Direct Numerical Simulation of Shock-Induced Turbulent Mixing with High-Resolution Methods

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A thesis submitted in fulfillment of the requirements of the degree of Doctor of Philosophy

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June 2020
Declaration

I hereby declare that this submission is my own work and that, to the best of my knowledge and belief, it contains no material previously published or written by another person nor material which to a substantial extent has been accepted for the award of any other degree or diploma of the University or other institute of higher learning, except where due acknowledgement has been made in the text.

Michael Groom

29 June 2020
Abstract

Turbulent mixing evolving from the Richtmyer–Meshkov instability, also known as shock-induced turbulent mixing, has been investigated using numerical simulations of fundamental test problems with high-resolution computational methods. Shock-induced turbulent mixing plays an important role in areas such as inertial confinement fusion, high-speed combustion and many astrophysical phenomena. The difficulty with which experimental data can be obtained in these types of applications means that gaining an understanding of the underlying physics relies considerably on the use of numerical simulation.

An existing state-of-the-art implicit large eddy simulation algorithm for compressible multispecies flows is extended to include the effects of viscous dissipation, thermal conductivity and species diffusion by deriving a novel set of governing equations for binary mixtures. This allows for direct numerical simulations of shock-induced turbulent mixing to be performed for arbitrary gas mixture cases where the ratio of specific heats may vary with mixture composition at much greater computational efficiency. A comprehensive set of test cases is used to demonstrate the advantages of the new algorithm.

Using direct numerical simulation, a detailed study is performed of the effects of Reynolds number on the transition to turbulence in shock-induced mixing evolving from narrowband initial conditions. The simulations are demonstrated to be grid converged for various integral and spectral quantities of interest, which is also shown to be equivalent to resolving the Kolmogorov microscales even though these may not be well defined for a developing flow. Despite the fact that the turbulence in the highest Reynolds number case is not fully developed, a careful analysis shows that the high Reynolds number limit of several key quantities is able to be estimated from the present data. For quantities such as the normalised dissipation rate, this high Reynolds number asymptotic behaviour is commonly used in reduced-order models for turbulence. The mixing layer is also shown to be persistently anisotropic at all Reynolds numbers, which also has important consequences for modelling. At the time of writing, the highest Reynolds number case from this set of simulations is the highest Reynolds number achieved in a fully-resolved direct numerical simulation presented in the open literature for this class of problems.
Implicit large eddy simulation is employed to investigate the influence of broadband initial conditions on the late-time evolution of a shock-induced turbulent mixing layer. Both the bandwidth of initial modes as well as their relative amplitudes are varied, showing that both the growth rate of the mixing layer width and the decay rate of fluctuating kinetic energy strongly depend on initial conditions. The results for the growth rate of integral width compare favourably with theoretical predictions in the limit of infinite bandwidth. However, the measured decay rates are found not to match the values predicted by dimensional analysis, which is shown to be due to a time-varying normalised dissipation rate. Finally, both implicit large eddy simulations and direct numerical simulations are performed of an idealised shock tube experiment to analyse the effects of additional long wavelength, low amplitude modes in the initial perturbation. By comparing with the results for a purely narrowband perturbation, plausible explanations are given for the behaviour observed in recent experiments of the Richtmyer–Meshkov instability with multi-mode initial conditions. These calculations also represent the first direct numerical simulations performed of Richtmyer–Meshkov instability evolving from broadband initial conditions.
Acknowledgements

This thesis would not have been possible without a considerable amount of assistance. There are a number of people I would like to thank for making the experience as enjoyable and fulfilling as it was.

Firstly, I would like to thank my supervisor A/Prof. Ben Thornber for his guidance and mentorship. You have always shown great enthusiasm for my research and it has been a pleasure working with you these last four years. I look forward to continuing to do so in some capacity in the years to come. I have also had the opportunity to collaborate with some other brilliant minds, in particular Prof. David Youngs, Prof. Evgeniy Romenski and Dr. Ye Zhou for whom, along with Ben, I would like to thank for greatly improving my thinking around numerical methods and the study of turbulent mixing. Completing a PhD also involves a substantial amount of non-technical work and I would like to thank my auxiliary supervisor Dr. Gareth Vio for his assistance with stipends, conference expenses and the like, as well as for his no-nonsense take on academia more generally.

I have been lucky to share an office with a number of other smart and motivated people who have all helped me in one way or another. In no particular order, thank you to Daniel Linton, Asiful Islam, Abhijeet Kumar, Hanxun Yao, Hee Sung Park, Moutassem El Rafei, Alex Coyle and Tom Cochrane. Also a big thank you to Tamas Bykerk, Adam Murray, David Munk and Nick Giannelis for providing a great deal of entertainment and the occasional but much needed break from work.

On a personal note, I would like to thank my former housemates Malcolm and Emma for all of their support and friendship. Whether it was helping me out with groceries while I was on crutches for three months or lending me the use of a car, I greatly appreciate all of your help. I am also immensely grateful to my partner Andrea. Our journey together began almost exactly to the day that I commenced my doctoral studies and you have been a huge part of my life ever since. I am especially indebted to you for your support over the last six months, thank you for your patience and understanding during all the late nights and weekends spent writing. Finally, I would have never got to where I am now without the love and support of my parents. You have always encouraged me to pursue my interests and have been a constant source of advice throughout my life so far.
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Nomenclature

List of Symbols

The following list of symbols is not exhaustive. It merely covers symbols that have the same definition throughout this entire thesis. The definition of all other symbols is given in the text whenever they are introduced.
Nomenclature

\((x, y, z)\) Cartesian coordinates in \(\mathbb{R}^3\)
\(t\) time
\(x\) position vector
\(u\) velocity vector
\(u_x\) \(x\)-direction component of velocity
\(v\) \(y\)-direction component of velocity
\(w\) \(z\)-direction component of velocity
\(\rho\) mass density
\(n\) particle number density
\(p\) pressure
\(T\) temperature
\(e\) internal energy per unit mass
\(E\) total energy per unit mass
\(s\) specific entropy
\(a\) speed of sound
\(c_v\) specific heat capacity at constant volume
\(c_p\) specific heat capacity at constant pressure
\(\gamma\) ratio of specific heats
\(\mathcal{R}_u\) universal gas constant
\(\mathcal{R}\) specific gas constant
\(k_b\) Boltzmann constant
\(\nu\) kinematic viscosity
\(\mu\) dynamic viscosity
\(\mu_b\) bulk viscosity
\(D\) mass diffusivity
\(\kappa\) thermal conductivity
\(Y_l\) mass fraction of species \(l\)
\(f_l\) volume fraction of species \(l\)
\(A\) Atwood number
Nomenclature

\[ M \quad \text{Mach number} \]
\[ Re \quad \text{Reynolds number} \]
\[ Pr \quad \text{Prandtl number} \]
\[ Sc \quad \text{Schmidt number} \]
\[ U \quad \text{vector of conserved variables} \]
\[ W \quad \text{vector of primitive variables} \]
\[ F \quad \text{numerical flux in } x\text{-direction} \]
\[ G \quad \text{numerical flux in } y\text{-direction} \]
\[ H \quad \text{numerical flux in } z\text{-direction} \]
\[ dS \quad \text{differential surface element} \]
\[ dV \quad \text{differential volume element} \]
\[ n \quad \text{unit normal vector} \]
\[ \delta \quad \text{Kronecker delta} \]

In addition, italicised bold symbols indicate vector or tensor quantities and roman bold symbols indicate discrete vector or tensor quantities.

List of Acronyms

- ALE: Arbitrary Lagrangian-Eulerian
- CFL: Courant–Friedrichs–Lewy
- DNS: Direct Numerical Simulation
- ENO: Essentially Non-Oscillatory
- HIT: Homogeneous Isotropic Turbulence
- ICF: Inertial Confinement Fusion
- KHI: Kelvin–Helmholtz Instability
- LEM: Linear Electric Motor
- MUSCL: Monotone Upstream-centred Scheme for Conservation Laws
- PAWCM: Parallel Adaptive Wavelet Collocation Method
- PPM: Piece-wise Parabolic Method
- RANS: Reynolds-Averaged Navier–Stokes
- RDE: Rotating Detonation Engine
- RMI: Richtmyer–Meshkov Instability
- RTI: Rayleigh–Taylor Instability
- TENO: Targeted Essentially Non-Oscillatory
- TKE: Turbulent Kinetic Energy
- TVD: Total Variation Diminishing
- WENO: Weighted Essentially Non-Oscillatory

List of Operators
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<tbody>
<tr>
<td>$\Delta$</td>
<td>Laplacian</td>
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<tr>
<td>$\nabla$</td>
<td>gradient</td>
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<td>$\cdot$</td>
<td>dot product</td>
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<td>$\times$</td>
<td>cross product</td>
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<td>partial differential</td>
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<tr>
<td>$\int_V$</td>
<td>volume integral</td>
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<tr>
<td>$\oint_S$</td>
<td>surface integral</td>
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<tr>
<td>$\langle \ldots \rangle$</td>
<td>plane average over statistically homogeneous directions</td>
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<tr>
<td>$(\ldots)^t$</td>
<td>transpose</td>
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<tr>
<td>$(\ldots)$</td>
<td>Fourier transform</td>
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<tr>
<td>$(\ldots)^\dagger$</td>
<td>complex conjugate</td>
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<td>$</td>
<td>\ldots</td>
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<tr>
<td>$(\ldots)'$</td>
<td>Reynolds-averaged fluctuating quantity</td>
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<tr>
<td>$(\ldots)''$</td>
<td>Favre-averaged fluctuating quantity</td>
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### List of Units

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<th>Symbol</th>
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<td>Kelvin</td>
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<td>N</td>
<td>Newtons</td>
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Chapter 1

Introduction

1.1 Background and motivation

This thesis is concerned with the study of turbulence, which may be defined as a spatially complex velocity field that evolves in a chaotic manner and exhibits a wide range of length and time scales [11]. In particular, the focus will be on the turbulence that is generated when two or more fluids mix together, referred to as turbulent mixing. The ‘amount’ of turbulence in a given flow is quantified by a non-dimensional number known as the Reynolds number. This will be defined in Chapter 2, but for now it is sufficient to state that the Reynolds number represents the ratio of the inertial forces that drive the motion of the flow to the viscous forces that dissipate kinetic energy. As an example, consider the flow shown in Figure 1.1 for the same experimental setup but at two different Reynolds numbers. The images shown are of a mixing layer that is produced between nitrogen and a mixture of helium and argon, matched to give the same density. The nitrogen is injected above at a velocity of 10 m/s and the helium-argon mixture is injected below at a velocity of 3.8 m/s, both at a pressure of 4 atm. A shear layer is produced due to the velocity difference and any small irregularities at the interface between the two streams get amplified. It is this amplification process that causes the gases to mix and eventually leads to turbulence, provided the Reynolds number is sufficiently large.
1.1 Background and motivation

(a) Mixing layer between nitrogen and a mixture of helium/argon.

(b) The same experiment above performed at twice the Reynolds number.

