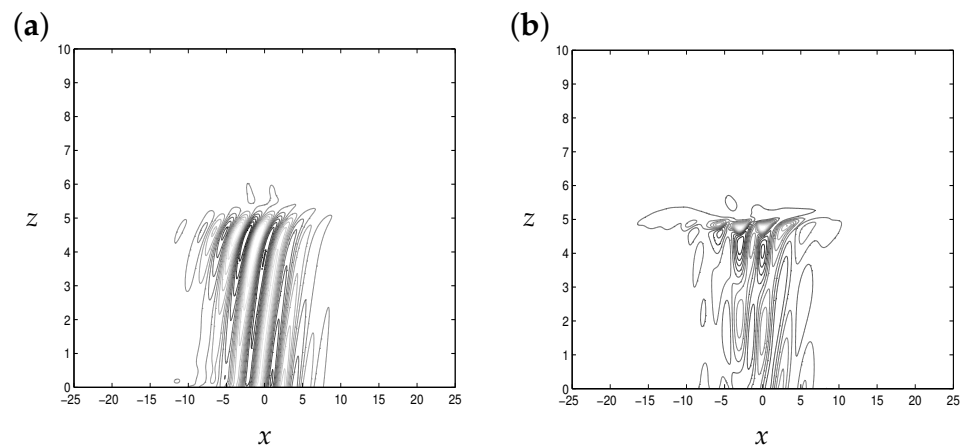


Figure 1. The horizontal velocity perturbation $u(x, z, t)$ at (a) $t = 10$ and (b) $t = 40$ with $\delta = 0.2$ and $\varepsilon = 0.05$.

We note that, in comparison to the results shown in Figure 1, using smaller values of ε reduces these nonlinear effects and increases the time frame for their onset. Using smaller values of δ results in a large vertical wavenumber and hence increases the slope of the lines of constant phase as the disturbance propagates upward.

The nonlinear interaction around the critical level gives rise to zero-wavenumber ($k = 0$) components, $\hat{\psi}(0, z, t)$, $\hat{\zeta}(0, z, t)$ and $\hat{\rho}(0, z, t)$, which correspond to changes in the mean streamfunction, vorticity and density, respectively, as discussed in Section 3.1. The corresponding change in the mean flow velocity is the zero-wavenumber component $\bar{u}_0(z, t) = -\hat{\psi}_z(0, z, t)$, which is given by (23), and this is shown in Figure 2. We note that the mean flow velocity is modified only in the vicinity of the critical level. The wave-induced mean flow varies rapidly with z around the critical level, but is almost constant away from the critical level. This is consistent with the analytical observation by [28], indicating that the momentum of the absorbed gravity waves is transferred to the mean flow in the critical layer.

The wave-induced mean flow velocity $\bar{u}_0(z, t)$ computed here is used in the numerical solution of the chemical transport equation in Section 4. For the analysis of Section 5, we express the wind speed U as

$$U(z) = \bar{u} + \varepsilon \tilde{u}(z), \quad (26)$$

where $\bar{u}$ is the background wind speed, $\varepsilon \ll 1$, and $\tilde{u}(z)$ is a perturbation to the wind speed such as that due to the gravity-wave interactions. We choose an expression for the wind speed perturbation $\tilde{u}(z)$ that takes a form similar to the vertical profile of the computed wave-induced mean flow velocity $\bar{u}_0$.

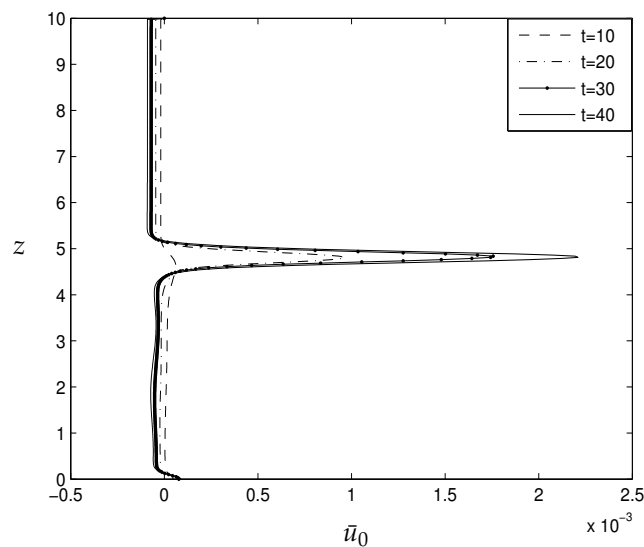


Figure 2. Wave-induced mean flow $\bar{u}_0(z, t)$ at different times.

4. Numerical Computation of the Chemical Distribution

4.1. Chemical Transport Formulation

In this section, we carry out numerical solutions of the system of Equations (13)–(17) to study the effect of a gravity-wave packet perturbation on the distribution of a chemical modelled by the Fisher-type Equation (16). In this configuration, the gravity waves affect the distribution of the chemical by modifying the advection velocity of the chemical. As before, it is assumed that the chemical heating has a negligible impact on the gravity-wave development. Configurations where the chemical heating affects the gravity waves through a coupled system of equations are examined in [27,38].

The concentration of chemicals, such as ClO, in the atmosphere is generally localized around some latitude and altitude. This can be seen, for example, from the measurements of heating in the atmosphere due to the effect of several chemicals including ozone and water vapour presented by Gille and Lyjak [39]. Their observations show that the initial profiles 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 for the chemical concentration C in our numerical solutions can be represented by a Gaussian function of the spatial variables x and z . A convergence theorem for travelling-wave solutions of Fisher's equation is given by Bramson [25] and gives the conditions on the initial function that would lead to a solution in form of a travelling wave. In [27], it is verified that the Gaussian function satisfies these conditions and some numerical computations are presented in [27] to illustrate this.

In the absence of gravity waves, the chemical is advected by a background wind with speed $\bar{u}(z) = \tanh(z - 5)$. However, in the presence of the gravity waves, the background mean flow is perturbed and the chemical is advected by the total wind with velocity components $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$ and $W = \varepsilon w(x, z, t)$, where $u(x, z, t)$ and $w(x, z, t)$ are the gravity-wave velocity components (17). As in Section 3, the gravity-wave phase speed is set to $c = 0$, and consequently, there is a critical level at $z = z_c = 5$.

We solve Equations (13)–(17) numerically on the rectangular domain given by $-50 \leq x \leq 50$ in the horizontal direction and $0 \leq z \leq 10$ in the vertical direction and with time variable $t \geq 0$. The equations are solved using the same numerical approximations and procedure as in Section 3, described in Appendix A. A detailed description is given in [27].

The results shown in this section are obtained with the parameter δ set to 0.2, the background density $\bar{\rho} = \rho_0 e^{-z/h}$, with $\rho_0 = 1$ and $h = 4.9$. In the boundary condition (18), we set $\mu = 0.2$ and $k_0 = 2$. We impose the initial condition for the chemical equation as

$$C(x, z, 0) = e^{-a^2 x^2} e^{-b^2 (z-z_1)^2}, \quad (27)$$

with $a^2 = 5$, $b^2 = 5$ and $z_1 = 5$. This means that the Gaussian profile is centered at the critical level $z_c = 5$. As in Section 3, a horizontally localized gravity-wave packet, is generated by a lower boundary condition with a Gaussian amplitude (18).

4.2. Chemical Transport Simulations

In this section, we present results obtained by numerically solving the chemical transport Equation (16) with the advection velocity $(U, W) = (\bar{u} + \varepsilon u, \varepsilon w)$, where u and w are the gravity-wave velocity components (17) obtained from solving the nonlinear gravity-wave problem (13)–(15). We first present, for reference, some results of numerical solutions of the chemical transport Equation (16) in the absence of gravity waves, i.e., with $U = \bar{u}$ and $W = \bar{w} = 0$. Figure 3 shows the evolution of the chemical concentration C at times $t = 0, 10, 30$, for the configuration with the background advection speed $\bar{u} = \tanh(z - 5)$. The value of the nonlinear parameter is set to $\sigma = 0.5$ and two different values of the diffusion coefficient are used, $\mathcal{D} = 0.01$ and $\mathcal{D} = 0.001$. A similar comparison is shown in Figure 4 with a value of $\sigma = 0.005$ and the same two values of $\mathcal{D} = 0.01$ and $\mathcal{D} = 0.001$. In each graph, the initial Gaussian profile of the function C generates travelling waves that propagate horizontally and vertically with advection speed that depends on $\bar{u}$ and hence on z , and also depends on the values of σ and $\mathcal{D}$. In each of these figures, comparing the graphs in the left column ($\mathcal{D} = 0.01$) to those in the right column ($\mathcal{D} = 0.001$) shows that increasing $\mathcal{D}$ increases the propagation speed. Comparing the graphs in Figure 3 with those in Figure 4 shows that increasing σ also increases the propagation speed. These dependences are consistent with the exact expression for the travelling wave speed (7) for the case with constant $\bar{u}$ that was discussed in Section 2.1.

Based on the results obtained with no gravity-wave effects which are illustrated in Figures 3 and 4, we choose appropriate values for $\mathcal{D}$ and σ so that the chemical wave front does not travel too fast, in order to ensure that, within the time frame of the computations, the wave front does not reach the boundaries of the domain. In the results shown in Section 3, we see that the wave-induced mean flow resulting from gravity waves attains a maximum value close to the critical level and increases over time, as shown in Figure 2. In order to investigate this critical-layer effect on the chemical concentration, we must choose small enough values for $\mathcal{D}$ and σ to allow the chemical wave front to remain in the vicinity of the critical layer during the time frame of the gravity-wave nonlinear development. From several simulations with different values $\mathcal{D}$ and σ , we find that, for the computations with gravity waves, the values of $\mathcal{D} = 0.001$ 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 specified chemicals discussed in related work [27].

Figure 5 shows the effect of the gravity waves on the chemical concentration in the vicinity of the critical level ($4 \leq z \leq 6$). Figure 5a,c,e show the chemical concentration at times $t = 10, 20, 40$, obtained by solving the linearized problem with $\varepsilon = 0$ and with no effect of the gravity waves on the chemical. Figure 5b,d,f show the chemical concentration at the same times, obtained by solving the nonlinear problem with $\varepsilon = 0.1$.

We see that the effect of the gravity waves on the chemical concentration is most significant close to the critical level. In the horizontal direction, we note that the effect is

mainly contained within the interval $-10 \leq x \leq 10$, which is the active domain of the gravity-wave packet.

Figure 6 shows the same result as Figure 5f, but over a smaller horizontal interval $-8 \leq x \leq 8$, in order to give a better visualization of the structure of the effects in the central part of the domain. Figures 5 and 6 show that the effect of the gravity waves on the chemical concentration takes the form of localized oscillations that have a similar structure to the oscillatory gravity-wave velocity perturbation shown in Figure 1. This effect is examined further and also seen in the asymptotic approximations for the solution in the configuration studied in Section 5.