Figure 1.1 – Spark shadow photographs of a turbulent mixing layer between nitrogen (top) and a mixture of helium/argon of the same density (bottom). The experiment is performed at two different Reynolds numbers, demonstrating how increasing the Reynolds number produces additional fine-scale structure without significantly altering the largest scales in the flow. Source: An Album of Fluid Motion, assembled by Milton Van Dyke.

In both cases the Reynolds number is large enough for the flow to transition to turbulence at some point downstream of the splitter plate (located at the left hand edge of the images). However, there are clear qualitative differences in the flow field that are produced when the Reynolds number is doubled (by increasing the background pressure to 8 atm). From the two images in Figure 1.1, it can be seen that increasing the Reynolds number produces additional fine-scale structure without significantly altering the largest scales in the flow. This has important consequences for the rate at which the two gas streams mix, as increasing the Reynolds number increases the overall surface area of the interface between the two streams and enables the otherwise slow process of molecular mixing via diffusion to occur much more rapidly.
The ability of a turbulent flow to transport and mix fluid much more effectively than a comparable laminar flow is an important characteristic of turbulence in general. When combined with the observation that the vast majority of flows in nature and industrial applications are turbulent, as well as the fact that promoting or inhibiting mixing is often of great importance in these flows, this gives ample motivation for the study of turbulence and turbulent mixing. In addition, due to its chaotic nature (i.e. extreme sensitivity to initial conditions) there is currently no ‘general theory’ of turbulence. This means that any predictions about the motion of a turbulent flow can only be statistical ones for classes of flows that have similar boundary conditions. These are informed by the results of repeated experiments, or more recently by numerically simulating the equations governing the motion of a fluid.

For the turbulent flow shown in Figure 1.1, the vorticity (or equivalently, the angular velocity) is generated by shear due to the different velocities of the two streams and any infinitesimal perturbation of the interface between them. It is this vorticity that drives the transition to turbulence, through a process known as the Kelvin–Helmholtz instability (KHI) [12]. Other sources of vorticity are also possible, for example due to buoyancy. In the presence of a gravitational field, fluids of differing densities will be accelerated into one another. In the case where the lighter fluid is accelerated into the heavier fluid, any infinitesimal perturbation of the interface between the two fluids will be amplified and increasing amounts of vorticity, referred to as baroclinic vorticity, will be generated. This process is known as the Rayleigh–Taylor instability (RTI) and it is the mechanism behind phenomena such as the mixing of temperature and salinity fields in large-scale ocean currents, the dynamics of which highly influence the climate and life on this planet [13, 14].

Although the gases used in the experiments shown in Figure 1.1 were at a relatively high pressure and hence the flow is approximately incompressible, in general gases can exhibit significant compressibility effects. For example, large-amplitude pressure disturbances in a compressible medium (i.e. one where the particle density can vary significantly) can steepen and form a shock wave, across which the pressure, temperature, density and velocity of the fluid all change almost discontinuously. The
interaction of a shock wave with an interface between two fluids of differing densities will also induce baroclinic vorticity, due to the misalignment of the pressure gradient across the shock and the local density gradient across the interface [15]. The process of amplification of any infinitesimal perturbations on the interface by interaction with a shock wave is known as the Richtmyer–Meshkov instability (RMI) [16, 17], which can be viewed as the impulsive limit of the more familiar Rayleigh-Taylor instability. There are some important distinctions to make however. Unlike RTI, RMI can be induced for both light to heavy and heavy to light configurations. In both RTI and RMI the transition to turbulence occurs through the development of secondary shear layer instabilities (i.e. KHI) due to differences in tangential velocity across the interface, however for RMI baroclinic vorticity is deposited almost instantaneously whereas in RTI it is continuously generated for as long as the acceleration persists. The various phases of development for both RTI and RMI will be discussed in Chapter 2.

This thesis primarily focuses on turbulent mixing evolving from the Richtmyer–Meshkov instability. Some motivating applications of RMI will be given here, however for a comprehensive and up-to-date review of the literature on both RTI and RMI, the reader is referred to Zhou [18, 19]. The understanding of mixing due to RMI is of great importance in many areas of high-energy density physics such as inertial confinement fusion (ICF), as well as in various aerospace applications. In ICF, a spherical capsule containing thermonuclear fuel is imploded using powerful lasers with the aim of compressing the contents to sufficient densities and temperatures so as to initiate nuclear fusion [20]. There are two main approaches, indirect-drive and direct-drive, which are illustrated in Figure 1.2. In both cases the compression is performed using a series of strong laser-driven shocks, which trigger hydrodynamic instabilities at the ablation front due to capsule defects [21]. The subsequent mixing of ablatur material and fuel that ensues can dilute and cool the hotspot, which reduces the overall efficiency of the implosion. In many ways nuclear fusion is the ultimate energy source, since it offers a lot of the benefits of nuclear fission power like zero carbon emissions while avoiding most of the downsides such as long-term radioactive waste and the risk of nuclear meltdown. If commercially viable fusion power plants can be built,
they will have access to effectively unlimited supplies of fuel; the amount of energy produced by burning a standard 44 gallon drum of oil could instead be obtained from a single glass of seawater\footnote{This is perhaps slightly misleading as it is based on the energy density of deuterium only, for which there is 33 grams per cubic metre of seawater.}. Hence it is very important that the mechanisms which cause degradation of the implosion quality, such as undesirable mixing of the fuel and ablator material, are well understood.

As a contrast to this, in high-speed combustion such as in a scramjet or rotating detonation engine (RDE), RMI due to weak shocks improves the mixing of fuel and oxidiser leading to more efficient combustion \cite{22, 23}. The use of air-breathing engines such as scramjets or RDEs for powering launch vehicles has the potential to dramatically lower costs and increase launch frequency. For example, even for reusable rocket-powered launch vehicles the majority of the gross take-off weight is taken up by the oxidiser. In the case of the SpaceX Falcon-9, approximately 65\% of the gross weight of the vehicle at launch corresponds to the weight of liquid oxygen. Currently

\begin{figure}[h!]
\centering
\includegraphics[width=\textwidth]{figure1.pdf}
\caption{A schematic of indirect- and direct-drive inertial confinement fusion. \textit{Source:} From Figure 1 of Betti and Hurricane \cite{1}.}
\end{figure}
the cost per kilogram of payload sent to low Earth orbit is somewhere in the range of $1,000 to $20,000 USD, therefore an attractive option for reducing this cost is to reduce the weight of the launch vehicle by using an air-breathing engine for the first-stage. This is possible because the oxidiser is supplied by the surrounding atmosphere and is mixed in the combustor with fuel carried on board. However, there are many challenges when trying to achieve sustained combustion at such high speeds as the total time available for the reactants to burn in the combustion chamber is typically on the order of less than a millisecond. A recent review by Urzay [24] summarised the problem in lay terms as like trying to light a match in a hurricane. It is for this reason that only a handful of powered flight tests of scramjets have been performed to date. Methods for improving the rate at which the fuel and oxidiser mix are therefore very important, and one of the main ways of achieving this is through the use of internal shock waves.

An understanding of mixing due to RTI and RMI is also important for many astrophysical phenomena such as supernovae and the dynamics of interstellar media. For example, Sano et al. [25] showed that RMI could be the cause of the amplification of interstellar magnetic fields and localised strong fields observed at the shock in supernova remnants. In Type 1a supernovae, which serve as standard candles for measuring the rate of expansion of the universe, the expansion of ash behind the thermonuclear flame front causes the flame to become Rayleigh–Taylor unstable as it propagates outwards, which is potentially responsible for the transition from a subsonic deflagration to a supersonic detonation [18]. For Type 2 supernovae, following the collapse of the core there is significant RMI-induced mixing between the stratified outer gas layers [26], which affects the appearance of the supernovae remnants [27]. For supernova remnants in general, their uneven shape is due in part to the combined influence of RTI and RMI acting on perturbations present within the star prior to the supernova itself [28].
1.2 Objectives and approach

In most of the applications and phenomena given above, quantitative experimental data is often difficult or expensive to obtain. Because of this, gaining an understanding of the underlying physics relies to a considerable extent upon the use of numerical simulation. There is also quite a broad range of length and time scales involved in these phenomena, and often other physics must be considered as well such as radiation or chemical/nuclear reactions. For this reason it is currently necessary to model the effects of mixing and turbulence to some degree in order to maintain computational tractability. This motivates the use of high-fidelity simulation techniques for studying fundamental problems with the purpose of increasing the understanding of turbulent mixing, in this case initiated by the interaction of a shock wave with a material interface. This has been the approach taken for a number of decades now on the fundamental problem of homogeneous isotropic turbulence [11], using the technique of direct numerical simulation (DNS) [29]. The results of these studies have lead to the development of various reduced-order modelling techniques and sub-grid models over the years, as well as tremendous insight into the physics of turbulence in its most pure form.

A similar approach is also adopted here, whereby the fundamental elements of turbulent mixing induced by the Richtmyer–Meshkov instability are studied computationally in an idealised setting. An important example of this approach is given by a study known as the $\theta$-group collaboration [30], where eight independent algorithms were used to simulate a canonical test problem of a 3D planar mixing layer evolving from RMI. All of the algorithms in this study used a technique known as implicit large eddy simulation (ILES), which along with DNS will be discussed in further detail in Chapter 2. The computational setup and results of the $\theta$-group collaboration also form the starting point for the core body of work presented in this thesis, which builds on those results to explore the effects of Reynolds number using DNS in the same way as has been successfully performed for homogeneous isotropic turbulence. In particular, these simulations are used to investigate the transition to turbulence in an RMI-induced mixing layer, which is a highly relevant issue in reduced-order
modelling of these types of flows. The other main body of work in this thesis involves investigating the influence of initial conditions in RMI, which is also of high practical importance. The approach for doing so is based on the pioneering study of Thornber et al. [31], which used a similar computational setup to the later θ-group collaboration. The methodology and results of that study are significantly extended here and are also combined with DNS to investigate the effects of both Reynolds number and initial conditions simultaneously for an experimentally motivated test problem.

Ultimately this thesis aims to make significant contributions to improving the understanding of shock-induced turbulent mixing through the use of carefully designed computational studies of canonical test problems. By rigorously analysing the data generated in these studies, the results may be used to inform the development and improvement of models for turbulent mixing in the applied contexts mentioned in Section 1.1.

1.3 Thesis structure

The structure of this thesis is given as follows. In Chapter 2 an overview is given of the fundamentals of shock-induced turbulent mixing, as well as variable-density interfacial instabilities more generally. The various growth regimes of the Rayleigh–Taylor and Richtmyer–Meshkov instabilities are detailed along with a review of the state-of-the-art in computational modelling of these flows. Chapter 3 gives a detailed presentation of the equations that govern the behaviour miscible mixtures of compressible fluids, along with how to solve these equation numerically using Godunov finite-volume methods. A novel quasi-conservative system of equations, that is suitable for cases where the ratio of specific heats varies with mixture composition, is also derived for binary mixtures and the existing finite-volume discretisation is extended to solve this new set of equations.

In Chapter 4 direct numerical simulations are presented of RMI evolving from the same initial condition that was used in the θ-group collaboration [30]. Comparisons are made between the ILES results from that study and the new DNS results for
various integral quantities, and the Reynolds number dependence of various statistics of the velocity and scalar fields is investigated. An evaluation of the unsteady mixing transition criterion is also given to assess how close the turbulence in the flow is to becoming fully developed. In Chapter 5 the focus is switched to the influence of initial conditions on the self-similar growth characteristics of an RMI mixing layer. ILES is used to compute the evolution of a series of different initial surface perturbations, using the same configuration and material properties as in Chapter 4 but with a much greater bandwidth of initial modes. The results of these simulations are used to validate theoretical predictions of various quantities in the self-similar regime for different initial perturbation power spectra. Finally in Chapter 6 both DNS and ILES are performed of an idealised shock tube experiment between air and sulphur hexafluoride, easily the most commonly used gas pair in experimental studies of RMI. The simulations are used to explore the effects of additional long wavelength, low amplitude modes on the growth rate of the mixing layer width and on the decay rate of fluctuating kinetic energy, which offer some plausible explanations for the behaviour observed in recent multi-mode shock tube experiments. Chapter 7 concludes the thesis with a summary of the key results and recommendations for future research.

1.4 Thesis contributions

The research conducted in this thesis has made several important contributions to the literature on shock-induced turbulent mixing and numerical methods for compressible multispecies flows. At the time of writing, this has resulted in the following journal papers being accepted for publication:


In addition, the following papers have also been published in conference proceedings:


Footnotes have been added to the introduction page of each chapter to indicate if any of the results have been included in the publications listed above. These footnotes also indicate if any of the results have been submitted for publication and are currently under review.

### 1.5 Attribution statement

This thesis contains material published in the journal article ‘Thornber, B., Groom, M., Youngs, D. (2018). *J. Comput. Phys.*, 372, 256-280’, for which I was not the lead author. This material is located in Section 3.3 of the thesis and my contributions are as follows:

- I wrote the literature survey presented in Section 3.3.1. I have also modified
and/or re-written much of the body of text, either for consistency with the rest of the thesis or to paraphrase in my own words.

- From Section 3.3.2 onwards I have modified the notation from that which was originally presented in the journal article so as to be consistent with the rest of the thesis.

- I created a new version of Figure 3.1, again to be consistent with notation.

- I performed the discretisation of the four-equation model, verified and finalised the discretisation of the five-equation model and combined both of these into a single codebase.

- I derived the Jacobian matrix given in Equation (3.65) and calculated its eigenvalues and eigenvectors.

- I implemented and ran all of the test cases in Section 3.3.5 and Section 3.3.6. I also derived the mathematical formulae for computing the cell averaged initial conditions.

- I performed all of the data analysis and generated all of the figures and tables for Section 3.3.5 and Section 3.3.6.
Chapter 2

Fundamentals of Turbulent Mixing

This chapter gives an overview of the fundamentals of shock-induced turbulent mixing as well as the current state-of-the-art in computational modelling for such flows\(^1\). The discussion is expanded to also include other variable-density interfacial instabilities such as the Rayleigh–Taylor instability, which is also present in many of the same applications as RMI and shares much of the same phenomenology. A description is given of the various growth regimes of these instabilities from initiation through to the development of a turbulent mixing layer. The various formulations of the mathematical equations used to describe these flows are also presented, along with the appropriate numerical methods used to solve each of these different formulations. Finally, the various approaches to modelling turbulence are discussed in the context of variable-density mixing, including where the present work fits within that picture.

\(^1\)The work presented in this chapter has been submitted for publication in the journal *Physica D: Nonlinear Phenomena* as part of a review article titled ‘Rayleigh-Taylor and Richtmyer-Meshkov instabilities: A journey through scales’ by Zhou, Y., Williams, R.J.R., Ramaprabhu, P., Groom, M., Thornber, B., Hillier, A., Mostert, W., Rollin, B., Balachandar, S., Powell, P.D., Mahalov, A. and Attal, N.
2.1 Instability development: linear through to turbulent regimes

Both the Rayleigh–Taylor and Richtmyer–Meshkov instabilities are initiated due to perturbations on the interface that initially separates the two fluids. The subsequent evolution of each instability is the result of a misalignment of the density gradient between the two materials and the pressure gradient, due to either a sustained (RTI) or impulsive (RMI) acceleration. For Rayleigh–Taylor, the instability is induced if the condition

\[ \nabla \rho \cdot \nabla p < 0 \]  

is satisfied. In other words, if the heavy fluid is accelerated into the light fluid then the configuration is unstable. This is the result of baroclinic vorticity being continuously generated at the interface due to the misalignment of density and pressure gradients, which in turn induces a velocity field that acts to create further misalignment. The evolution of vorticity \( \omega = \nabla \times u \) is described (ignoring viscous effects) by the following equation

\[ \frac{\partial \omega}{\partial t} = -u \cdot \nabla \omega + \omega \cdot \nabla u - \omega (\nabla \cdot u) + \frac{1}{\rho^2} \nabla \rho \times \nabla p, \]  

where the last term on the right hand side is the baroclinic term \([32]\). Clearly this is only present when \( \nabla \rho \cdot \nabla p \neq 0 \). The second term on the right hand side of Equation (2.2) accounts for vortex stretching and is only present in three-dimensional flows.

For Richtmyer–Meshkov, both heavy-light and light-heavy configurations are unstable when impulsively accelerated as baroclinic vorticity is instantaneously deposited at the interface. In the heavy-light case where \( \nabla \rho \cdot \nabla p > 0 \), the sense (i.e. clockwise or counter-clockwise) of the vorticity causes the instability to evolve in the opposite direction to that of the light-heavy case, reversing the initial phase of the perturbation. This is illustrated in Figure 2.1, which shows the sense of the vorticity generated by both instabilities when the acceleration \( g \) and impulse \( \Delta u \) are in the same direction.

Figure 2.1 depicts the evolution of both RTI and RMI for a single, sinusoidal perturbation of the interface with a given amplitude and wavelength, referred to as a
2.1 Instability development: linear through to turbulent regimes

Figure 2.1 – Schematic outlining the mechanisms by which baroclinic vorticity is generated/deposited at the interface between heavy and light fluids.

single mode. In most cases however, the interface perturbation will consist of many such modes of varying amplitude and wavelength and it is these multimodal perturbations that are of primary interest here. If each mode \( k \) in such a perturbation has an amplitude \( a_k \) that is sufficiently small with respect to its wavelength \( \lambda_k \), then its initial growth rate \( \dot{a}_k \) is well described by linear stability analysis [12]. For the Rayleigh–Taylor instability, the initial motion is governed by

\[
\dot{a}_k = Agka_k,
\]

the solution of which is an exponential with exponent \( \psi = \sqrt{Agk} \). Here \( g \) is the acceleration perpendicular to the interface (typically due to gravity). For Richtmyer–Meshkov, the growth rate due to the initial impulse can be derived by replacing \( g \) with \( \Delta u \delta(t) \) in Equation (2.3), where \( \Delta u \) is the impulsive change in velocity of the interface and \( \delta(t) \) is the Dirac delta function. This leads to

\[
\dot{a}_k = k\Delta u A^+ a_0^+,
\]

where \( a_0 \) is the initial amplitude of mode \( k \). The parameter \( A \) common to both Equation (2.3) and Equation (2.4) is the Atwood number, which characterises changes in mixing that occur due to different density ratios across the interface and is given
by

\[ A = \frac{\rho_2 - \rho_1}{\rho_1 + \rho_2}, \quad (2.5) \]

where \( \rho_2 > \rho_1 \) are the partial densities of the two fluids. Hence \( 0 < A < 1 \), with \( A \to 0 \) corresponding to mixing of fluids of almost identical properties, known as the Boussinesq limit, and \( A \to 1 \) corresponding to the case where the two fluids have greatly disparate properties, such that a turbulent mixing layer may not form. This difference in qualitative behaviour that occurs for different Atwood numbers must be taken into account in the formulation of the governing equations, which is discussed in greater detail in Section 2.2.

The + superscripts in Equation (2.4) indicate post-shock quantities. This means that \( A^+ \) is calculated using the post-shock partial densities \( \rho_2^+ \) and \( \rho_1^+ \), while \( a_0^+ = (1 - \Delta u/U_s)a_0 \) where \( U_s \) is the velocity of the incident shock wave. This introduces another key non-dimensional parameter, the Mach number \( M \) which governs compressibility effects. The Mach number \( M_s \) of the incident shock appears implicitly in Equation (2.4) through the compression factor that pre-multiplies \( a_0 \) and the induced velocity, hence modifying the growth rate. Two other Mach numbers that are important for characterising the effects of compressibility on both RT and RM mixing layers are (local) Mach numbers based on mean and fluctuating velocities [33]. As with the Atwood number, for Mach numbers significantly greater than zero the difference in qualitative behaviour must be taken into account in the governing equations and numerical method used to simulate them.

In the following sections, each distinct stage of development in multimodal RTI and RMI will be discussed in greater detail alongside visualisations relating to each stage. Note that although the discussion pertains to planar geometries, it may be qualitatively applied to more complicated configurations, for example cylindrical and spherical geometries.
2.1 Instability development: linear through to turbulent regimes

2.1.1 Linear regime

The simplest regime is that in which all modes in the interfacial perturbation are linear. An implicit assumption here is that the interface separating the two fluids is initially smooth and continuous, such that it can be described as an expansion in some orthonormal basis (e.g. as a Fourier series). This allows for analysis in terms of amplitudes and wavelengths of individual modes (i.e. harmonics) in the perturbation. A mode $k$ is considered linear if the growth of its amplitude $a_k$ is well described by linear stability analysis, as outlined above. Experimentally, linear theory has been shown to remain valid up until $ka_k \approx 1$ in three dimensions [34, 35], provided $ka_k \ll 1$ initially. Typically a more conservative estimate is taken, such as $a_k \leq 0.1 \lambda_k$ [15], beyond which the mode is considered saturated. Note that there are a wide range of factors such as viscosity, finite thickness, strong shocks and additional physics that modify the initial growth rate compared to the basic forms given in Equation (2.3) and Equation (2.4), a detailed discussion of which can be found in Zhou [18, 19]. This may also affect the amplitude at which each mode saturates, however for simplicity it will be assumed here that a multimode perturbation is growing in the linear regime provided all modes satisfy $a_k \leq 0.1 \lambda_k$.

Figure 2.2a shows the initial condition used in the $\theta$-group collaboration [30]. While the following image sequence will be taken from that study, the same general trends also apply to Rayleigh–Taylor mixing layers, for example see Youngs [36] for visualisations of an analogous RTI case. The initial surface perturbation shown in Figure 2.2a contains modes ranging from $k_{\min} = 4$ to $k_{\max} = 8$ and the total standard deviation of the perturbation is set to be $\sigma = 0.1 \lambda_{\min}$ to ensure that all modes are initially linear (see Chapter 4 for further details). The interface also has an initial diffuse thickness, which modifies the initial growth rate but has a negligible impact on the subsequent evolution [37].