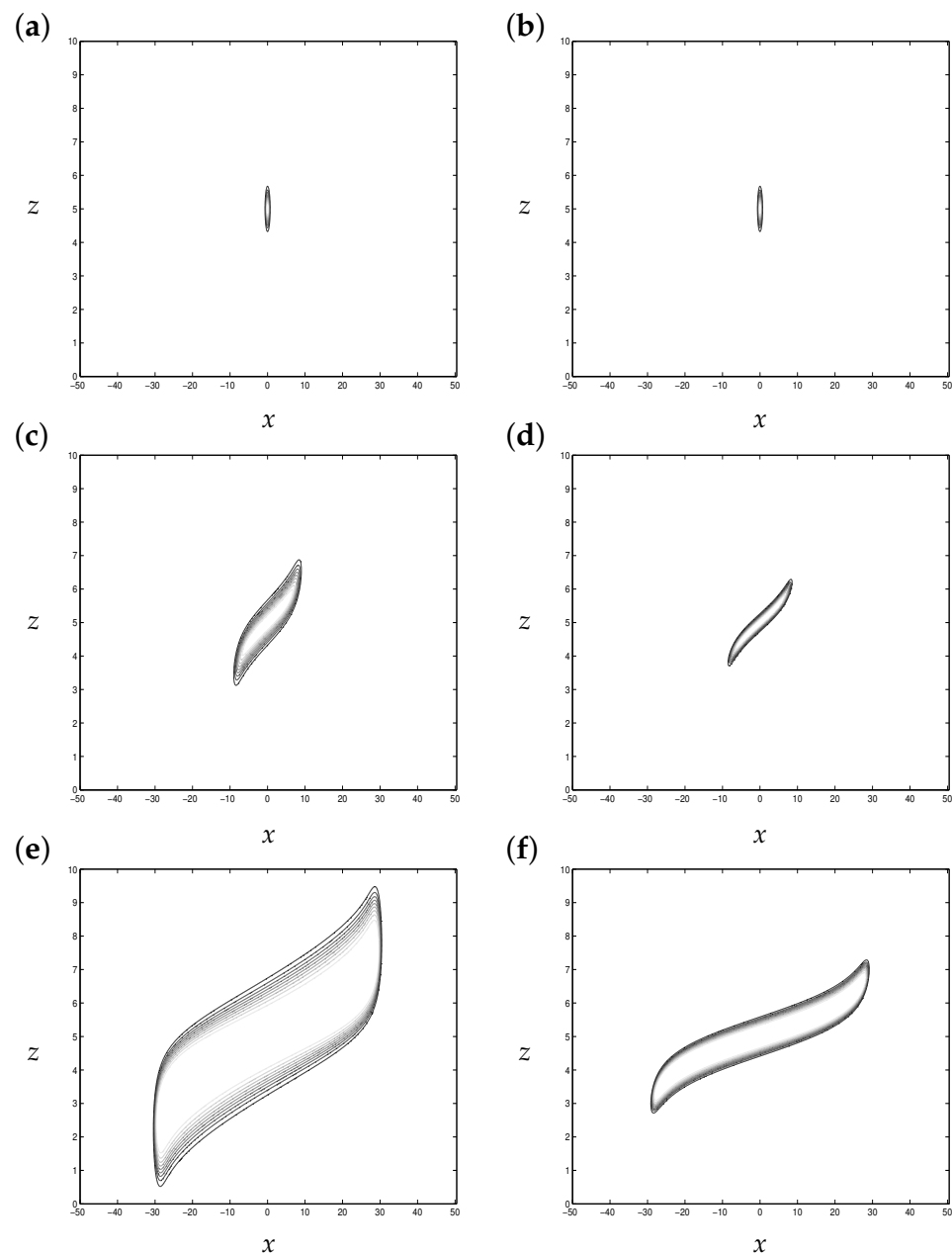


Figure 3. Contour plots of the concentration $C(x, z, t)$ of the two-dimensional Fisher's equation with $U = \tanh(z - 5)$, $W = 0$ and $\sigma = 0.5$. In the first column, (a,c,e), $D = 0.01$, and in the second column, (b,d,f), $D = 0.001$. The plots (a,b) are at $t = 0$, the plots (c,d) are at $t = 10$, and the plots (e,f) are at $t = 30$.

The chemical concentration $C(x, z, t)$, at a fixed horizontal location $x = 0$, is illustrated in Figure 7a. The figure shows the concentration as a function of z at times $t = 10$, $t = 20$ and $t = 40$ for the case with $\sigma = 0.005$ and $\mathcal{D} = 0.001$. These correspond to the contour plots in Figure 5b,d,f, respectively, and show how the vertical profile of the concentration changes as a result of the gravity-wave perturbation. The profile takes the form of an oscillation in z superimposed on the initial Gaussian profile (27). We shall see in Section 5 that this form for the chemical concentration profile is consistent with the asymptotic expressions that are obtained for related configuration.

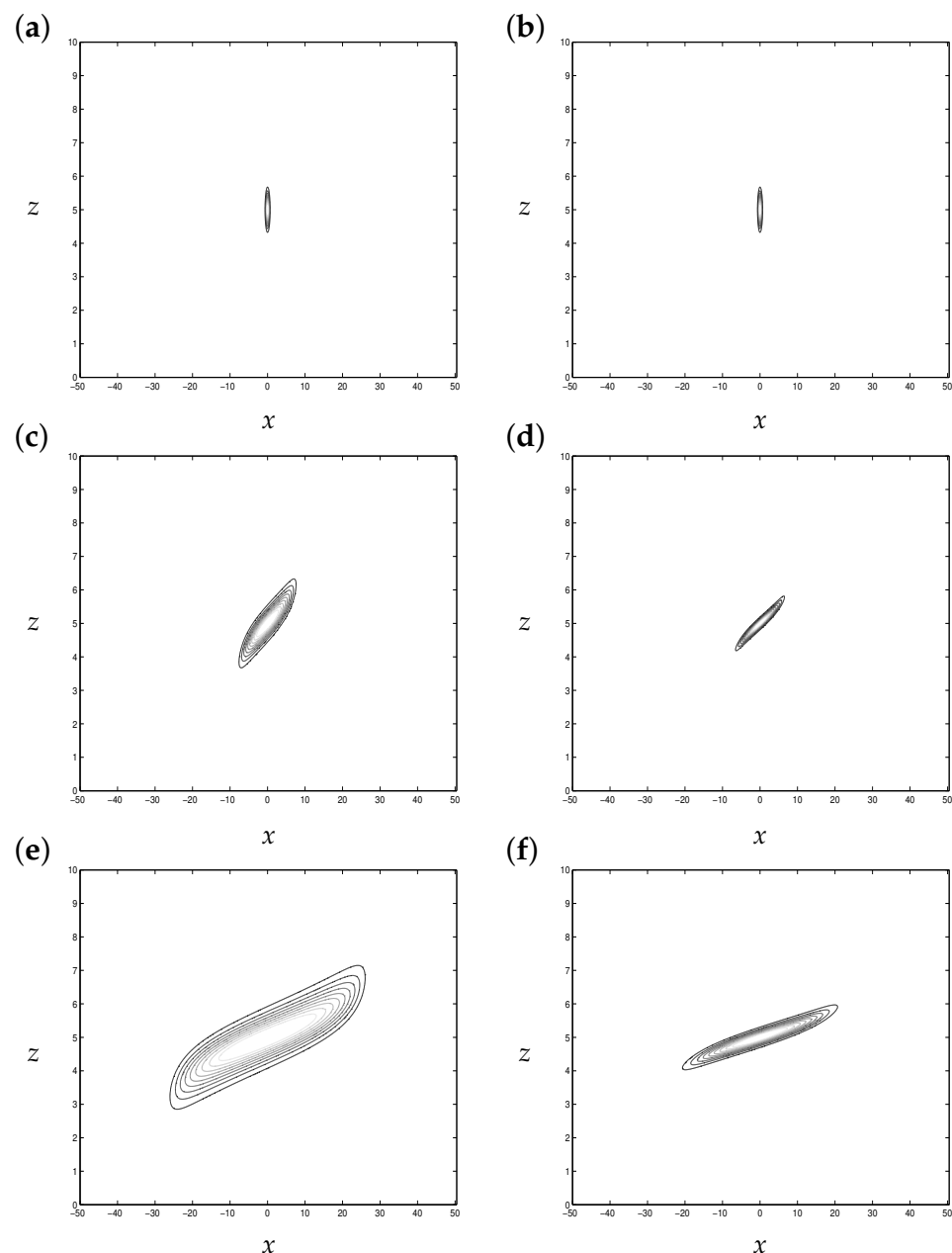


Figure 4. Contour plots of the concentration $C(x, z, t)$ from the solution of Fisher's Equation (5) with $U = \tanh(z - 5)$, $W = 0$ and $\sigma = 0.005$. In the first column, (a,c,e), $\mathcal{D} = 0.01$, and in the second column, (b,d,f), $\mathcal{D} = 0.001$. The plots (a,b) are at $t = 0$, the plots (c,d) are at $t = 10$, and the plots (e,f) are at $t = 30$.

Figure 8 shows the Fourier spectrum of the streamfunction perturbation at the two times $t = 10$ and $t = 40$ corresponding to the contour plots in Figure 5. We note that,

at early time, the magnitude of the zero-wavenumber component is comparable to that of the components of forced wavenumber $k = \pm 2$. At later time, as a result of nonlinearity, the zero-wavenumber component grows and exceeds the $k = \pm 2$ components. The Fourier spectrum of the chemical concentration with and without the effect of gravity waves is shown in Figure 9 at the same two different times. We note that, in the absence of gravity waves, the Fourier spectrum for the chemical (dashed curve) has a Gaussian form centred around the zero wavenumber at both early and late time. However, when gravity waves are present (solid curve) 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 the higher wavenumbers.

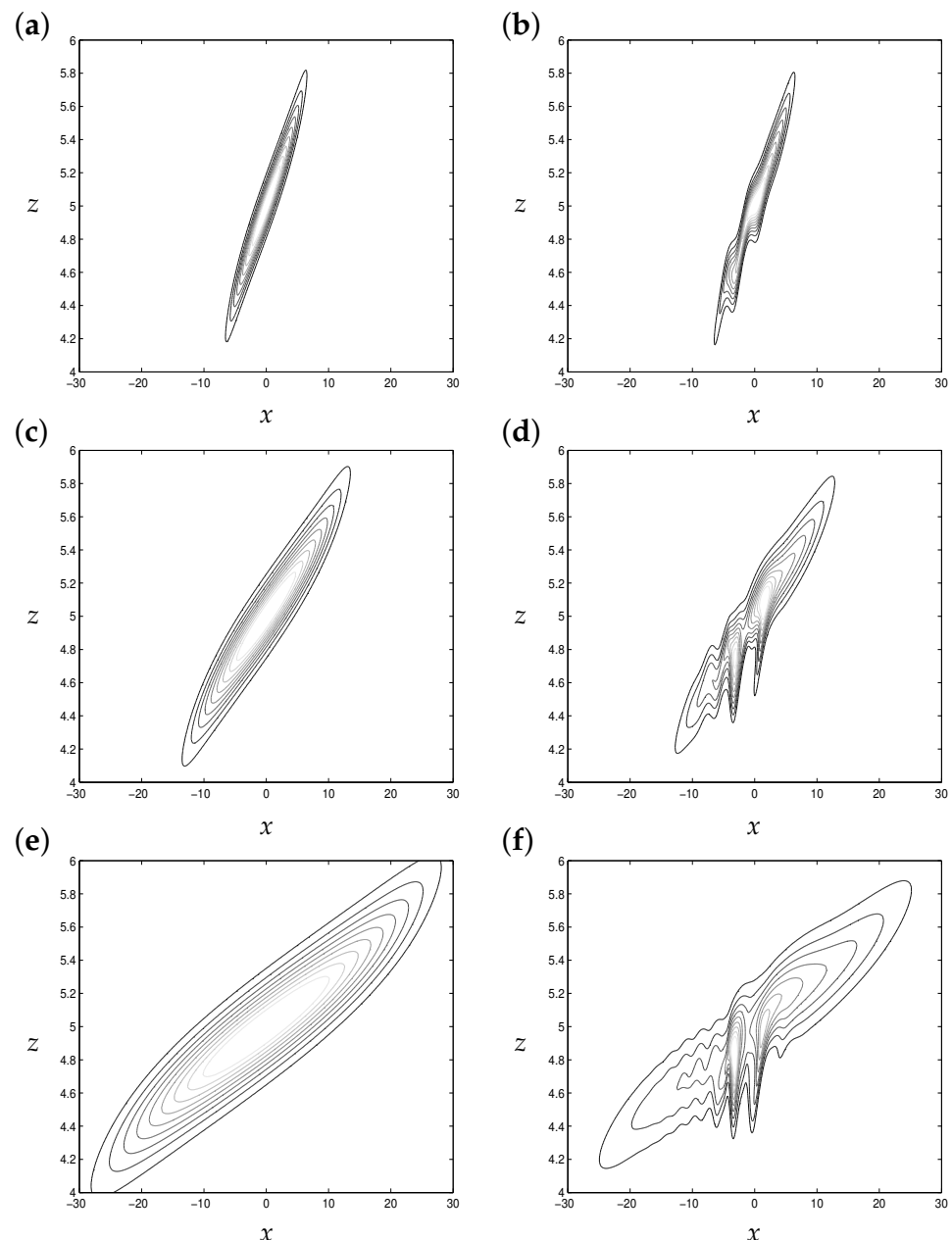


Figure 5. Contour plots of the chemical concentration $C(x, z, t)$ from the numerical solution of (16) with $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$, $W = \varepsilon w(x, z, t)$, $\sigma = 0.005$ and $\mathcal{D} = 0.001$: in the first column, (a,c,e), $\varepsilon = 0$, and in the second column, (b,d,f), $\varepsilon = 0.1$. The plots (a,b) are at $t = 10$, the plots (c,d) are at $t = 20$, and the plots (e,f) are at $t = 40$.