Shortly after initiation of the instability (in this case by a $M_s = 1.84$ shock wave), the layer is growing in the linear regime, as shown in Figure 2.2b. For this particular RMI case, the incident shock travels from heavy to light fluids and hence the perturbation has reversed in phase. The initial diffuse thickness of the interface has
2.1 Instability development: linear through to turbulent regimes

(a) Initial condition.

(b) Linear regime.

(c) Weakly nonlinear regime.

(d) Strongly nonlinear regime.

Figure 2.2 – Early time evolution of multimode Richtmyer-Meshkov instability. Shown are contours of volume fraction $f_1$ where $f_1 = 1$ (red) indicates unmixed heavy fluid and $f_1 = 0$ (blue) indicates unmixed light fluid. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
also been compressed by the shock. While the evolution of RTI from the same initial surface perturbation would differ, at an equivalent early time the layer would look qualitatively similar. In both cases the evolution of the instability is due to baroclinic torque at the interface, as given in Equation (2.2).

2.1.2 Nonlinear regime

Once the smallest initial wavelength mode has become nonlinear, i.e. \( a_{k_{\text{max}}} > 0.1 \lambda_{\text{min}} \), then the layer as a whole can be considered to have entered the weakly nonlinear regime. In this regime the growth of the highest modes is no longer well described by linear theory, however the interface is still smooth and simply connected. Figure 2.2c shows a visualisation of the RMI mixing layer in this regime. For \( A > 0 \), the structures on either side of the interface begin to grow asymmetrically and are referred to as bubbles (light fluid penetrating heavy fluid) and spikes (heavy fluid penetrating light fluid). For a single mode, the bubble/spike amplitudes are defined by considering the distance between the peak of the bubble/spike and the centre of the layer. This can be defined multiple ways, however a definition that is robust is to take the peak of the bubble and spike as the minimum and maximum \( x \) positions where the volume fraction of fluid 1 \( f_1 = 0.5 \) (assuming \( x \) points in the direction of gravity/shock for a heavy-light configuration). The mixing layer centre \( x_c \) can then be defined as the position of equal mixed volumes [38], given by

\[
\int_{-\infty}^{x_c} \langle f_2 \rangle \, dx = \int_{x_c}^{\infty} \langle f_1 \rangle \, dx, \tag{2.6}
\]

where \( \langle \ldots \rangle \) indicates a plane average in the statistically homogeneous direction(s). For multimode perturbations, average amplitudes of the bubble and spike fronts, denoted as \( h_b \) and \( h_s \), are used rather than the amplitudes of individual peaks. \( h_b \) and \( h_s \) are defined as the distance between the mixing layer centre and the \( x \) positions where \( \langle f_1 \rangle = 0.01 \) and \( \langle f_1 \rangle = 0.99 \) respectively (other thresholds may also be used e.g. 0.05 and 0.95 [39]), with the overall width of the layer given by \( h = h_b + h_s \) [5]. This definition can be subject to statistical fluctuations however, whereby a few outliers
can dominate the overall width of the layer. Therefore it is common for results from simulations to be presented in terms of the integral width instead \[40\], defined as

\[ W = \int_{-\infty}^{\infty} \langle f_1 \rangle \langle f_2 \rangle \, dx. \quad (2.7) \]

For a symmetric, linear volume fraction profile, it can be shown that \( h = 6W \). Using the previous definition for \( x_c \) given in Equation (2.6), bubble and spike integral widths may also be defined following Krivets et al. \[6\] as

\[ W_b = \int_{-\infty}^{x_c} \langle f_1 \rangle \langle f_2 \rangle \, dx, \quad (2.8) \]
\[ W_s = \int_{x_c}^{\infty} \langle f_1 \rangle \langle f_2 \rangle \, dx. \quad (2.9) \]

This allows for the assessment of asymmetries in the growth of the bubbles and spikes, while also retaining the favourable statistical properties of \( W \).

A distinction is generally made between weakly nonlinear and strongly nonlinear regimes. An RTI/RMI mixing layer can be considered strongly nonlinear when the interface has become multi-valued, as shown in Figure 2.2d. This occurs due to the intense vorticity that is generated/deposited at the interface, causing it to roll up. These roll-ups are also where the two fluids mix most readily due to the stirring motion and increased surface area. The interface may also no longer be simply connected as regions of strong circulation cause material to pinch off and advect away from the main layer. This is more pertinent to RMI than RTI, due to the initial impulsive acceleration.

### 2.1.3 Transition to turbulence

In addition to the primary roll-ups that occur due to baroclinic vorticity, as the mixing layer continues to evolve it begins to develop secondary instabilities within these roll-ups and at other locations along the interface. This is because of shearing motion that occurs at the interface, across which there is a jump in the tangential component of velocity. In regions where there is misalignment between the gradients
of density and tangential velocity, the interface becomes Kelvin–Helmholtz unstable and thus increasingly fine-scale vortical motions are produced. It is these motions that drive the transition of the mixing layer from laminar to turbulent, generating modes outside the range present in the initial perturbation. Since the interfacial surface area also rapidly increases, mixing occurs much more effectively as the layer becomes progressively more turbulent. Figure 2.3a shows a visualisation of the RMI mixing layer in this transitional regime.

It is often useful to quantify the degree to which the two fluids are mixed by considering a dimensionless measure of the mixing state. One such measure is the molecular mixing fraction [41], given by

\[ \Theta = \frac{\int \langle f_1 f_2 \rangle \, dx}{\int \langle f_1 \rangle \langle f_2 \rangle \, dx}. \]  

(2.10)

\( \Theta \) can takes values anywhere between 0 and 1, with \( \Theta = 0 \) corresponding to complete heterogeneity and \( \Theta = 1 \) corresponding to complete homogeneity of mixing. It can also be shown that \( \Theta \) is related to the variance of the density PDF [42]. The variation of \( \Theta \) in time can be used to estimate when the layer has entered the transitional regime. For a typical simulation of a conventional RTI/RMI configuration \( \Theta \) will start out close to 1, as the only heterogeneity present is due to the surface perturbation. As the instability develops, \( \Theta \) will decrease and eventually reach a minimum, beyond which it increases again and tends towards some asymptotic value. The decrease in \( \Theta \) is due to the penetration of bubbles and spikes and a stretching of the layer. As the roll-ups of the primary and secondary instabilities develop however, fine-scale mixing begins to occur and eventually overcomes the stretching effect. Thus the time of minimum \( \Theta \) can be considered to be approximately the time when the layer has begun to transition.

It is important to note that dissipative effects (viscosity, diffusivity, conductivity) will act against the fluid instabilities, most strongly at small scales, which has potentially important ramifications for how the layer evolves. In order to quantify how important, it is necessary to introduce the Reynolds, Schmidt and Prandtl numbers. The
Figure 2.3 – Transition to turbulence in a multimode RMI mixing layer. Shown are contours of volume fraction $f_1$ where $f_1 = 1$ (red) indicates unmixed heavy fluid and $f_1 = 0$ (blue) indicates unmixed light fluid. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
2.1 Instability development: linear through to turbulent regimes

Reynolds number is a measure of the ratio between inertial and viscous forces and is given by

\[ Re = \frac{LU}{\nu}, \quad (2.11) \]

where \( L \) and \( U \) are some characteristic length scale and velocity of the flow and \( \nu \) is the kinematic viscosity. An appropriate choice must be made for the characteristic length scale and velocity, with one such choice being to set \( L = h \) and \( U = \dot{h} \), resulting in the outer-scale Reynolds number [43]. For sufficiently low values of this Reynolds number, the growth of secondary instabilities will be suppressed and the mixing layer will not reach a state of fully developed turbulence. In the most severe case, that is, for extremely low Reynolds numbers, the growth of the primary instability will be significantly suppressed, even to the point of remaining completely stable.

Considering the Reynolds number in isolation does not give the full picture however, as in addition to viscous dissipation (diffusion of momentum) there will invariably also be some diffusion of mass and heat. To characterise the degree to which these processes affect the flow, the Schmidt number \( Sc \) and Prandtl number \( Pr \) are required. These parameters are a measure of the ratio of the rate of momentum diffusion to mass and heat diffusion respectively, and are given by

\[ Sc = \frac{\nu}{D}, \quad (2.12) \]
\[ Pr = \frac{\nu}{\alpha}. \quad (2.13) \]

Here \( D \) is the mass diffusivity and \( \alpha = \kappa/(\rho c_p) \) is the thermal diffusivity, with \( \kappa \) being the thermal conductivity and \( c_p \) the specific heat capacity at constant pressure. For many gases, \( Sc \approx Pr \approx 0.7 \), and it is common in fundamental turbulent mixing studies to set \( Sc = Pr = 1 \) [36]. Thus at very low Reynolds numbers, for \( Pr \) and \( Sc \) of \( O(1) \) there will be significant amounts of heat and mass transfer and the two fluids will mix via these mechanisms rather than by turbulent stirring.

The particular case being used here to illustrate the various stages of instability development initially contains only a narrow range of modes, hence saturation and transition of the lowest modes in the initial perturbation occurs relatively soon after
that of the highest modes. If there is a sufficiently broad range of modes in the initial perturbation however, then the lowest modes will still be growing in the linear regime while higher modes have saturated and begun to transition. Youngs [44] proposed that it is possible for this linear growth of the lowest modes to overtake that of the higher, saturated modes and thus dominate the overall growth rate of the layer. In addition, it also implies that the growth rate of the layer for RT and RM in this regime is dependent on the initial conditions [31].

2.1.4 Fully developed turbulence

For a sufficiently high Reynolds number, the mixing layer will eventually transition to a state of fully developed turbulence. A visualisation of the fully turbulent RM mixing layer is shown in Figure 2.3b. In this regime, the RM mixing layer will enter into self-similar decay in a manner analogous to homogeneous decaying turbulence. During this period, integral mix measures such as the mixing fraction $\Theta$ will approach an asymptotic value and the width grows as $h = h_b + h_s = \alpha_{RM} t^\theta$ for some constant exponent $\theta$. The specific value of $\theta$ depends weakly on the Atwood number as well as the initial conditions as mentioned previously, a consequence of the permanence of large eddies [45], while $\alpha_{RM}$ also depends on the initial conditions [46]. Note that experimental results have indicated that the bubble and spike amplitudes may grow as $h_b \sim t^{\theta_b}$ and $h_s \sim t^{\theta_s}$ where $\theta_s > \theta_b$, particularly for large Atwood numbers, implying that the layer does not grow self-similarly [47]. However, recent numerical results show for $0.5 < A < 0.9$ that while the ratio $h_s/h_b$ varies initially, it eventually approaches a constant value which implies that $\theta_b = \theta_s$ [48, 49]. This is also in agreement with the analysis of Elbaz & Shvarts [46], who showed that at least $G = 3$ mode coupling generations must occur in order for self-similar growth to be obtained. For the impulsive linear electric motor (LEM) experiments cited above it is estimated that $G = 1.25–1.85$ generations, hence it can be concluded that they did not reach self-similarity.

For the fully turbulent RT mixing layer, self-similar growth occurs of the form $h =$
2.1 Instability development: linear through to turbulent regimes

\[ \alpha_{RT} A g t^2 \] where \( \alpha_{RT} = \alpha_b + \alpha_s \). As with \( \theta \), the constant \( \alpha_{RT} \) depends on \( A \) as well as on the initial conditions [36]. For immiscible fluids, surface tension may also influence the value of \( \alpha_{RT} \) obtained [50]. Results from the LEM experiments show that the ratio \( \alpha_s/\alpha_b \) varies significantly with Atwood number, however this still implies that the layer grows self-similarly as both the bubble and spike amplitudes have the same temporal scaling. In terms of mode coupling generations, it was estimated that the constant acceleration LEM experiments achieved \( G = 3.3–4.9 \) and therefore the reported values of \( \alpha_{RT} \) are representative of the self-similar asymptotic limit. It is important to note that, in general, a RT mixing layer will achieve self-similarity on a shorter timescale than a RM mixing layer due to the different dependence on \( t \), hence why it is easier to achieve self-similarity in experiments and simulations. This can also be explained in terms of the time between successive mode generations, which becomes progressively shorter for RT but longer for RM, where each new mode generation requires \( \sim 10 \) times longer to reach than the previous one [46]. The different dependence of \( h \) on \( t \) also implies that the dependence of the Reynolds number on \( t \) is different. For Rayleigh–Taylor, the outer-scale Reynolds number grows as \( Re \propto t^3 \), whereas for Richtmyer–Meshkov it grows as \( Re \propto t^{2\theta-1} \) (see Chapter 4 for details). Thus for \( \theta < 1/2 \) (as is the case for narrowband perturbations), the outer-scale Reynolds number decreases in time.

As for what constitutes a sufficiently high Reynolds number in order to achieve fully developed turbulence, the mixing transition concept of Dimotakis [51] for statistically stationary flows can be adapted to flows that are evolving in time [52]. For stationary flows, the transition to fully developed turbulence, characterised by a reduction in the sensitivity of the flow to the specific value of the Reynolds (and Schmidt) number, occurs for an outer-scale Reynolds number of \( Re \approx 1–2 \times 10^4 \). It was shown by Dimotakis [51] that this corresponds to the requirement that \( \lambda_L \geq \lambda_v \), where \( \lambda_L \) and \( \lambda_v \) are the Liepmann–Taylor and inner-viscous length scales and are estimates for the upper and lower bounds of the inertial range in the turbulent kinetic energy spectrum. Zhou et al. [52] extended this theory to unsteady flows, showing that an additional, temporally developing length scale, the diffusion layer scale \( \lambda_D \), must be considered.
and that the criteria for fully developed turbulence becomes $\min(\lambda_L, \lambda_D) \geq \lambda_c$. This also allows for an estimate of the time for turbulence to fully develop in unsteady flows. Zhou [53] further refined this concept to introduce a minimum outer-scale Reynolds number of $Re^* = 1.6 \times 10^5$ beyond which there is a complete decoupling between the energy-containing scales and those in the dissipation range. For flows that have achieved this "minimum state", statistics of the energy-containing scales should be independent of Reynolds number. The mixing transition and associated concepts are discussed in greater detail in Chapter 4.

2.2 Choice of governing equations and numerical method

In numerical studies of turbulence induced by RTI and RMI, it is important to choose an appropriate set of governing equations to solve, along with a suitable numerical method. All formulations of the equations governing fluid flow are statements of the physical laws of conservation of mass, momentum and energy combined with a varying number of assumptions and approximations to derive tractable mathematical systems of equations. The tradeoff between tractability and complexity is an important one as it is generally what guides the choice of governing equations for a particular study. Assumptions are made to improve tractability but also place restrictions on the range of validity of the results with respect to real flows due to the increasing level of approximation. An additional level of approximation is made when the equations are discretised and solved numerically, which the researcher seeks to minimise by choosing an appropriate numerical method. However, the amount of complexity contained in the system of governing equations creates a certain number of requirements that the numerical method must satisfy, which restricts which numerical methods are appropriate for a given problem. Note that only continuum descriptions of the underlying physics are considered in the discussion that follows.

Broadly speaking, the different formulations of governing equations used to study
RTI/RMI may be grouped according to their treatment of the advective terms and the mixture. Starting from the assumption that the mixture may be treated as a continuum, a hierarchy of descriptions can be derived where each successive level becomes increasingly tractable but has a decreasing range of validity. Generally the first aspect that must be considered is whether the mixture contains multiple phases of matter. Historically, numerical studies of turbulence arising from RTI/RMI have focused almost exclusively on single-phase fluids as this greatly reduces the number of different physical phenomena that must be considered. A distinction is also made between whether fluids of the same phase are miscible of immiscible, as each case typically requires a different numerical approach. This distinction is important as many experiments, particularly for Rayleigh–Taylor, use immiscible fluids to study turbulent mixing.

Perhaps the biggest distinction however, from an algorithmic point of view, is whether advection of the fluids may be treated as compressible or incompressible. Assuming incompressibility greatly improves the numerical tractability of the problem, as now the pressure and velocity fields may be considered to remain smooth and continuous, which allows for the use of numerical methods that can take advantage of this assumption. Needless to say this also reduces the range of validity of the results, which will be limited to applications where acoustic effects are negligible. If acoustic effects are important, as quantified by the Mach number, then a fully compressible formulation must be used which allows for the possibility of discontinuous changes in the flow properties. Typically, departures from incompressibility are considered to occur starting at a Mach number (mean and/or fluctuating) of $M \approx 0.3$ [54]. This requires the use of numerical methods that converge to (or approximate) the weak solution of the governing equations, which places restrictions on the ability of the method to resolve fine-scale turbulent features. One further assumption commonly made within the context of incompressible formulations relates to another non-dimensional parameter; the Atwood number. In the limit of $A \to 0$, variations in density can be assumed to be small and the governing equations may be simplified, known as the Boussinesq approximation. This may be considered as the simplest formulation that still permits
the study of buoyancy-driven turbulence. Based on this hierarchy of descriptions, the following subsections will detail each of the main formulations used for the study of turbulence induced by RTI and RMI; incompressible Boussinesq, incompressible variable-density and fully compressible formulations, as well as the use of various forms of interface tracking for simulating immiscible fluids. This constitutes a review of studies that investigate the effects of viscosity, conductivity, diffusion, variable-density, compressibility and surface tension on turbulence arising from these instabilities. The different approaches to modelling turbulence in these settings will also be discussed. For the sake of brevity, studies of the effects of other phenomena such as reactions [55], phase transition [56] and magnetohydrodynamics [57] on RMI and RTI will be neglected here. For a review of the application of non-continuum, particle-based methods such as the lattice Boltzmann method [58] to these flows, see Livescu [59].

2.2.1 Incompressible formulations

Boussinesq approximation

The basic formulation for buoyancy-driven incompressible flow with the Boussinesq approximation is given in Batchelor et al. [60]. In the Boussinesq approximation, fluctuations in density $\rho'$ are assumed to be small relative to the mean density $\rho_0$ and are due to the dependence of instantaneous density $\rho = \rho_0 + \rho'$ on a conserved scalar $\phi = \phi_0 + \phi'$ (e.g. concentration, temperature). Fluctuations in $\rho$ and $\phi$ are related by

$$\rho' = \beta \phi',$$

where $\beta$ is a constant (e.g. in the case where $\phi$ is temperature, $\beta = -\rho_0 \alpha$ where $\alpha$ is the coefficient of thermal expansion). In the Boussinesq approximation, density variations are assumed to affect the flow only through changes in the buoyancy force.
The equations governing the motion of Boussinesq fluids can therefore be written as

\[ \nabla \cdot \mathbf{u} = 0, \]  
\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} = \nu \Delta \mathbf{u} + \frac{\rho' \mathbf{g} - \nabla (\rho - \rho_0 \mathbf{g} \cdot x)}{\rho_0}, \]  
\[ \frac{\partial \rho'}{\partial t} + \mathbf{u} \cdot \nabla \rho' = D \Delta \rho', \]

where \( \nu = \mu / \rho_0 \) is the kinematic viscosity and \( D \) is the diffusivity associated with \( \phi \). The dot product of the acceleration vector \( \mathbf{g} \) and the position vector \( \mathbf{x} \) gives the specific potential energy (e.g. due to gravity). The equations may also be equivalently formulated in terms of the fluctuation \( \phi' \), for example see Landau and Lifshitz \cite{landau1976} for full details of the derivation of Equation (2.15) in the context of free convection. A recent review of Boussinesq Rayleigh–Taylor turbulence is given in Boffetta and Mazzino \cite{boffetta2015}.

In \cite{rodgers2015}, Equation (2.15a)–(2.15c) were solved numerically using the Fourier pseudospectral code of Rogallo \cite{rogallo1981}, developed for homogeneous turbulence. This is an important advantage of using the Boussinesq approximation; accurate and efficient codes developed for studying homogeneous turbulence may be applied with little modification to study buoyancy-driven effects. In general for DNS studies, the choice of numerical method is guided by wanting to minimise dissipation and dispersion errors for a given amount of computational effort. For incompressible flows, this is typically achieved with spectral methods \cite{schroeder2007}.

A triply periodic domain was used in \cite{rodgers2015} and the flow was initialised with homogeneous, isotropic perturbations to the density field. This homogeneous configuration may be considered to be an approximation of the interior of a fully developed Rayleigh–Taylor mixing layer at small Atwood number. Planar Rayleigh–Taylor mixing layers have also been studied using the Boussinesq approximation, with various approaches taken for dealing with modelling the inhomogeneous direction. Young et al. \cite{young2015} applied no flux, no slip boundary conditions in the inhomogeneous direction and used spatial discretisation with a Chebyshev polynomial basis to handle the aperiodicity. That same study also used a spectral-element method for comparison,
an approach that was also taken by Vladimirova and Chertkov [66] for a similar configuration. An alternative approach is to retain periodicity in all three directions by applying a second density interface far away from the primary mixing layer, which will remain Rayleigh–Taylor stable since the top fluid is lighter. This allows for the use of a Fourier pseudo-spectral code in all three directions, as in the studies of Boffetta et al. [67] and Matsumoto [2]. This can be seen at the top of Figure 2.4, taken from the study of Matsumoto [2].

Given that changes in density only produce changes in momentum through the buoyancy force in the Boussinesq approximation, the equations of motion are independent of the Atwood number, defined as $A = \Delta \rho/(2\rho_0)$. In this formulation, the role of the Atwood number is merely to rescale the non-dimensional time of the simulation. As explained in Section 2.1.4, for RTI in the self-similar regime $h = \alpha_{RT}Agt^2$ and
therefore $Re \propto h \dot{h} \propto A^2$, meaning that higher Reynolds numbers may be obtained for the same computational effort if the Atwood number is increased. This is why studies exploring the scaling of various quantities in the self-similar regime have used a relatively high Atwood number of $A = 0.1$ [67, 68] or even $A = 0.15$ [2]. Physically, the Boussinesq approximation is valid only for very low Atwood number. For Rayleigh–Bénard convection in air at standard atmospheric conditions, Gray and Giorgini [69] found the Boussinesq approximation to give results with at most a $\pm 10\%$ error so long as the maximum temperature difference does not exceed 28.6 K (i.e. roughly 10% of the mean). This corresponds to an Atwood number of $A = 0.05$, hence why studies aiming to match laboratory conditions or investigate transition to turbulence have typically used $A = 0.01$ or lower [65, 70].