Figure 10 shows the chemical concentration $C(x, z, t)$, at the critical level, as a function of x in the cases with and without the effect of gravity waves. The dashed curve shows the chemical concentration for the case where the advection speed is $\bar{u} = \tanh(z - 5)$ is shown with the dashed curve and the solid curve for the case where the advection speed of the chemical is modified by the gravity-wave perturbation and given by $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$. The effect of the gravity-wave perturbation can be seen especially at later time, in Figure 10b, where we note that these gravity-wave perturbations cause the chemical distribution to have an oscillatory form in the part of the domain where the gravity waves are present.

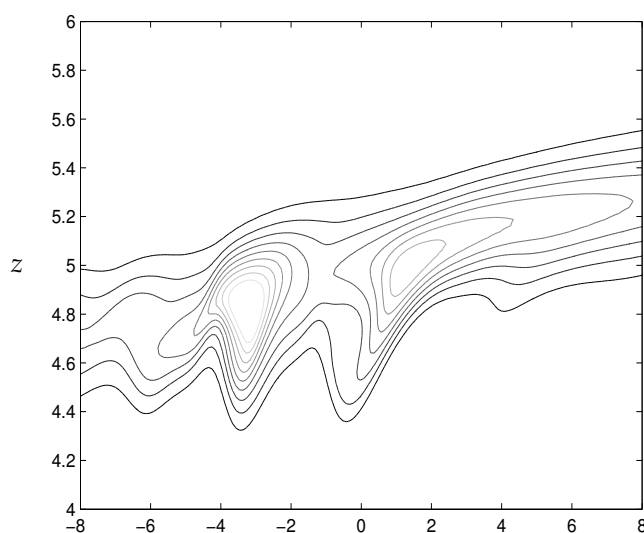


Figure 6. Contour plot of the chemical concentration $C(x, z, t)$ from the numerical solution of (16) with $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$, $W = \varepsilon w(x, z, t)$, $\varepsilon = 0.1$, $\sigma = 0.005$, $\mathcal{D} = 0.001$, $\varepsilon = 0.1$, at $t = 40$. Same as Figure 5f, but over a narrower horizontal interval $-8 \leq x \leq 8$.

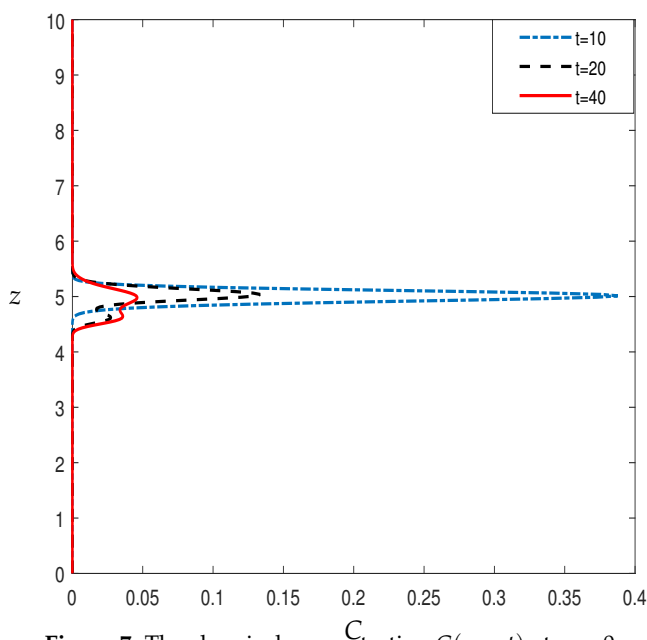


Figure 7. The chemical concentration $C(x, z, t)$ at $x = 0$ as a function of z from the numerical solution of (16) with $U(x, z, t) = \tanh(z - 5) + \varepsilon u(x, z, t)$, $W = \varepsilon w(x, z, t)$, $\varepsilon = 0.1$, $\sigma = 0.005$ and $\mathcal{D} = 0.001$. The dashed-dotted blue curve shows the chemical concentration at $t = 10$, the dashed black curve represents $t = 20$, and the solid red curve represents $t = 40$; these correspond to the contour plots in Figures 5b,d,f, respectively.

These results show that the nonlinear critical level effects of the gravity-wave packet on the background flow have a significant influence on the chemical concentration. This mechanism for dynamical-chemical interactions differs from situations that are addressed in the previous related studies that were discussed in Section 1. The investigation of Xu et al. [14] considered linear equations for gravity waves, with a horizontally oscillatory representation for both the waves and the chemical concentration and no wave-induced mean flow. Xu et al. [15] developed a nonlinear gravity-wave model and showed that gravity-wave effects can induce significant changes in the distribution of several different chemical species; however, the focus of their investigation was on the variations that result from the temperature profile, rather than from the wave-induced mean flow. Liu et al. [16] also developed a nonlinear gravity-wave model and part of their investigation focuses on the effects on chemical species distributions; however, the focus was on gravity waves that break at high altitudes as a result of density-weighted increase in amplitude.

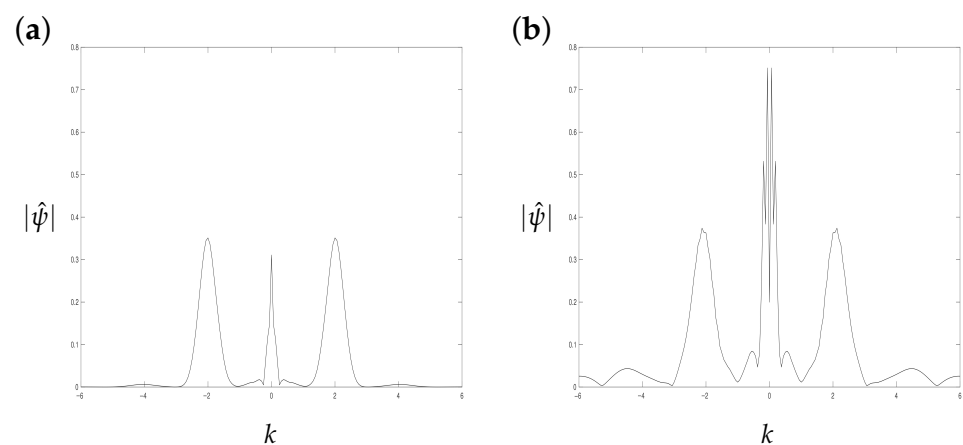


Figure 8. The Fourier spectrum of the perturbation streamfunction $\hat{\psi}(k, z, t)$ at the critical level with $\varepsilon = 0.1$ at (a) $t = 10$ and (b) $t = 40$.

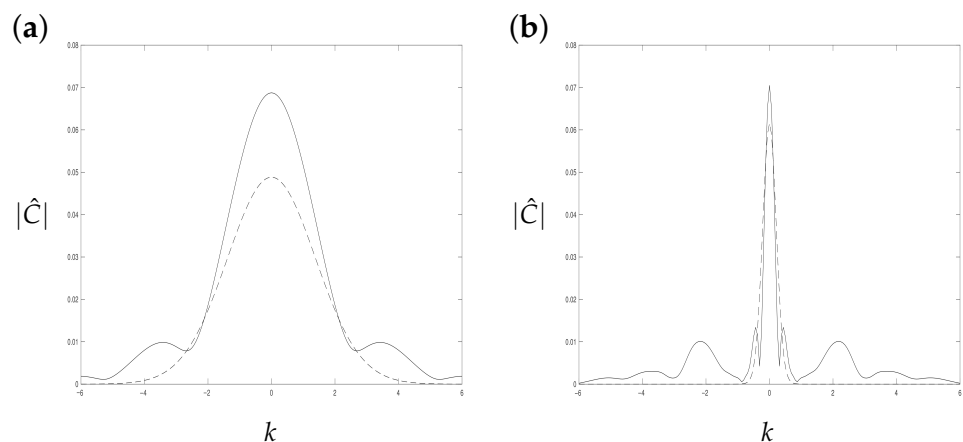


Figure 9. The Fourier spectrum of the chemical concentration $\hat{C}(k, z, t)$ at the critical level at (a) $t = 10$ and (b) $t = 40$. The dashed curves show the Fourier spectrum of the chemical concentration without the effect of gravity-wave perturbation ($\varepsilon = 0$ in (16)), while the solid curves show the Fourier spectrum of the chemical concentration where its advection is affected by the gravity-wave perturbation with $\varepsilon = 0.1$.

We would seek to obtain additional insight into the dependence of the horizontal and vertical profile of the chemical concentration on the forced gravity-wave packet and wave-induced mean flow. We can explore this using asymptotic analyses; however, our choice of background flow and the form of the wave-induced mean flow profile result

in a problem that is not readily tractable to asymptotic methods. In the next section, we introduce a simpler configuration that is qualitatively similar to the configuration that we solved numerically and we present an asymptotic analysis that gives us information on the dominant behaviour of the solutions for the chemical concentration.

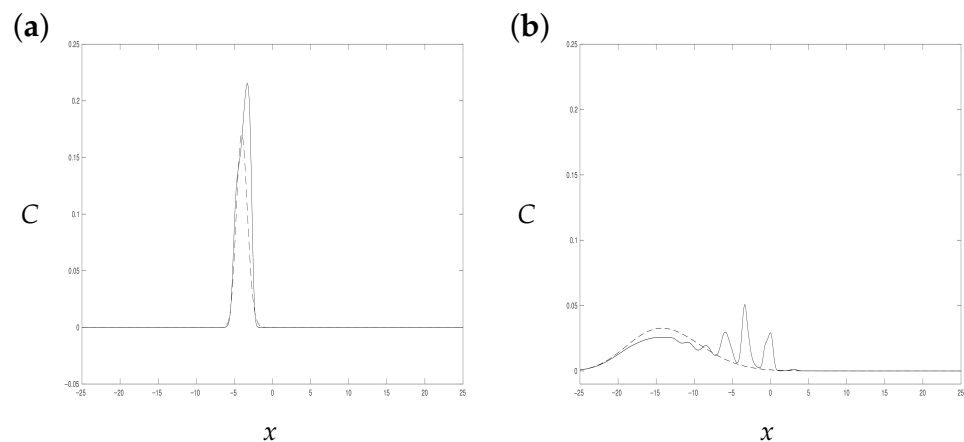


Figure 10. The chemical concentration $C(x, z, t)$ at the critical level as a function of x at (a) $t = 10$ and (b) $t = 40$. The dashed curves show the chemical concentration without the effect of gravity-wave perturbation ($\varepsilon = 0$ in (16)), while the solid curves show the chemical concentration where its advection is affected by the gravity-wave perturbation with $\varepsilon = 0.1$.

5. Asymptotic Analysis

In this section, we present a weakly nonlinear analysis of Equation (16), with $\varepsilon \neq 0$, $\varepsilon \ll 1$, on the domain $-\infty < x < \infty$ and $-\infty < z < \infty$ with $t > 0$. We consider the situation where $\varepsilon \ll \delta$; hence, the $O(\delta)$ x -derivative term in (16) is included at all orders of the analysis in terms of powers of ε .

We consider an initial condition of the form $C(x, z, 0) = \bar{C}(x)$, where $\bar{C}$ is a continuously differentiable function for all x . This corresponds to a wave front, with $\theta = 0$, which propagates in the x direction. We impose the boundary conditions

$$C(x, z, t) \rightarrow 1 \text{ as } x \rightarrow -\infty, \quad (28)$$

and

$$C(x, z, t) \rightarrow 0 \text{ as } x \rightarrow \infty. \quad (29)$$

In general, the background wind speed u is a smooth (infinitely differentiable) function of z , but in this analysis, we consider the case where it varies so slowly with respect to z , i.e., its z -derivatives are small enough relative to ε , that we are able to approximate it by a constant in the analysis at leading order and at $O(\varepsilon)$.

For the purpose of carrying out the asymptotic analysis in this section, the function $\tilde{u}(z)$ is chosen to have a qualitatively similar profile to the wave-induced mean flow profile which we computed numerically in Section 3 and which is shown in Figure 2. Specifically, we impose a form in which $\tilde{u}(z) \rightarrow 0$ as $z \rightarrow \pm\infty$. In the analysis below, we represent $\tilde{u}(z)$ by a function of the form

$$\tilde{u}(z) = e^{-b|z-z_c|} \text{ or } \tilde{u}(z) = e^{-b^2(z-z_c)^2}, \quad (30)$$

where, in each case, b is a positive constant and z_c is the critical level for the gravity waves. The latter choice, the Gaussian profile is illustrated by the dashed blue curve in Figure 11, for the choice of parameter value $b = 5$. This gives a good approximation to the graph of

the numerically computed gravity-wave-induced flow velocity at $t = 40$, the red curve in Figure 2, which is included in Figure 11 for comparison.

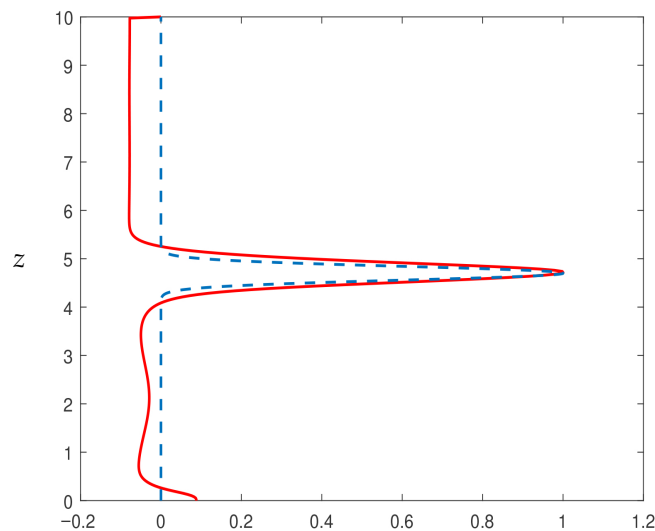


Figure 11. The function $\tilde{u} = e^{-b^2(z-z_c)^2}$ with $b = 5$ is shown by the dashed blue curve. The red curve shows the numerically computed gravity-wave-induced flow velocity given by the solid curve in Figure 2.

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

$$C(x, z, t) = C^{(0)}(x, z, t) + \varepsilon C^{(1)}(x, z, t) + O(\varepsilon^2). \quad (31)$$

We substitute this into Equation (16) and obtain the leading-order equation

$$O(\varepsilon^0) : C_t^{(0)} + \tilde{u} C_x^{(0)} = \delta \mathcal{D} C_{xx}^{(0)} + \mathcal{D} C_{zz}^{(0)} + \sigma C^{(0)}(1 - C^{(0)}). \quad (32)$$

The subscripts denote partial derivatives with respect to x , z and t . When the mean flow is constant, we know that the exact solution of (5) is (6).

Now we consider the case where $W = 0$ and $\theta = 0$. Equation (32) then has an exact z -independent travelling-wave solution given by (6) with $W = 0$ and $\theta = 0$,

$$C^{(0)}(x, z, t) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\delta \mathcal{D}}}(x-ct)}{\sqrt{6}}\right)\right)^2}, \quad (33)$$

where $c = \frac{5\sqrt{\sigma \delta \mathcal{D}}}{\sqrt{6}} + \tilde{u}$. This solution corresponds to the initial condition

$$C^{(0)}(x, z, 0) = \bar{C}(x) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\delta \mathcal{D}}}x}{\sqrt{6}}\right)\right)^2}. \quad (34)$$

and can be expressed in form $C^{(0)}(\xi) = C^{(0)}(x - ct)$, with $\xi = x - ct$, as

$$C^{(0)}(\xi) = \frac{1}{\left(1 + \exp\left(\frac{\sqrt{\frac{\sigma}{\delta \mathcal{D}}}\xi}{\sqrt{6}}\right)\right)^2}. \quad (35)$$

This exact solution is shown in Figure 12 as a function of x at times $t = 0$ and $t = 40$.

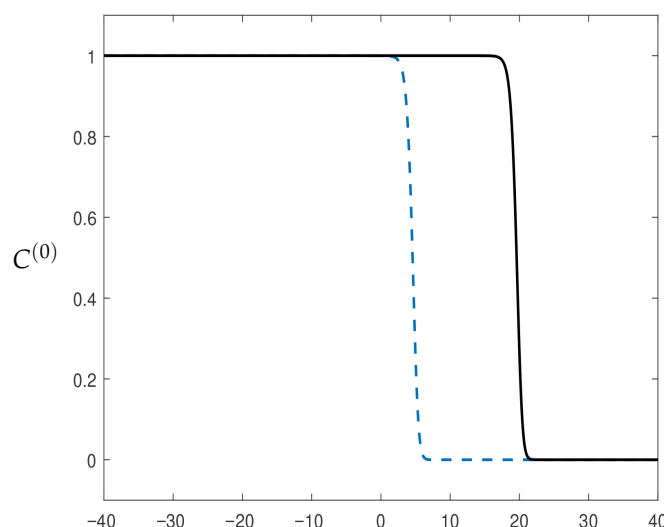


Figure 12. The leading-order solution $C^{(0)}(x, z, t)$ given by the exact expression (33) at different times. The dashed blue curve represents $t = 10$ and the solid black curve represents $t = 40$.

At $O(\varepsilon)$, we have

$$O(\varepsilon) : C_t^{(1)} + \bar{u} C_x^{(1)} - \delta \mathcal{D} C_{xx}^{(1)} - \sigma C^{(1)}(1 - 2C^{(0)}) - \mathcal{D} C_{zz}^{(1)} = -\bar{u}(z) C_x^{(0)}, \quad (36)$$

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

$$C^{(1)}(x, z, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty, \quad (37)$$

and

$$C^{(1)}(x, z, t) \rightarrow 0 \text{ as } z \rightarrow \pm\infty. \quad (38)$$

The solution of (36) depends on $(x - ct)$ and z . Setting $\xi = x - ct$ and $C^{(1)}(\xi, z) = C^{(1)}(x, z, t)$, Equation (36) is rewritten as

$$C_{\xi\xi}^{(1)} + \gamma C_{\xi}^{(1)} - \beta(\xi) C^{(1)} + \frac{1}{\delta} C_{zz}^{(1)} = \bar{u}(z) f(\xi), \quad (39)$$

where $\gamma = \frac{5\sqrt{\sigma}}{\sqrt{6\delta\mathcal{D}}}$, $\beta(\xi) = \frac{\sigma}{\delta\mathcal{D}}(2C^{(0)} - 1)$, $f(\xi) = \frac{1}{\delta\mathcal{D}} C_{\xi}^{(0)}$, 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 with respect to ξ and z .

Equation (39) can be solved using the Fourier transform method. We define $\hat{C}(\xi, \lambda)$ and $\hat{u}(\lambda)$, the Fourier transforms of $C(\xi, \lambda)$ and $\bar{u}(\lambda)$ with respect to z , as

$$\hat{C}(\xi, \lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} C^{(1)}(\xi, z) e^{-i\lambda z} dz \quad (40)$$

and

$$\hat{u}(\lambda) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{u}(z) e^{-i\lambda z} dz. \quad (41)$$

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

$$C^{(1)}(\xi, z) = \int_{-\infty}^{\infty} \hat{C}(\xi, \lambda) e^{i\lambda z} d\lambda \quad (42)$$

and

$$\bar{u}(z) = \int_{-\infty}^{\infty} \hat{u}(\lambda) e^{i\lambda z} d\lambda. \quad (43)$$

Taking the Fourier transform of Equation (39) using the definitions (40) and (41), the transformed equation, for each Fourier mode λ , is

$$\hat{C}_{\xi\xi}(\xi, \lambda) + \gamma\hat{C}_{\xi}(\xi, \lambda) - \left(\beta(\xi) + \frac{1}{\delta}\lambda^2\right)\hat{C}(\xi, \lambda) = f(\xi)\hat{u}(\lambda), \quad (44)$$

with $\hat{C}(\xi, \lambda) \rightarrow 0$ as $\xi \rightarrow \pm\infty$. Equation (44) is a nonhomogeneous 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 homogeneous equation and a particular solution of the corresponding nonhomogeneous equation. We first discuss the solution of the corresponding homogeneous equation

$$\hat{C}_{\xi\xi} + \gamma\hat{C}_{\xi} - \left(\beta(\xi) + \frac{1}{\delta}\lambda^2\right)\hat{C} = 0, \quad (45)$$

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 [40]) to obtain an asymptotic approximations.

We rewrite Equation (45) in a form that is compatible with the WKB theory by introducing $Q(\xi, \lambda)$ and writing the solution as $\hat{C}_h(\xi, \lambda) = e^{-\frac{\gamma}{2}\xi}Q(\xi, \lambda)$. Equation (45) can then be written as

$$Q_{\xi\xi}(\xi, \lambda) - \left(\frac{\gamma^2}{4} + \beta(\xi) + \frac{1}{\delta}\lambda^2\right)Q(\xi, \lambda) = 0. \quad (46)$$

Setting $P(\xi, \lambda) = \beta(\xi) + \frac{1}{\delta}\lambda^2 + \frac{\gamma^2}{4}$, Equation (46) is rewritten as

$$Q_{\xi\xi}(\xi, \lambda) - P(\xi, \lambda)Q(\xi, \lambda) = 0. \quad (47)$$

As is known about the WKB method, if $P_{\xi} \ll P^{\frac{3}{2}}$, then P is slowly varying with respect to ξ , and the WKB method is valid.

We first consider the limit $\xi \rightarrow -\infty$,

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

As $\xi \rightarrow \infty$, we have

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

which indicates that $\frac{P_{\xi}}{2P^{\frac{3}{2}}} \ll 1$ as $\xi \rightarrow \pm\infty$ and means that P is slowly varying and the WKB approximation is valid as $\xi \rightarrow \pm\infty$.