**Variable density**

The generalisation of the equations governing buoyancy-driven incompressible flow to arbitrary density ratios is given in Sandoval [71], who considered the incompressible limit of a two-fluid mixture of ideal gases. For a general derivation including non-ideal gas effects and heat conduction, as well as the associated discussion, see Livescu [72]. Note that the incompressible limit may be obtained mathematically as either $p \to \infty$ or $\gamma \to \infty$ [59]. The $p \to \infty$ limit leads to uniform density in regions of pure fluid (as opposed to a non-constant background density) and is the one used in [71]. In this limit the ideal gas equation of state reduces to

$$\rho = \frac{1}{Y_1/\rho_1 + Y_2/\rho_2}.$$  \hfill (2.16)

where $Y_1$, $\rho_1$ and $Y_2$, $\rho_2$ are the mass fractions and partial densities of species 1 and species 2 respectively and $Y_1 + Y_2 = 1$. Each species mass fraction obeys a transport equation (of the same form as Equation (2.19d) in Section 2.2.2), which when summed over both species yields the continuity equation. The governing equations
are therefore

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{2.17a}
\]
\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}^t \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g}, \tag{2.17b}
\]
\[
\nabla \cdot \mathbf{u} = -\nabla \cdot \left( \frac{D}{\rho} \nabla \rho \right), \tag{2.17c}
\]

where \( D \) is the mass diffusion coefficient (assumed constant) and the viscous stress tensor is given by

\[
\mathbf{\sigma} = \mu \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^t - \frac{2}{3} (\nabla \cdot \mathbf{u}) \delta \right). \tag{2.18}
\]

Compared to the Boussinesq approximation, the inclusion of variable density introduces additional cubic nonlinearities in the momentum equations as well as a non-zero divergence of velocity. This divergence term on the right-hand side of Equation (2.17c) is derived from Equation (2.16) and the species mass fraction equations, with the full diffusion operator in the infinite speed of sound limit. It is a consequence of the change in specific volume that occurs when the two fluids mix.

This term is also the principal source of additional difficulty that is encountered when solving these equations numerically, compared to incompressible constant-density and Boussinesq formulations. In incompressible solvers, the velocity divergence constraint is satisfied by deriving an elliptic equation for pressure. This equation is obtained by taking the divergence of the momentum equation, combined with the divergence constraint. In constant-density and Boussinesq formulations, combining Equation (2.15a) and the divergence of Equation (2.15b) results in a constant-coefficient Poisson equation for pressure, which is readily solved through a variety of techniques [73]. For the variable-density formulation however, combining Equation (2.17c) and the divergence of Equation (2.17b) leads to a Poisson equation with a factor of \( 1/\rho \) in the coefficients, making its solution more complicated.

Approaches for tackling this problem vary. Sandoval [71] and Cook and Dimotakis [43] used a constant-coefficient Poisson equation for pressure and estimate the \( \nabla \cdot (\rho \mathbf{u})^{n+1} \) term using finite differences of \( \mathbf{u} \) from previous timesteps \( n \) and \( n - 1 \), the divergence...
constraint and the fact that $\rho^{n+1}$ is already known at that point in the solution process. This approach has the advantage that no iteration is required for pressure, however the overall accuracy of the temporal discretisation is reduced. When used in conjunction with a third-order Adams-Bashforth-Moulton time integration method, the scheme remains stable up to a density ratio of 4, while with third-order Runge-Kutta timestepping density ratios up to 10 are able to be simulated (A. Cook, private communication).

Livescu and Ristorcelli [74] overcome the reduction in accuracy of the temporal discretisation by deriving an exact nonlinear equation for pressure (i.e. no finite difference approximation required for $u^{n+1}$). The trade-off for eliminating temporal discretisation errors is that this pressure equation now requires an iterative solution, increasing the overall computational cost of the scheme. This approach also only works for triply periodic flows. A third approach is given by Chung and Pullin [75], who use a Helmholtz-Hodge decomposition on the pressure gradient terms in the momentum equation. This leads to a constant-coefficient Poisson equation being obtained for the scalar potential of this decomposition and a nonlinear equation for the divergence-free component that is solved by iteration. This approach ensures that temporal discretisation errors are isolated to divergence-free component. The iteration introduces additional computational cost however, with the convergence rate depending on the Atwood number. In addition, $\ln(\rho)$ is used instead of $\rho$ in the timestepping as this ensures $\rho$ is always positive after dealiasing, but at the cost of not discretely conserving mass (D. Chung, private communication).

To date, computations have been run using this method up to a density ratio of 10 [76]. A similar procedure was used by Livescu et al. [77] to simulate planar RTI between fluids with density ratios as high as 19. Recent simulations have also been performed of shear-driven mixing layers between hydrogen and air (density ratio 16) using this method [78]. A key difference with the method of Chung and Pullin [75] is that $\rho$ is advanced in the timestepping, which ensures that mass is conserved but at the cost of a smaller timestep (D. Livescu, private communication). Other approaches have also been presented, typically in the context of incompressible two-phase flows,
such as the method of Dodd and Ferrante [79] who use a pressure-correction technique coupled with a volume-of-fluid method. This approach is quite similar to that of [74], but using only the first step of the iteration.

There are also a variety of different configurations used in studies of variable-density turbulent mixing. Sandoval [71] and Livescu and Ristorcelli [74] considered the variable-density extension of the homogeneous problem studied by Batchelor et al. [60]. Chung and Pullin [75] also used a triply periodic domain but with the fringe-region technique [80], thus producing a statistically stationary flow. Cook and Dimotakis [43], Cabot and Cook [3] performed simulations of a planar Rayleigh–Taylor mixing layer at an Atwood number of $A = 0.5$ and Schmidt number $Sc = 1$. Spatial derivatives in the inhomogeneous direction were computed using an eighth-order compact difference scheme to account for aperiodicity. Due to the decreased fidelity of the compact difference scheme versus the spectral scheme used in the homogeneous directions, the grid spacing used in the inhomogeneous direction was decreased by a factor of $8/13$. Figure 2.5 shows a visualisation of the highest Reynolds simulation of this configuration. Mueschke and Schilling [81] used this same numerical method to perform a direct numerical simulation of planar RTI with experimentally measured initial conditions. Livescu et al. [77] used a similar approach in the inhomogeneous direction (sixth-order compact differences) to perform DNS of planar Rayleigh–Taylor mixing layers for Atwood numbers ranging from 0.04 to 0.9.

While the variable-density formulation allows for accurate results to be obtained for mixtures of miscible fluids at high Atwood number, its range of applicability is still limited to low-speed flows. In general this precludes the study of the Richtmyer–Meshkov instability using this formulation, as although the development of the instability at late time is virtually incompressible for small to moderate shock Mach numbers, the shock wave itself is an inherently compressible phenomenon. This is not necessarily the case however and there are two approaches to tackling this that are worth mentioning here. The first is to use a hybrid solver that switches between compressible and incompressible formulations based on the maximum local Mach number. This was the approach taken by Oggian et al. [82], who found that a thresh-
old value of \( M = 0.2 \) was optimal for performing this switch. The second approach, valid for initial perturbations that are entirely linear, is to use an equivalent velocity perturbation [31], thus circumventing the need to initialise a shock wave. This second approach has been used in conjunction with compressible solvers [31, 83, 45], however it also represents an intriguing way to apply state-of-the-art incompressible solvers to RMI flows.

### 2.2.2 Compressible formulations

The governing equations for multicomponent mixtures of compressible, inert, miscible materials are given in Livescu [59] in a very general form. Here the presentation will be restricted to binary mixtures of ideal gases with linear constitutive relations. With these restrictions, the standard form of the governing equations is

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}^t + p \mathbf{\delta}) &= \nabla \cdot \mathbf{\sigma} + \rho \mathbf{g}, \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho E + p \mathbf{u}) &= \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{u} - \mathbf{q}_c - \mathbf{q}_d) + \rho \mathbf{g} \cdot \mathbf{u},
\end{align*}
\]
In Equation (2.19) above, (2.19a), (2.19b) and (2.19c) are statements of the conservation of mass, momentum and total energy of the mixture, while (2.19d) describes the conservation of mass for species 1. The velocity $u$ is the mass-weighted velocity of the mixture and each species $l$ has its own velocity, which differs from the mixture velocity by a diffusion velocity $V_l$. The total energy is given by $E = e + \frac{1}{2}u \cdot u$, where the internal energy $e$ is related to the state variables $\rho$ and $p$ through the equation of state. For ideal gases this relation is

$$\rho e = \frac{p}{\gamma - 1},$$

where $\gamma$ is the ratio of mass-weighted specific heats, given by

$$\gamma = \frac{\sum Y_l c_{p,l}}{\sum Y_l c_{v,l}}.$$
invoked), while the heat flux vector is given by Fourier’s law of conductivity to be

$$q_c = -\kappa \nabla T. \quad (2.22)$$

The mass flux for species 1 is given by $J_1 = -\rho Y_1 V_1$, and the application of Fick’s law of diffusion gives

$$J_1 = \rho D \nabla Y_1, \quad (2.23)$$

where $D$ is the binary mass diffusion coefficient as before. Often in fundamental studies $D$ (as well as the viscosity $\mu$ and conductivity $\kappa$) is assumed to be constant, however this need not be the case in general. For mixtures of more than two species, Fick’s law is often still used but with an additional correction velocity to ensure mass conservation [90], while a more accurate representation is the Hirschfelder–Curtiss approximation [91]. Finally, changes in mixture composition due to species diffusion give rise to changes in energy which must be accounted for. This is done via the enthalpy diffusion flux, defined as

$$q_d = \sum h_l J_l, \quad (2.24)$$

where $h_l = e_l + p/\rho_l$ is the enthalpy of species $l$. Note that in general, the system of equations and constitutive laws given above does not satisfy the second law of thermodynamics due to the exclusion of terms relating to the diffusion of mass due to pressure and temperature gradients and the energy changes associated with these processes [61]. These terms are typically neglected for the sake of simplicity but may be non-negligible at large molecular weight ratios [59], see Section 3.1 for a complete description.

Comparing the (already simplified) compressible formulation above to the incompressible variable-density formulation given in Section 2.2.1, numerical methods must be able to robustly handle shocks and resolve acoustic waves, in addition to capturing fine-scale vortical motions and material interfaces. This represents the key challenge that compressible solvers must overcome and in general some form of trade-off must be made between stably capturing discontinuities and resolving fine-scale structures.
2.2 Choice of governing equations and numerical method

For this reason, a more diverse range of numerical methods is present in the literature for compressible formulations as each approach has its own strengths and weaknesses. For example, Gauthier [33] used an auto-adaptive multidomain Chebyshev-Fourier spectral method to perform direct numerical simulations of the compressible Rayleigh–Taylor instability. However, for this study the maximum (fluctuating and mean) Mach number was $M < 0.04$ to prevent the formation of shock waves, which lead to Gibbs oscillations and non-uniform convergence in spectral methods. This inability of spectral methods to robustly handle shock waves is one of the main reasons why fundamental studies of compressible turbulence induced by RTI and RMI are typically performed using some form of high-order finite-difference, finite-volume or arbitrary Lagrangian-Eulerian (ALE) method.