As $\xi \rightarrow 0$, we find that

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

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

Since $\frac{P_\xi}{P^2} \ll 1$ as $\xi \rightarrow \pm\infty$ and $P(\xi)$ varies slowly, the WKB approximations are expressed in terms of ξ as

$$Q(\xi, \lambda) \sim \frac{e^{\pm i \int \sqrt{-P(\xi, \lambda)} d\xi}}{(-P(\xi, \lambda))^{\frac{1}{4}}}, \quad \text{if } P(\xi, \lambda) < 0, \quad (48)$$

and

$$Q(\xi, \lambda) \sim \frac{e^{\pm i \int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}}, \quad \text{if } P(\xi, \lambda) > 0. \quad (49)$$

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

From (35), 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 $1 > C^{(0)}(\xi) > 0$ which implies that $1 > 2C^{(0)}(\xi) - 1 > -1$ and

$$\frac{\sigma}{\delta \mathcal{D}} > \frac{\sigma}{\delta \mathcal{D}} (2C^{(0)}(\xi) - 1) > -\frac{\sigma}{\delta \mathcal{D}}$$

which implies

$$\frac{\sigma}{\delta \mathcal{D}} + \frac{\gamma^2}{4} + \frac{1}{\delta} \lambda^2 > \frac{\sigma}{\delta \mathcal{D}} (2C^{(0)}(\xi) - 1) + \frac{\gamma^2}{4} + \frac{1}{\delta} \lambda^2 > -\frac{\sigma}{\delta \mathcal{D}} + \frac{\gamma^2}{4} + \frac{1}{\delta} \lambda^2.$$

The last inequality can be written as

$$L(\lambda) > P(\xi, \lambda) > R(\lambda),$$

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 the function $Q(\xi, \lambda)$ in (49) can be approximated by an exponentially growing or decaying function.

Thus, the solution of the homogeneous Equation (45), $\hat{C}(\xi, \lambda) = e^{-\frac{\gamma}{2}\xi} Q(\xi, \lambda)$ can be written as an asymptotic approximation

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi} + a_2(\lambda) \frac{e^{-\int \sqrt{P(\xi, \lambda)} d\xi}}{P(\xi, \lambda)^{\frac{1}{4}}} e^{-\frac{\gamma}{2}\xi} \quad \text{as } \xi \rightarrow \pm\infty. \quad (50)$$

The solution of the nonhomogeneous Equation (44) is

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

where $\hat{C}_h(\xi, \lambda)$ is the homogeneous solution given by (50) and $\hat{C}_p(\xi, \lambda)$ is the particular solution $\hat{C}_p(\xi, \lambda)$. Using the method of variation in parameters, the particular solution can be found as

$$\hat{C}_p(\xi, \lambda) = -\hat{C}_1 \int \frac{\hat{u}(\lambda) \hat{C}_2 f(\xi)}{W(\hat{C}_1, \hat{C}_2)} d\xi + \hat{C}_2 \int \frac{\hat{u}(\lambda) \hat{C}_1 f(\xi)}{W(\hat{C}_1, \hat{C}_2)} d\xi, \quad (51)$$

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 $W(\hat{C}_1, \hat{C}_2)(\xi, \lambda)$ is the Wronskian, given by $W(\hat{C}_1, \hat{C}_2) = \hat{C}_1 \frac{\partial}{\partial \xi} \hat{C}_2 - \hat{C}_2 \frac{\partial}{\partial \xi} \hat{C}_1$.

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

$$\hat{C}_h(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}}, \quad \text{as } \xi \rightarrow -\infty. \quad (52)$$

The particular solution $\hat{C}_p$ can then be approximated as $\xi \rightarrow -\infty$, by

$$\begin{aligned} \hat{C}_p(\xi, \lambda) &\sim -\hat{u}(\lambda) \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} L^{\frac{1}{2}}} \int e^{(-\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi} d\xi \\ &\quad + \hat{u}(\lambda) \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} L^{\frac{1}{2}}} \int e^{(\sqrt{L}+\frac{\gamma}{2}+\frac{1}{\sqrt{6}})\xi} d\xi \\ &\sim \frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-L + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right). \end{aligned} \quad (53)$$

Thus, the asymptotic solution of the nonhomogeneous Equation (44), as $\xi \rightarrow -\infty$, is

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{L}-\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{L}+\frac{\gamma}{2})\xi}}{L^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-L + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right). \quad (54)$$

In order to satisfy the boundary condition that $\hat{C} \rightarrow 0$ as $\xi \rightarrow -\infty$, given in (44), we note that since $\gamma > 0$ we must choose $a_2(\lambda) = 0$, and, for $a_1(\lambda) \neq 0$, we need to have $\sqrt{L} - \frac{\gamma}{2} > 0$; i.e., we need $\sqrt{\frac{\gamma^2}{4} + \frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2} > \frac{\gamma}{2}$ which means $\frac{\sigma}{\delta \mathcal{D}} + \frac{1}{\delta} \lambda^2 > 0$. This inequality is always satisfied since all the parameters are positive.

Next we consider the limit $\xi \rightarrow \infty$, and following the same procedure as above, the WKB approximation for the homogeneous Equation (45), valid as $\xi \rightarrow \infty$, is

$$\hat{C}_h(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}}, \quad (55)$$

and a particular solution of the nonhomogeneous Equation (44) can be approximated, as $\xi \rightarrow \infty$, by

$$\begin{aligned} \hat{C}_p(\xi, \lambda) &\sim \hat{u}(\lambda) \frac{2e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} R^{\frac{1}{2}}} \int \left(\frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi} e^{\frac{-2\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi \\ &\quad - \hat{u}(\lambda) \frac{2e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{\delta \mathcal{D} \sqrt{6} R^{\frac{1}{2}}} \int \left(\frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi} e^{\frac{-2\xi}{\sqrt{6}}}}{-2e^{-\gamma\xi}} \right) d\xi \\ &\sim \frac{\hat{u}(\lambda) e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-R - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right). \end{aligned} \quad (56)$$

Therefore, an asymptotic approximation for the solution of the nonhomogeneous Equation (44), as $\xi \rightarrow \infty$, is

$$\hat{C}(\xi, \lambda) \sim a_1(\lambda) \frac{e^{(\sqrt{R}-\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + a_2(\lambda) \frac{e^{-(\sqrt{R}+\frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-R - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right). \quad (57)$$

As noted before, $\sqrt{R} > 0$ and $\gamma > 0$ and in order to satisfy the boundary condition $\hat{C} \rightarrow 0$ as $\xi \rightarrow \infty$, given in (44), we must choose $a_1(\lambda) = 0$ if $\sqrt{R} - \frac{\gamma}{2} \geq 0$. To satisfy the zero boundary condition with $a_1(\lambda) \neq 0$, we must have

$$\sqrt{R} - \frac{\gamma}{2} < 0$$

which means $\sqrt{\frac{\gamma^2}{4} - \frac{\sigma}{\delta D} + \frac{1}{\delta} \lambda^2} < \frac{\gamma}{2}$ or $\lambda^2 < \frac{\sigma}{D}$.

In summary, an asymptotic solution of the nonhomogeneous Equation (44), as $\xi \rightarrow -\infty$, is (54). As $\xi \rightarrow \infty$, an asymptotic solution of (44) is (57); i.e., we have

$$\hat{C}(\xi, \lambda) \sim \begin{cases} \text{Expression (54)}, & \text{as } \xi \rightarrow -\infty; \\ \text{Expression (57)}, & \text{as } \xi \rightarrow \infty. \end{cases}$$

To find $C^{(1)}(\xi, z)$ as $\xi \rightarrow \pm\infty$, we apply the inverse Fourier transform given by (42). As $\xi \rightarrow -\infty$, we find

$$C^{(1)}(\xi, z) \sim \int_{-\infty}^{\infty} \left(a_1(\lambda) \frac{e^{(\sqrt{L(\lambda)} - \frac{\gamma}{2})\xi}}{L(\lambda)^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta D \sqrt{6}} \left(\frac{-2}{-L(\lambda) + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right) \right) e^{i\lambda z} d\lambda. \quad (58)$$

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. The inequality $\sqrt{L(\lambda)} - \frac{\gamma}{2} > \frac{1}{\sqrt{6}}$ means that $\sqrt{\frac{\gamma^2}{4} + \frac{\sigma}{\delta D} + \frac{1}{\delta} \lambda^2} > \frac{\gamma}{2} + \frac{1}{\sqrt{6}}$ and this holds if and only if

$$\lambda^2 > -\frac{\sigma}{D} + \delta \left(\frac{\gamma}{\sqrt{6}} + \frac{1}{6} \right). \quad (59)$$

For wave modes where the condition (59) is satisfied, the second term on the right-hand side of (58) is dominant; otherwise, the first term is dominant. If the parameters are chosen such that the right-hand side of (59) is negative, then the condition (59) is satisfied for all λ . In that case, the second term which corresponds to the particular solution is the dominant term and $C^{(1)}(\xi, z)$ can be approximated as $\xi \rightarrow -\infty$, by

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \int_{-\infty}^{\infty} \left(\frac{\hat{u}(\lambda) e^{\frac{\xi}{\sqrt{6}}}}{\delta D \sqrt{6}} \left(\frac{-2}{-L(\lambda) + \frac{\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{1}{6}} \right) \right) e^{i\lambda z} d\lambda \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{D \sqrt{6}} \int_{-\infty}^{\infty} \hat{u}(\lambda) \frac{1}{(\lambda^2 + \frac{\sigma}{D} - \frac{\delta \gamma}{\sqrt{6}} - \frac{\delta}{6})} e^{i\lambda z} d\lambda \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{D \sqrt{6}} \int_{-\infty}^{\infty} G(\lambda) \hat{u}(\lambda) e^{i\lambda z} d\lambda, \end{aligned} \quad (60)$$

where $G(\lambda) = \frac{1}{(\lambda^2 + a^2)}$ and $a^2 = \frac{\sigma}{D} - \delta \left(\frac{\gamma}{\sqrt{6}} + \frac{1}{6} \right)$. Comparing the expression (60) with the condition (59), we note that a^2 has the opposite sign to the right-hand side of (59). Thus, the expression for a^2 is positive and a is real.

The expression (60) depends on the choice of the function $\tilde{u}$. We consider the two choices suggested in (30).

5.1. The Case with $\tilde{u} = e^{-b|z-z_c|}$

To evaluate the expression (60) with the choice of $\tilde{u} = e^{-b|z-z_c|}$, we make use of the Fourier transform

$$\mathcal{F}(e^{-a|z|}) = \frac{1}{\pi} \left(\frac{a}{\lambda^2 + a^2} \right) \quad (61)$$

The Fourier transform of $\tilde{u}(z) = e^{-b|z-z_c|}$ is

$$\hat{u}(\lambda) = \mathcal{F}(e^{-b|z-z_c|}) = e^{-i\lambda z_c} \mathcal{F}(e^{-b|z|}) = \frac{e^{-i\lambda z_c}}{\pi} \left(\frac{b}{b^2 + \lambda^2} \right), \quad (62)$$

by the Fourier shifting theorem. Using Formula (61), we note that $G(\lambda) = \frac{1}{2a} \mathcal{F}(e^{-a|z|})$ and thus the inverse transform of $G(\lambda)$ is $g(z) = e^{-a|z|}$.

The asymptotic approximation (60) can be expressed using the Fourier convolution theorem as

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} \mathcal{F}(g)\mathcal{F}(\tilde{u}) e^{i\lambda z} d\lambda \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \mathcal{F}^{-1}(\mathcal{F}(g)\mathcal{F}(\tilde{u})) \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} g(\tau) \tilde{u}(z - \tau) d\tau \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \int_{-\infty}^{\infty} e^{-a|\tau|} e^{-b|\tilde{z}-\tau|} d\tau, \end{aligned} \quad (63)$$

where $\tilde{z} = z - z_c$.

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

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\int_{-\infty}^{\tilde{z}} e^{a\tau} e^{-b(\tilde{z}-\tau)} d\tau + \int_{\tilde{z}}^0 e^{a\tau} e^{b(\tilde{z}-\tau)} d\tau + \int_0^{\infty} e^{-a\tau} e^{b(\tilde{z}-\tau)} d\tau \right) \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(e^{-b\tilde{z}} \left[\frac{e^{(a+b)\tau}}{a+b} \right]_{-\infty}^{\tilde{z}} + e^{b\tilde{z}} \left[\frac{e^{(a-b)\tau}}{a-b} \right]_{\tilde{z}}^0 - e^{b\tilde{z}} \left[\frac{e^{-(a+b)\tau}}{a+b} \right]_0^{\infty} \right), \end{aligned} \quad (64)$$

If $a \geq 0$ or $a < 0$ with $|a| < b$, we have

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\frac{e^{a\tilde{z}}}{a+b} + \frac{e^{b\tilde{z}} - e^{a\tilde{z}}}{a-b} + \frac{e^{b\tilde{z}}}{a+b} \right), \quad (65)$$

otherwise, we could have a divergent approximation. For $\tilde{z} \geq 0$, we have

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\int_{-\infty}^0 e^{a\tau} e^{-b(\tilde{z}-\tau)} d\tau + \int_0^{\tilde{z}} e^{-a\tau} e^{-b(\tilde{z}-\tau)} d\tau + \int_{\tilde{z}}^{\infty} e^{-a\tau} e^{b(\tilde{z}-\tau)} d\tau \right) \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(e^{-b\tilde{z}} \left[\frac{e^{(a+b)\tau}}{a+b} \right]_{-\infty}^0 + e^{-b\tilde{z}} \left[\frac{e^{(b-a)\tau}}{b-a} \right]_0^{\tilde{z}} - e^{b\tilde{z}} \left[\frac{e^{-(a+b)\tau}}{a+b} \right]_{\tilde{z}}^{\infty} \right) \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2a\mathcal{D}\sqrt{6}} \left(\frac{e^{-b\tilde{z}}}{a+b} + \frac{e^{-a\tilde{z}} - e^{-b\tilde{z}}}{b-a} + \frac{e^{-a\tilde{z}}}{a+b} \right), \end{aligned} \quad (66)$$

for $a \geq 0$ or $a < 0$ with $|a| < b$.

An asymptotic approximation for $C^{(1)}(\xi, z)$, as $\xi \rightarrow \infty$, is

$$C^{(1)}(\xi, z) \sim \int_{-\infty}^{\infty} \left(a_2(\lambda) \frac{e^{-(\sqrt{R} + \frac{\gamma}{2})\xi}}{R^{\frac{1}{4}}} + \frac{\hat{u}(\lambda) e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \left(\frac{-2}{-R(\lambda) - \frac{2\gamma}{\sqrt{6}} + \frac{\gamma^2}{4} + \frac{2}{3}} \right) \right) e^{i\lambda z} d\lambda \quad (67)$$

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 , i.e., if

$$\sqrt{\frac{\lambda^2}{\delta} + \frac{\sigma}{24\delta\mathcal{D}}} > \frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6\delta\mathcal{D}}}. \quad (68)$$

If $\frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6\delta\mathcal{D}}} < 0$, then (68) is satisfied for all λ . Otherwise, if $\frac{2}{\sqrt{6}} - \frac{5\sqrt{\sigma}}{2\sqrt{6\delta\mathcal{D}}} > 0$, then (68) holds if and only if

$$\begin{aligned} \frac{\lambda^2}{\delta} + \frac{\sigma}{24\delta\mathcal{D}} &> \frac{25\sigma}{24\delta\mathcal{D}} - \frac{10\sqrt{\sigma}}{6\sqrt{\delta\mathcal{D}}} + \frac{4}{6} \\ \lambda^2 &> \frac{\sigma}{\mathcal{D}} + \delta \left(\frac{4}{6} - \frac{10\sqrt{\sigma}}{6\sqrt{\delta\mathcal{D}}} \right). \end{aligned} \quad (69)$$

If the condition (69) is satisfied for all λ , we can approximate $C^{(1)}(\xi, z)$ as $\xi \rightarrow \infty$ by

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{-2\xi}{\sqrt{6}}}}{\delta \mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \frac{1}{(-\frac{\lambda^2}{\delta} + \frac{\sigma}{\delta\mathcal{D}} - \frac{2\gamma}{\sqrt{6}} + \frac{2}{3})} \hat{u} e^{i\lambda z} d\lambda \\ &\sim \frac{e^{\frac{-2\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \frac{1}{\lambda^2 - \frac{\sigma}{\mathcal{D}} + \delta \left(\frac{2\gamma}{\sqrt{6}} - \frac{2}{3} \right)} \hat{u} e^{i\lambda z} d\lambda \\ &\sim \frac{e^{\frac{-2\xi}{\sqrt{6}}}}{\mathcal{D} \sqrt{6}} \int_{-\infty}^{\infty} \tilde{G}(\lambda) \hat{u} e^{i\lambda z} d\lambda, \end{aligned} \quad (70)$$

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 (69), $\tilde{a}^2$ 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 $\tilde{z} \leq 0$, (70) is approximated as

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{-2\xi}{\sqrt{6}}}}{2\tilde{a}\mathcal{D}\sqrt{6}} \left(\frac{e^{\tilde{a}\tilde{z}}}{\tilde{a} + b} + \frac{e^{b\tilde{z}} - e^{\tilde{a}\tilde{z}}}{\tilde{a} - b} + \frac{e^{b\tilde{z}}}{\tilde{a} + b} \right), \quad (71)$$

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

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{-2\xi}{\sqrt{6}}}}{2\tilde{a}\mathcal{D}\sqrt{6}} \left(\frac{e^{-b\tilde{z}}}{\tilde{a} + b} + \frac{e^{-\tilde{a}\tilde{z}} - e^{-b\tilde{z}}}{b - \tilde{a}} + \frac{e^{-\tilde{a}\tilde{z}}}{\tilde{a} + b} \right). \quad (72)$$

In summary, for the case where $\tilde{u} = e^{-b|z-z_c|}$, the asymptotic approximation for $C^{(1)}(\xi, z)$ takes the form

$$C^{(1)}(\xi, z) \sim \frac{f(\xi)}{a\mathcal{D}\sqrt{6}} \left(\frac{a e^{-b|z-z_c|} - b e^{-a|z-z_c|}}{a^2 - b^2} \right). \quad (73)$$

This approximation is valid as for all z . For $\xi \rightarrow -\infty$, we have $f(\xi) = e^{\frac{\xi}{\sqrt{6}}}$ and for $\xi \rightarrow \infty$, we have $f(\xi) = e^{\frac{-2\xi}{\sqrt{6}}}$ and a is replaced by $\tilde{a}$. In each case, the dominant term in the expression as $z \rightarrow \infty$ depends on the magnitude of the constant a or $\tilde{a}$, relative to the value of the parameter b .

5.2. The Case with $\tilde{u} = e^{-b^2(z-z_c)^2}$

In this subsection, we consider the configuration in which $\tilde{u} = e^{-b^2(z-z_c)^2}$, as shown in Figure 11. This form of $\tilde{u}$ is comparable with the gravity-wave-induced mean flow shown in Figure 2; thus, it is mathematically considered here to imitate the wave-induced mean flow.

To evaluate the expression (60) with the choice of $\tilde{u} = e^{-b^2(z-z_c)^2}$, we again apply the shifting theorem and evaluate the Fourier transform

$$\begin{aligned} \hat{u}(\lambda) &= \mathcal{F}(e^{-b^2(z-z_c)^2}) = e^{-i\lambda z_c} \mathcal{F}(e^{-b^2 z^2}) \\ &= \frac{e^{-i\lambda z_c}}{2\pi} \int_{-\infty}^{\infty} e^{-b^2 z^2} e^{-i\lambda z} d\bar{z} = \frac{e^{-i\lambda z_c}}{2b\sqrt{\pi}} e^{\frac{-\lambda^2}{4b^2}}. \end{aligned} \quad (74)$$

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

$$C^{(1)}(\xi, z) \sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{2b\mathcal{D}\sqrt{\pi}\sqrt{6}} \int_{-\infty}^{\infty} G(\lambda) e^{\frac{-\lambda^2}{4b^2}} e^{-i\lambda z_c} e^{i\lambda z} d\lambda. \quad (75)$$

We note that the Gaussian function $e^{\frac{-\lambda^2}{4b^2}}$ is the controlling factor in the integrand in (75), and that the dominant contribution to the integral comes from an interval of λ values around $\lambda = 0$ where the Gaussian function is maximum. Thus, we expand $G(\lambda)$ about $\lambda = 0$ in (75) and obtain

$$\begin{aligned} C^{(1)}(\xi, z) &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}b\sqrt{\pi}\sqrt{6}} \int_{-\infty}^{\infty} \left(\frac{1}{a^2} - \frac{1}{a^4}\lambda^2 + \frac{1}{a^6}\lambda^4 + O(\lambda^6) \right) e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda \\ &\sim \frac{e^{\frac{\xi}{\sqrt{6}}}}{\mathcal{D}b\sqrt{\pi}\sqrt{6}} \left[\frac{1}{a^2} \int_{-\infty}^{\infty} e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda - \frac{1}{a^4} \int_{-\infty}^{\infty} \lambda^2 e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda \right. \\ &\quad \left. + \frac{1}{a^6} \int_{-\infty}^{\infty} \lambda^4 e^{\frac{-\lambda^2}{4b^2}} e^{i\lambda(z-z_c)} d\lambda + O(\lambda^6) \right]. \end{aligned} \quad (76)$$

We evaluate the following integrals using integration by parts:

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}}, \quad (77)$$

$$\int_{-\infty}^{\infty} x^2 e^{-ax^2+bx} dx = \frac{\sqrt{\pi}(2a+b^2)}{4a^{5/2}} e^{\frac{b^2}{4a}}, \quad (78)$$

and

$$\int_{-\infty}^{\infty} x^4 e^{-ax^2+bx} dx = \frac{\sqrt{\pi}(12a^2+12ab^2+b^4)}{16a^{9/2}} e^{\frac{b^2}{4a}}. \quad (79)$$

Evaluating the integrals in (76) using (77)–(79), we obtain an asymptotic approximation for $C^{(1)}(\xi, z)$, as $\xi \rightarrow -\infty$. Similarly, following the same approach, we find that an asymptotic approximation for $C^{(1)}(\xi, z)$, as $\xi \rightarrow \infty$.

In summary, for the case where $\tilde{u} = e^{-b(z-z_c)^2}$, the asymptotic approximation for $C^{(1)}(\xi, z)$ takes the form

$$C^{(1)}(\xi, z) \sim \frac{f(\xi)e^{-b^2(z-z_c)^2}}{\mathcal{D}b\sqrt{6}} \left[\frac{2b}{a^2} - \frac{1}{a^4} \left(\frac{\frac{1}{2b^2} - (z-z_c)^2}{4\left(\frac{1}{2b}\right)^5} \right) + \frac{1}{a^6} \left(\frac{\frac{6}{8b^4} - \frac{12}{4b^2}(z-z_c)^2 + (z-z_c)^4}{16\left(\frac{1}{2b}\right)^9} \right) \right]. \quad (80)$$

For $\xi \rightarrow -\infty$, we have $f(\xi) = e^{\frac{\xi}{\sqrt{6}}}$ and for $\xi \rightarrow \infty$, we have $f(\xi) = e^{-\frac{2\xi}{\sqrt{6}}}$ and a is replaced by $\tilde{a}$. In each case, the controlling factor which describes the dominant behaviour as $z \rightarrow \infty$, is given by the Gaussian function with the parameter b . This indicates that, at this order, the profile of the chemical concentration perturbation takes the same form as the profile of the imposed mean flow perturbation $\tilde{u}(z)$.