Compact difference schemes are one such substitute for spectral methods in fundamental studies of compressible turbulence, and their performance relative to spectral methods is reasonably well known from studies using incompressible formulations such as Cook and Dimotakis [43]. Olson and Greenough [92] assessed the resolution requirements for DNS and LES of a RMI-induced turbulent mixing layer using the Miranda and ARES simulation codes. A similar study was also performed using the same codes for compressible RTI [93]. Miranda uses a tenth-order compact difference scheme for spatial differentiation combined with a five-stage, fourth-order Runge–Kutta scheme for temporal integration. Artificial fluid properties are used to regularise sharp gradients and discontinuities in the flow. An eighth-order compact filter is also applied to the conserved variables at each time step to smoothly remove the top 10% of wavenumbers to ensure numerical stability. The other code used in these studies, ARES, is an arbitrary Lagrangian-Eulerian method that uses a second-order predictor-corrector method in the Lagrange step and second-order finite-difference for spatial gradients. Artificial viscosity is used to damp oscillations that occur near shocks and material interfaces. Comparisons between these two methods showed that, as expected, the higher order of accuracy in the Miranda code was important for capturing a broader range of length scales and also resulted in better convergence of large-scale integral quantities. Note that ARES has an adaptive mesh refinement
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capability that was not used in these studies, which would significantly enhance the
efficiency of the method. In both methods, a downside with the use of artificial vis-
cosity for capturing shock waves is that a penalty is incurred on the timestep size
in order to meet the viscous stability condition, particularly for strong shocks where
a lot of artificial viscosity is required. For an explicit time-stepping scheme in one
dimension, von Neumann stability analysis yields the following requirement

\[
\frac{\alpha \Delta t}{(\Delta x)^2} \leq \frac{1}{2},
\]

(2.25)

where \(\Delta t\) and \(\Delta x\) are the timestep size and grid spacing respectively and \(\alpha\) is the
diffusivity of the physical process in question (e.g. mass diffusion, heat conduction,
viscosity). This shows that for large values of \(\alpha\), which in this case represents artificial
+ actual viscosity, the timestep size depends on \((\Delta x)^2\), as opposed to the usual \(\Delta x\)
dependence given by the inviscid stability condition (given in Equation (2.26) below).

The Miranda code was also compared to INCA, a conservative finite-difference scheme
that employs a hybrid central-upwind reconstruction method for the numerical fluxes,
for simulations of 3D planar RMI in Tritschler et al. [4]. This method consists of a
sixth-order stencil in smooth regions and a nonlinear convex combination of third-
order stencils in regions with steep gradients. The reconstruction uses a projection
onto local characteristics, which requires the Roe-averaged Jacobian matrix, and a
positivity-preserving flux limiter is used in regions of low density or pressure. Temp-
al integration is performed with a third-order total variation diminishing Runge–
Kutta method. Results from this study showed that Miranda was able to resolve more
of the fine-scale turbulent kinetic energy and enstrophy, particularly at late-time. This
result follows the observation that high-order compact difference schemes are capable
of resolving higher modes than explicit finite-difference methods, based on modified
wavenumber analysis [94]. Overall this study is a good example of the differences that
arise due to dominantly dissipative (Miranda) versus dominantly dispersive (INCA)
truncation errors when simulating compressible turbulent mixing problems. These
can be observed qualitatively in Figure 2.6.
Another example of the successful application of central-upwind schemes to study RTI/RMI is the hybrid method of Hill et al. [95], which uses a combination of a fifth-order weighted essentially non-oscillatory (WENO) conservative finite difference scheme for shock capturing and a five-point tuned centre-difference (TCD) scheme away from shocks. The TCD scheme is optimised for low-dissipation by minimising the spatial truncation error, at the price of a reduction in order of accuracy from fourth- to second-order. To ensure numerical stability, the momentum, energy and scalar convective terms are written in a skew-symmetric form and time integration is performed using a third-order strong stability-preserving Runge–Kutta scheme. An issue that is pertinent to all hybrid numerical methods of this form is how to efficiently detect shocks and other discontinuities such that the more dissipative upwind method is isolated to the region surrounding the discontinuity and is not activated prematurely or in a large region of the flow. There is also an additional computational cost associated with this detection function; see Johnsen et al. [96] for a comparison of various numerical methods for shock-turbulence interaction, including hybrid central-

\[ \text{Figure 2.6} \] – Plots of heavy fluid mass fraction from (a) Miranda and (b) INCA in a 3D planar RMI calculation. *Source:* From Figure 5 of Tritschler et al. [4].
upwind schemes, and their respective computational cost estimates.

The two most relevant and comprehensive studies in the context of this discussion are the comparative numerical studies of turbulence induced by RTI/RMI, known as the \( \alpha \)-group and \( \theta \)-group collaborations respectively. In the \( \alpha \)-group study [5], six compressible codes and one incompressible code were used to investigate self-similar Rayleigh–Taylor turbulence evolving from a high-wavenumber, narrowband, multi-modal perturbation in the nearly incompressible regime. The choice of performing simulations in the nearly incompressible regime was made so as to conform with most previous RTI experiments, however for the compressible codes used this incurs a significant penalty in computational expense due to the restriction on the timestep size required by the inviscid stability condition, known as the Courant–Friedrichs–Lewy (CFL) condition. Again for an explicit time-stepping scheme in one dimension, von Neumann stability analysis shows that

\[
\frac{S_{\text{max}}^n \Delta t}{\Delta x} \leq 1.
\] (2.26)

Here \( S_{\text{max}}^n \) refers to the maximum wave speed present in the domain at time \( n \), which is commonly approximated by \( S_{\text{max}}^n = \max(|u_i^n| + a_i^n) \) where \( u_i^n \) and \( a_i^n \) are the velocity and speed of sound in cell \( i \) at time \( n \) [97]. Thus for small \( M = u_i^n / a_i^n \) the timestep size is dominated by \( a_i^n \) in a compressible algorithm and many timesteps are required to simulate the same amount of time as one timestep of an incompressible method for the same problem.

Upwind schemes are also known to exhibit excessive numerical dissipation and a deterioration in accuracy in the low Mach number limit [98, 99]. Of the codes used in the \( \alpha \)-group study, this includes the three solvers based on the Piecewise Parabolic Method (PPM); FLASH, WP/PPM and NAV/STK. The three other compressible codes used include ALEGRA and HYDRA, both ALE codes with optional interface reconstruction capabilities, and the Lagrange-remap code Turmoil. The Lagrange-remap method used in Turmoil is similar to an ALE method and operates on a staggered grid. Multiple Lagrangian advection steps may be run, particularly at low
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Mach number, prior to a remap back to the initial grid. A distinguishing feature of this approach is that the Lagrangian phase is non-dissipative in the absence of shocks, while the dissipation in the remap phase is independent of the Mach number, making it well suited for computing nearly incompressible flows. A direct quantification of the amount of numerical dissipation introduced in the remap phase is also available with this method, which is useful for estimating the level of grid independence obtained when performing DNS [36]. The relative resolving power of each of the codes in the \( \alpha \)-group study may be compared by examining the critical wavenumber \( N_{\text{crit}} \), beyond which the spectra of fluctuating volume fraction depart from the expected Kolmogorov inertial range. This metric indicates that WP/PPM and Turmoil were the least dissipative codes, followed by NAV/STK.

For the \( \theta \)-group study, seven compressible codes (and an additional interface reconstruction code) were used to perform simulations of turbulent mixing induced by the multimode, narrowband Richtmyer–Meshkov instability. The codes used in the study include the previously discussed ARES, Miranda, FLASH and Turmoil as well as the conservative finite difference code Triclade [100] and two high-order Godunov methods, Flamenco [101] (the same code used in this thesis) and NUT3D [102]. For the two cases that were simulated, the late-time evolution is close to incompressible and therefore the same considerations apply as in the \( \alpha \)-group study with regards to using compressible codes in the nearly incompressible regime. For standard Godunov methods, pressure and density fluctuations scale as \( O(M) \) in the incompressible limit, contrary to the theoretical \( O(M^2) \) scaling [103]. This results in a kinetic energy dissipation rate of \( \epsilon \propto 1/M \) in the standard formulation of these schemes and hence any low Mach features in the flow are heavily damped. In Flamenco, a correction for this behaviour is applied in the reconstruction phase [9], restoring the correct scaling of pressure and density in the incompressible limit and significantly enhancing the fidelity of the numerical method for little additional computational cost. This approach maintains the favourable properties of Godunov finite-volume methods, namely robust shock capturing and good resolution of material interfaces, while also improving the ability to resolve fine-scale vortical motions. The algorithm has been extended
to include a DNS capability, which is discussed in detail in Chapter 3, as well as a semi-Lagrangian moving mesh option [104].

Comparisons between the various codes in the $\theta$-group collaboration found that there was very good agreement in the representation of the large scales of motion for quantities such as turbulent kinetic energy spectra. The main sources of disagreement between the codes were in general confined to higher wavenumbers and were determined to be due to the different dissipative properties of the various numerical methods. The study also gave some insight into the relative advantages and disadvantages of each of the main approaches to modelling compressible turbulent mixing. One such issue is in the definition of initial conditions, with algorithms based on finite-differences requiring that there be a smoothly varying profile across the material interface. Other algorithms, such as finite-volume methods, are able to initialise with a sharp profile, provided an appropriate cell-average is specified. The high-wavenumber cutoff behaviour is also an important point of comparison, as this is a good indication of the ability of the scheme to resolve fine-scale turbulence. Results from the $\theta$-group study show that for fluctuating kinetic energy spectra, Flamenco and Miranda both have very similar spectral fidelity (up until the activation of the eighth-order filter in Miranda), followed closely by Triclade and then with ARES and FLASH being more dissipative. Turmoil predicted consistently higher levels of kinetic energy throughout the layer than the other codes, which may be due to the treatment of acoustic waves in the Lagrange-remap method [105]. It should also be mentioned that due to their efficiency (as well as availability of computational resources), both Turmoil and Triclade were able to be run at double the grid resolution of the other codes.