We illustrate the form of this asymptotic solution in Figure 13a by plotting $\varepsilon C^{(1)}$ as a function of z for the fixed horizontal location, $x = 0$, and at times $t = 10, 20, 40$. We set parameter values $\sigma = 0.5$, $\mathcal{D} = 0.001$, $\delta = 0.2$, $b = 5$ and a constant initial flow speed of $\tilde{u} = 0.1$. These values give a travelling wave speed of $c > 0$; thus, $\xi = x - ct$ is negative, and the asymptotic approximation is (80) with $f(\xi) = e^{\frac{\xi}{\sqrt{6}}}$. The profile of the solution is localized in the vertical direction due to the Gaussian controlling factor.

We may compare this with the corresponding plots of the numerical solution shown in Figure 7. However, it is important to note that there are significant differences between the configuration used for the numerical solutions in Section 4 and that studied analytically in this section. Specifically, in the numerical study, the initial chemical concentration is given by a Gaussian function of x and z (27), the background wind has vertical shear and takes the form $\tilde{u} = \tanh(z - z_c)$, and the gravity-wave perturbation has horizontal and vertical velocity components u and w which modify the background flow and affect the chemical propagation. In contrast, for the asymptotic analysis in this section, we considered a simpler configuration that allows us to obtain asymptotic approximations. The initial chemical concentration (34) is independent of z , the background wind is constant, and the perturbation to the background wind has a horizontal component only, given by (30). We, therefore, cannot expect close agreement with the numerical solutions of Section 4. In spite of these differences, we note that the asymptotic solutions in Figure 13a are consistent with the numerical solutions shown in Figure 7; in particular, we note that the controlling factor of the chemical concentration profile is of the same form as the profile of the gravity-wave perturbation.

In order to carry out a more consistent comparison, we present the results of some additional numerical computations carried out for the same configuration that was studied in the asymptotic analysis with initial chemical concentration $\tilde{C}(x)$, given by (34) and background wind perturbation (30). We use the same numerical discretization methods as in Section 4 and set the same parameter values used for Figure 13a with $\varepsilon = 0.1$ and with the same initial amplitude.

The numerical solution $C_{\text{numerical}}(x, z, t)$ can be compared with the asymptotic solution $C^{(0)} + \varepsilon C^{(1)}$. To do so, we compute $\Delta C(x, z, t) = C_{\text{numerical}}(x, z, t) - C^{(0)}(x, z, t)$, the difference between the numerical solution and the exact leading-order solution. In Figure 13b, we plot ΔC for $x = 0$ and at the same times used for the graphs of $\varepsilon C^{(1)}$ in Figure 13a.

We recall that in making the asymptotic approximation, the neglected terms are $O(\varepsilon^2)$, according to (31). Thus, we expect a difference of this order between the numerical solution and the asymptotic approximation. As t increases, the amplitude of the asymptotic approximation decreases according to $e^{-ct/\sqrt{6}}$, while the vertical profile takes the form $e^{-b^2(z-z_c)^2}$. The numerical solution ΔC decreases more rapidly with t for early time ($t < 20$) and more slowly at later time ($t > 20$). The vertical variation is less rapid and thus, the peak in the chemical concentration profile is less narrow than for the asymptotic solution. The absolute difference between the numerical solution and the asymptotic approximation is $|\Delta C - \varepsilon C^{(1)}| < 0.02$ over the time interval shown, which is consistent with the value of $\varepsilon = 0.1$ used in the computations.

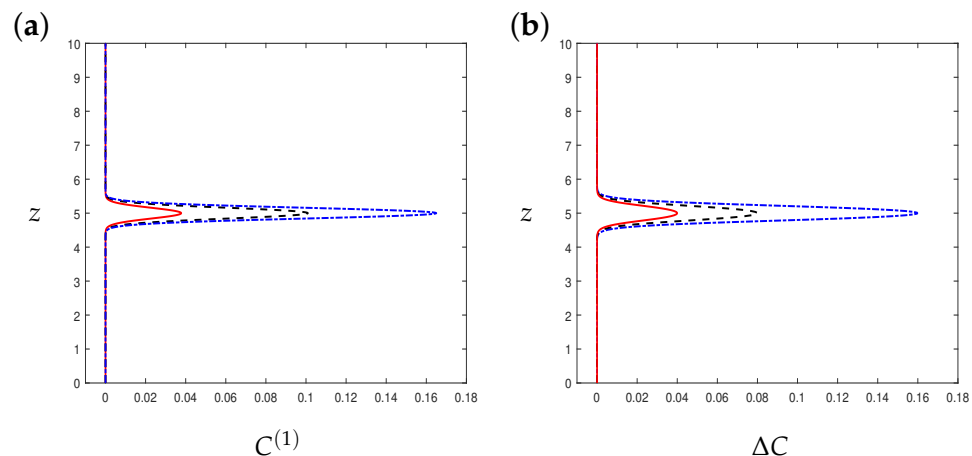


Figure 13. (a) The asymptotic solution $\varepsilon C^{(1)}(x, z, t)$ given by Equation (80) at $x = 0$ as a function of z at several times with $\sigma = 0.5$ and $\mathcal{D} = 0.001$. (b) The corresponding numerical solution $\Delta C = C_{\text{numerical}}(x, z, t) - C^{(0)}(x, z, t)$. In each case, the dashed-dotted blue curve shows the chemical concentration at $t = 10$, the dashed black curve represents $t = 20$, and the solid red curve represents $t = 40$.

6. Conclusions

The interaction of internal gravity waves with chemical constituents in the atmosphere was studied in this paper. Internal gravity waves were represented by a system of equations obtained by applying the Boussinesq approximation. The chemical transport was represented by an advection–diffusion–reaction equation of Fisher type.

The effect of gravity waves on the distribution of the chemical was studied numerically. We examined a configuration where a horizontally localized gravity-wave packet with a zero phase speed is generated at the lower boundary of a rectangular domain and propagates upwards towards a critical level. Nonlinear interactions occur at the critical level and generate a wave-induced mean flow perturbation. This is added as a modification to the background flow speed in the chemical transport equation and it thus affects the advection and the distribution of the chemical. We found that the 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 takes the same form as the profile of the wave-induced perturbation.

To explore the observed dependence of the chemical concentration perturbation on the wave-induced mean flow perturbation, we carried out a weakly nonlinear analysis of the chemical transport problem for a configuration where the advection speed is the sum of a constant and a small-amplitude $O(\varepsilon)$ z -dependent perturbation. The form of the

perturbation was specified to be qualitatively similar to the profile of the the gravity-wave-induced mean flow that develops around the critical level in the gravity-wave numerical solutions. The solution of the perturbed equation was represented as a perturbation series in powers of ε . The leading-order term satisfies the unperturbed Fisher chemical transport equation with constant advection speed, unaffected by the gravity-wave perturbation. This exact analytical expression for this term is in the form of the well-known travelling-wave solution.

The $O(\varepsilon)$ term in the series was approximated asymptotically by the WKB approximation. We found that the controlling factor of this term is proportional to the specified vertical profile for the perturbation to the wind speed. This is consistent with the numerical results obtained for the more realistic configuration involving the gravity-wave perturbation, where we observed that the profile of the gravity-wave-induced change in the chemical concentration is of the same form as the profile of the gravity-wave velocity perturbation. For further comparison, we also carried out numerical solutions for the same configuration that was studied in the asymptotic analysis. In that case, comparing the numerical and asymptotic solutions, we found the same qualitative form for the vertical profile of the chemical concentration with a maximum difference of the order of magnitude of the terms that were neglected in the asymptotic approximation.

Our results showing the effect of gravity waves on the distribution of a chemical species can be compared with the work of previous researchers [14–16]. However, there are some key features that distinguish our investigation. These studies focused on different chemical species that are modelled by different forms of the nonlinear reaction term in the transport equation. Our focus was on chemicals such as ClO, which can be modelled by an equation of Fisher type. This allowed us to carry out asymptotic analyses making use of the known properties of travelling wave solutions of Fisher-type equations. Most significantly, our model included nonlinear gravity-wave equations and a background flow with vertical shear and a critical level, whereas previous studies used linear gravity-wave equations or studied other interaction mechanisms. We specified a spatially localized initial profile for the chemical species and introduced the gravity waves in the form of horizontally localized wave packet with several wavelengths within the packet extent. Our results reflect the effect of the wave-induced mean flow due to the presence of the critical level that occurs in the vertically sheared flow. In spite of these differences, we note that our results are in general agreement with the conclusions of [15], where the gravity-wave effects cause perturbations in the chemical concentration, which are eventually seen to follow the same qualitative behaviour as the gravity-wave velocity perturbations.

We conclude, therefore, that nonlinearity and vertical shear play a vital role in the interplay between gravity-wave dynamics and chemical distributions in the atmosphere. This conclusion underscores the importance of correctly representing gravity-wave effects in large-scale GCMs [11]. Our analytical approach gives expressions for the chemical concentration that depend on the form of the nonlinear reaction term in the transport equation and on the form of the gravity-wave profile. Such information can be incorporated into a parameterization scheme in a GCM to represent the effects of small-scale gravity waves that are unresolved by the model.

Author Contributions: Conceptualization, A.S.A. and L.J.C.; Methodology, A.S.A. and L.J.C.; Formal Analysis, A.S.A. and L.J.C.; Investigation, A.S.A. and L.J.C.; Resources, A.S.A. and L.J.C.; Writing—original draft preparation, A.S.A.; Writing—review and editing, L.J.C.; Visualization, A.S.A.; Supervision, L.J.C.; Project administration, L.J.C.; Funding acquisition, A.S.A. and L.J.C. All authors have read and agreed to the published version of the manuscript.

Funding: The Researchers would like to thank the Deanship of Graduate Studies and Scientific Research at Qassim University for financial support (QU-APC-2025). The research was also supported by the Natural Sciences and Engineering Research Council of Canada (RGPIN-201805296).

Data Availability Statement: The original contributions presented in this study are included in the article. Further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

Nomenclature

V	fixed control volume
n	the number density of the chemical
t	time
$\mathcal{D}$	the constant diffusion coefficient
D	the nondimensional constant diffusion coefficient
C	the the mixing ratio of a chemical
S	the source term that represents the effect of chemical reactions
J	the rate of heat added to the control volume due to the chemical
U	the horizontal component of the fluid velocity
W	the vertical component of the fluid velocity
L_x	the reference value of the dimensional horizontal scale
L_z	the reference value of the dimensional vertical scale
τ	the reference time scale
δ	the square of the vertical-to-horizontal aspect ratio
Ψ	the total streamfunction
ρ	the total density
ψ	the streamfunction perturbation
ρ	the density perturbation
ν	the kinematic viscosity coefficient
κ	the thermal diffusivity coefficient
α	the chemical heating coefficient
φ	the reference value of the streamfunction perturbation
D_p	the reference value of density perturbation
D	the reference value of density
ε	the magnitude of the perturbations relative to the background flow
$\bar{u}$	the horizontal component of the background flow velocity
$\bar{\rho}$	the background density
u	the horizontal perturbation
w	the vertical perturbation
Re	the Reynolds number
Pr	the Prandtl number
ζ	the vorticity perturbation

Appendix A. Numerical Approximations

For the numerical solution of Equations (13)–(15), we first take the Fourier transform of each equation, defining the functions $\hat{\zeta}(k, z, t)$, $\hat{\rho}(k, z, t)$ and $\hat{\psi}(k, z, t)$ as the transforms of $\zeta(x, z, t)$, $\rho(x, z, t)$ and $\psi(x, z, t)$, respectively. The transformed equations are then solved numerically using a finite difference method in the vertical direction and the fourth-order Adams–Bashforth method for the time discretization and a pseudo-spectral method to represent the nonlinear terms. At each time step, the functions $\hat{\zeta}$ and $\hat{\rho}$ are computed using the transforms of Equations (13) and (15) at the new time level and $\hat{\psi}$ is computed from the transform of Equation (14). The functions ζ , ρ and ψ and their spatial derivatives are obtained by numerically inverting the Fourier transforms. The nonlinear terms are

then calculated at the new time level using a pseudo-spectral representation and added to the time-marching computation at the next time step. A detailed description of the numerical procedure is given in [27]. For comparison and verification of our results, we carry out numerical computations with the same input parameters used by [32] and confirm agreement between our results and those presented by [32].

Taking the Fourier transform of (13)–(15), we obtain the transformed equations

$$\hat{\zeta}_t + ik\bar{u}\hat{\zeta} - ik\bar{u}''\hat{\psi} + ik\frac{\delta}{\bar{\rho}}\hat{\rho} + \varepsilon\mathcal{F}[\psi_x\zeta_z - \psi_z\zeta_x] = 0, \quad (\text{A1})$$

$$\hat{\rho}_t + ik\bar{u}\hat{\rho} + ik\bar{\rho}'\hat{\psi} + \varepsilon\mathcal{F}[\psi_x\rho_z - \psi_z\rho_x] = 0, \quad (\text{A2})$$

$$\hat{\psi}_{zz} - \delta k^2\hat{\psi} = \hat{\zeta}. \quad (\text{A3})$$

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 is computed numerically in the form of a summation as

$$\begin{aligned} \hat{\psi}(k, z, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \psi(x, z, t) e^{-ikx} dx \\ &\approx \frac{\Delta x}{2\pi} \sum_{x=-\infty}^{\infty} \psi(x, z, t) e^{-ikx} \\ &= \frac{\Delta x}{2\pi} \sum_{j=0}^{N-1} \psi(x, z, t) e^{-i(k_0+m\Delta k)(x_0+j\Delta x)}. \end{aligned} \quad (\text{A4})$$

Rearranging, we get

$$\hat{\psi}(k, z, t) = \frac{\Delta x}{2\pi} e^{-ikx_0} \sum_{j=0}^{N-1} \psi(x, z, t) e^{-ik_0j\Delta x} e^{-imj\Delta k\Delta x}. \quad (\text{A5})$$

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. For efficiency reasons, it is preferable for the FFT that the number of points N is a power of 2.

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.

The vertical grid size is chosen based on grid sensitivity analysis. In the vertical direction, we repeat the computation of the solution with successively smaller values of 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 $2\Delta z$ which lies within a tolerance of 3×10^{-2} .

The choice of Δx and Δk is made following the same procedure of grid sensitivity analysis. With the choice of $N = 1024$ which gives $\Delta k = 0.0625$, the maximum error of

solutions computed with this Δk compared with the corresponding ones computed with $2\Delta k$ corresponding to $N = 512$ is 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} . For the numerical solution of the chemical transport Equation (16), with the gravity-wave induced velocity components (17), we use the same procedure as described above. At each time step, the gravity-wave vorticity ζ , density ρ and stream-function ψ , as well as the chemical concentration C , are all computed at the new time level using the Fourier transforms of (13)–(17). The computation of C uses the advection velocity perturbations u and w computed at the previous time step.

References

1. Shepherd, T.G. Transport in the middle atmosphere. *J. Meteorol. Soc. Jpn. Ser. II* **2007**, *85*, 165–191.
2. Li, M.; Karu, E.; Brenninkmeijer, C.; Fischer, H.; Lelieveld, J.; Williams, J. Tropospheric OH and stratospheric OH and Cl concentrations determined from CH₄, CH₃, Cl, and SF₆ measurements. *Npj Clim. Atmos. Sci.* **2018**, *1*, 29.
3. Marshall, J.; Plumb, R.A. *Atmosphere, Ocean, and Climate Dynamics: An Introductory Text*; Elsevier: Amsterdam, The Netherlands, 2008; Volume 93.
4. Jacob, D. *Introduction to Atmospheric Chemistry*; Princeton University Press: Princeton, NJ, USA, 1999.
5. Pendlebury, D.; Shepherd, T.G.; Pritchard, M.; McLandress, C. Normal mode Rossby waves and their effects on chemical composition in the late summer stratosphere. *Atmos. Chem. Phys.* **2008**, *8*, 1925–1935.
6. Leovy, C.B. Photochemical destabilization of gravity waves near the mesopause. *J. Atmos. Sci.* **1966**, *23*, 223–232.
7. Zhu, X.; Holton, J.R. Photochemical damping of inertio-gravity waves. *J. Atmos. Sci.* **1986**, *43*, 2578–2584.
8. Xu, J. The influence of photochemistry on gravity waves in the middle atmosphere. *Earth Planets Space* **1999**, *51*, 855–861.
9. Nappo, C.J. *An Introduction to Atmospheric Gravity Waves*; Academic Press: Cambridge, MA, USA, 2002; Volume 85.
10. Sutherland, B.R. *Internal Gravity Waves*; Cambridge University Press: Cambridge, UK, 2010.
11. Guarino, M.; Gardner, C.S.; Feng, W.; Funke, B.; García-Comas, M.; López-Puertas, M.; Kupilas, M.M.; Marsh, D.R.; Plane, J.M.C. A novel gravity wave transport parametrization for global chemistry climate models: Description and validation. *J. Adv. Model. Earth Syst.* **2024**, *16*, e2023MS003938.
12. Achatz, U.; Alexander, M.J.; Becker, E.; Chun, H.-Y.; Dörnbrack, A.; Holt, L.; Plougonven, R.; Polichtchouk, I.; Sato, K.; Sheshadri, A.; et al. Atmospheric gravity waves: Processes and parameterization. *J. Atmos. Sci.* **2024**, *81*, 237–262.
13. Hickey, M.P.; Plane, J. A chemical-dynamical model of wave-driven sodium fluctuations. *Geophys. Res. Lett.* **1995**, *22*, 2861–2864.
14. Xu, J.; Smith, A.K.; Brasseur, G.P. The effects of gravity waves on distributions of chemically active constituents in the mesopause region. *J. Geophys. Res. Atmos.* **2000**, *105*, 26593–26602.
15. Xu, J.; Smith, A.K.; Ma, R. A numerical study of the effect of gravity-wave propagation on minor species distributions in the mesopause region. *J. Geophys. Res. Atmos.* **2003**, *108*, 4119.
16. Liu, H.L.; Hays, P.B.; Roble, R.G. A numerical study of gravity wave breaking and impacts on turbulence and mean state. *J. Atmos. Sci.* **1999**, *56*, 2152–2177.
17. Spiegel, E.A.; Veronis, G. On the Boussinesq approximation for a compressible fluid. *Astrophys. J.* **1960**, *131*, 442.
18. Fowler, A. *Mathematical Geoscience*; Springer Science & Business Media: Berlin/Heidelberg, Germany, 2011; Volume 36.
19. Bird, R.B.; Stewart, W.E.; Lightfoot, E.N. *Transport Phenomena*; Wiley: Hoboken, NJ, USA, 2002.
20. Brasseur, G.; Solomon, S. *Chemistry and Physics of the Stratosphere and Mesosphere*; D. Reidel Publishing Company: Dordrecht, The Netherlands, 1984.
21. Brasseur, G.P.; Jacob, D.J. *Modeling of Atmospheric Chemistry*; Cambridge University Press: Cambridge, UK, 2017.
22. Fitzgibbon, W.E.; Langlais, M.; Morgan, J.J. A degenerate reaction–diffusion system modeling atmospheric dispersion of pollutants. *J. Math. Anal. Appl.* **2005**, *307*, 415–432.
23. Carpenter, L.J.; Reimann, S.; Burkholder, J.B.; Clerbaux, C.; Hall, B.D.; Hossaini, R. Laube, JC, and Yvon-Lewis, SA: Ozone-Depleting Substances (ODSs) and other gases of interest to the Montreal Protocol. Scientific Assessment of Ozone Depletion. 2014. Available online: <https://csl.noaa.gov/assessments/ozone/2014/report/2014OzoneAssessment.pdf> (accessed on 1 January 2019).
24. Tham, Y.J.; Sarnela, N.; Iyer, S.; Li, Q.; Angot, H.; Quéléver, L.L.J.; Beck, I.; Laurila, T.; Beck, L.J.; Boyer, M.; et al. Widespread detection of chlorine oxyacids in the Arctic atmosphere. *Nat. Comm.* **2023**, *14*, 1769.
25. Bramson, M. *Convergence of Solutions of the Kolmogorov Equation to Travelling Waves*; American Mathematical Society: Providence, RI, USA, 1983; Volume 285.
26. Tyson, J.J.; Brazhnik, P.K. On traveling wave solutions of Fisher’s equation in two spatial dimensions. *SIAM J. Appl. Math.* **2000**, *60*, 371–391.

27. Almohaimeed, A. Internal-Gravity-Wave Interactions in the Presence of Localized Chemical Heating in the Atmosphere. Ph.D. Thesis, Carleton University, Ottawa, ON, Canada, 2019.
28. Booker, J.R.; Bretherton, F.P. The critical layer for internal gravity waves in a shear flow. *J. Fluid Mech.* **1967**, *27*, 513–539.
29. Brown, S.; Stewartson, K. On the nonlinear reflexion of a gravity wave at a critical level. Part 1. *J. Fluid Mech.* **1980**, *100*, 577–595.
30. Brown, S.N.; Stewartson, K. On the nonlinear reflection of a gravity wave at a critical level. Part 2. *J. Fluid Mech.* **1982**, *115*, 217–230.
31. Brown, S.N.; Stewartson, K. On the nonlinear reflection of a gravity wave at a critical level. Part 3. *J. Fluid Mech.* **1982**, *115*, 231–250.
32. Campbell, L.J.; Maslowe, S.A. Nonlinear critical-layer evolution of a forced gravity wave packet. *J. Fluid Mech.* **2003**, *493*, 151–179.
33. Campbell, L.J.; Nikitina, L.V. Weakly non-linear analysis of small-amplitude internal gravity waves forced by isolated topography. *Geophys. Astrophys. Fluid Dyn.* **2014**, *108*, 503–535.
34. Whiteway, J.A.; Duck, T.J. Evidence for critical level filtering of atmospheric gravity waves. *Geophys. Res. Lett.* **1996**, *23*, 145–148.
35. Ejiri, M.K.; Taylor, M.J.; Nakamura, T.; Franke, S.J. Critical level interaction of a gravity wave with background winds driven by a large-scale wave perturbation. *J. Geophys. Res.* **2009**, *114*, D18117. <https://doi.org/10.1029/2008JD011381>.
36. Holton, J.R. *An Introduction to Dynamic Meteorology*; Elsevier: Amsterdam, The Netherlands, 2004; Volume 88.
37. Eliassen, A.; Palm, E. On the transfer of energy in stationary mountain waves. *Geophys. Publ.* **1961**, *22*, 1–23.
38. Almohaimeed, A.S. Mathematical modelling for gravity waves interactions coupled with localized water vapor and ozone in the atmosphere. *Front. Earth Sci.* **2024**, *12*, 1385305.
39. Gille, J.C.; Lyjak, L.V. Radiative heating and cooling rates in the middle atmosphere. *J. Atmos. Sci.* **1986**, *43*, 2215–2229.
40. Bender, C.M.; Orszag, S.A. *Advanced Mathematical Methods for Scientists and Engineers I: Asymptotic Methods and Perturbation Theory*; Springer: Berlin/Heidelberg, Germany, 1999.

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.