To conclude this section, some other computational approaches to modelling compressible turbulent mixing will now be discussed. One is the use of front tracking (discussed in further detail in Section 2.2.3) in conjunction with physical mass diffusion to model mixing between miscible fluids [106]. The main idea behind this approach is to minimise numerical diffusion across an interface so that it does not dominate contributions from physical diffusion and/or sub-grid models. In Glimm et al. [107], the use of front tracking and large eddy simulation with dynamically
modelled sub-grid terms gave favourable comparisons with data from the Rayleigh–Taylor water channel experiment of Mueschke et al. [108]. Another unconventional and potentially very effective approach for simulating compressible turbulent mixing is the use of wavelet-based grid adaptivity such as in the Parallel Adaptive Wavelet Collocation Method (PAWCM) of Nejadmalayeri et al. [109]. PAWCM uses wavelet compression to dynamically adapt the grid to the scale of local flow structures, and a wavelet collocation method is used to ensure a one-to-one correspondence between grid points and wavelets. The evaluation of nonlinear terms in adaptive wavelet collocation methods is performed in the physical domain, similar to pseudo-spectral methods, and in PAWCM derivatives are calculated at the corresponding grid points using finite differences (of variable order). A key challenge in scaling adaptive wavelet collocation methods is achieving effective load balancing between processes. In PAWCM this is achieved using a tree-like data structure and domain repartitioning. Reckinger et al. [110] applied PAWCM to perform DNS of the 2D single-mode compressible Rayleigh–Taylor instability and provide a good discussion on how to consistently initialise the interface perturbation to reduce the generation of acoustic waves, as well as treatments at the domain boundaries to help avoid spurious acoustic reflections.

This last point forms another important consideration when going from incompressible to compressible formulations, namely how to maintain stability and high-order accuracy at non-periodic boundaries while also avoiding unwanted wave reflections, as often the aim of the simulation is to represent a very large (or even infinite) physical domain with a much smaller computational one. In incompressible simulations of RTI, the boundary conditions applied in the inhomogeneous direction are typically no-slip or free-slip conditions, placed far enough away such that the pressure and velocity fields are always uniform at the boundaries. For compressible simulations, acoustic phenomena mean that more advanced treatments are required. These fall broadly into two categories; the use of an absorbing buffer zone or the use of analytical solutions of the system external to the domain. In the buffer zone approach, the computational domain is extended (but typically calculations are only performed in one dimension) and numerical/physical viscosity is gradually increased such that
the intensity of any reflected waves is reduced to the point where the impact on the interior domain is negligible. Buffer zones are generally quite effective for arbitrary systems of equations and are also easy to implement, however they often require user interaction and tuning for different simulations.

Analytical approaches use one-dimensional characteristic analysis of the hyperbolic part of the governing equations to relate the amplitudes of incoming and outgoing waves [111]. For non-reflecting boundary conditions, setting the reflected amplitude to zero results in the system of equations becoming ill-posed and hence some degree of reflection must be allowed. In practice, the amount of reflection required to maintain well-posedness is minimal and is typically still smaller than reflections that occur using buffer zones. Incoming waves must also be sufficiently planar for the analysis to be valid and the viscosity must be sufficiently small (i.e. the Reynolds number must be large) if the full Navier–Stokes equations are being simulated, since the wave propagation is assumed to only be due to the inviscid part of the equations. The choice by researchers of whether to use one approach over the other therefore depends on the nature of the flow field being simulated, as well as other factors such as ease of implementation and computational cost (with characteristic boundary conditions typically being slightly more expensive).

### 2.2.3 Interface tracking

All of the various formulations and numerical approaches discussed thus far are only strictly valid for studying turbulence between miscible fluids. That is, either physical diffusion across a material interface is explicitly modelled and/or interface capturing schemes are used where interface is 'smeared' across some region of finite width in the computational domain. However, often there are very good reasons for modelling an interface as exactly discontinuous with no numerical or physical diffusion. One such scenario is when the fluids being studied are immiscible (or partially so), or multiphase. Another is when thickness of the interface is negligible with respect to the size of the computational grid, such as for flame fronts or the early stage
development of RMI or RTI. Indeed, early research into RT and RM instabilities focussed on understanding single-mode growth and typically some form of interface tracking was used for this purpose, particularly due to the limited computational resources available at the time [112]. Such simulations were also typically run as inviscid. When examining turbulence induced by RTI/RMI, interface tracking was deemed to no longer be appropriate in situations where significant fine-scale breakup of the interface occurs. However, for situations where the interface radius of curvature is greater than the grid size, such as those discussed above, some form of interface tracking remains a viable and sometimes necessary approach to modelling its evolution in time. In addition to studies of turbulence, other areas of application include the modelling of various multiphase processes such as RTI/RMI in liquid-gas mixtures and shock-induced ejecta.

In general, there are three main approaches that have been used to perform interface tracking in fluid dynamics simulations; (Eulerian) level set methods [113], (Lagrangian) front tracking methods [114] and volume-of-fluid or interface reconstruction methods [115]. In level set methods, the location of the interface is implicitly defined through the use of a level set function $\phi$, the evolution of which is given by

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0.$$  

(2.27)

The zero level set $\phi = 0$ corresponds to the location of the interface and the level set method consists of approximating the solution of Equation (2.27) by discretising the operators on a fixed grid. In general, $\phi$ is initially equal to the signed distance function, is advected according to the numerical solution of Equation (2.27), and is reinitialised to remain approximately equal to the distance function whenever information about the interface location is required. In front tracking methods, the interface is described explicitly by topologically-linked marker particles which are propagated according to the underlying velocity field (which may depend on the front geometry). A key part of such methods is the handling of topological bifurcations, particularly in 3D, and typically some form of interface reconstruction is used in regions where bifurcation is detected. Interface reconstruction methods, specifically the volume-of-
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fluid method, represent the interface implicitly through a scalar field $C$ that gives the volume fraction of a reference fluid in each cell. The colour function $C$ takes values $0 < C < 1$ in cells cut by the interface, either 0 or 1 away from the interface, and is governed by an advection equation of the same form as Equation (2.27). At each timestep, a reconstruction (typically piecewise linear) of the interface is performed based on the $C$ field. Each interface segment is then advected according to the velocity field and the resulting volume, mass and momentum fluxes are determined.

The relative advantages and disadvantages of each approach are discussed in Sethian and Smereka [113] for level set methods, Du et al. [116] for front tracking methods and Scardovelli and Zaleski [117] for volume-of-fluid methods and will be briefly summarised here. Level set methods are advantageous for their ease of calculating geometric quantities such as curvature, extension to three-dimensions, and the handling of topological changes. Volume-of-fluid methods also handle topological changes implicitly, can also be relatively easily extended to 3D and conserve mass well. They are also simple to parallelise since the reconstruction scheme is local. Front tracking methods are inherently more accurate than the other two approaches, due to their ability to represent the interface with a much larger number of points. This increased accuracy comes at the cost of requiring explicit handling of topological changes however.

The use of interface tracking methods in simulations of turbulent mixing due to RTI and RMI has primarily been to study the effects of immiscibility. The level set method was used by Young and Ham [118] to simulate the incompressible RTI between two viscous fluids with varying amounts of surface tension. George et al. [119] also performed simulations of RTI with physical surface tension, using the front tracking code FronTier. Indeed, front tracking has proven useful in determining the degree to which surface tension influences mixing between partially immiscible fluids [50]. Volume-of-fluid methods have also been used in simulations of turbulent RTI/RMI [5, 30, 120], however, due to a lack of surface tension the results are only useful in distinguishing between heterogeneous and homogeneous mixing by inhibiting numerical diffusion and do not constitute a true study on the effects of immiscibility.
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Figure 2.7 – Volume fraction of light fluid across a slice located at $z = 0$ for various codes used in the $\alpha$-group collaboration. Source: From Figure 32 of Dimonte et al. [5].

For example, see the results shown in Figure 2.7 for the ALEGRA code with and without interface reconstruction. This is not a fundamental limitation of the volume-of-fluid approach however and there is potential to use a volume-of-fluid approach to study the effects of immiscibility on RTI/RMI, with surface tension implemented through the continuum surface force method [115].

The use of some form of interface tracking to resolve gradients that are sharp with respect to the computational grid is also potentially very beneficial for modelling early time development of RMI and RTI between miscible fluids. As previously mentioned, front tracking has also been used to simulate mixing between miscible fluids [106], where the front being tracked is typically an isosurface of concentration or temperature. This area of application has not received as much attention as the modelling of immiscible fluids, though not due to a lack of possibility. In addition to the front tracking approach, there is potential for combining volume-of-fluid interface reconstruction with a diffuse interface model, such as the newly proposed five-equation model of Thornber et al. [89] that is discussed in Chapter 3. This would allow for steep gradients present during early time evolution of RMI and RTI to be accurately resolved, while also retaining the simplicity of a diffuse interface approach once the gradients are captured sufficiently on the computational grid.
2.3 Turbulence modelling

All of the mathematical formulations discussed in Section 2.2 describe completely, at the continuum level, the evolution of the flow field that ensues from a given initial condition (assuming it is well-posed). Given sufficient conditions, as discussed in Section 2.1.4, the flow will become turbulent. Turbulence is characterised by chaotic motion across a wide range of time and length scales, as well as a substantial increase in the efficiency with which fluid is mixed [29]. This wide range of scales is described in full by the governing equations, however, in order to obtain a numerical solution these equations must be discretised, and a significant amount of information about the fine-scale structure of the flow can be lost in this discretisation. In particular, turbulent motions that are smaller than the Nyquist frequency of the computational grid employed will be lost, while scales that are close to the grid scale will be influenced by the numerics. This may affect how the part of the flow field that is resolved by the grid evolves in time, as there is a cascade of energy from larger scales to smaller ones and this energy is only dissipated at the very smallest scales where viscosity is active [11]. How the impacts of this finite grid resolution are handled when simulating unsteady, turbulent flow is the topic of this section.

2.3.1 Direct numerical simulation

In order to retain a complete description of the turbulent flow field numerically, the smallest scale motions of the flow must be resolved in the discretisation (both spatially and temporally). This is referred to as direct numerical simulation (DNS), whereby the numerical solution that is obtained is considered to be independent of the numerical method and grid resolution used. However, in computational terms DNS is often prohibitively expensive, particularly for problems of practical interest (i.e. flows at high Reynolds number). This is due to the broad range of scales that are present in these flows, which extend far beyond the range that can be directly resolved (and then simulated for sufficient time) using current available computational resources. Nevertheless DNS still plays an important role in fundamental studies of turbulent
mixing, where the problem can be designed such that it only contains a manageable
range of scales, which is the approach employed in the present work. These canonical
problems, such as the ones presented in Chapter 4 and Chapter 5, are used to gain
insight into the nature of turbulent mixing in its various configurations, so that this
may be applied to the modelling of more complex scenarios such as those discussed
in Chapter 1.

There are various ways in which numerical errors arise and affect the flow field during
a simulation. One major source of errors are truncation errors that result from ap-
proximating gradients or interpolation, which reduce the level of fidelity with which
fine-scale motions in the flow can be resolved. These are often referred to as numerical
dissipation and dispersion, due to similarities with their physical counterparts in how
they affect the flow field. As an example, consider the second-order finite difference
approximation for the first derivative of $u$ at a point $x_i$. The Taylor series expansions
for $u_{i+1} = u(x_i + \Delta x)$ and $u_{i-1} = u(x_i - \Delta x)$ are

$$u(x_i + \Delta x) = u(x_i) + u'(x_i)\Delta x + \frac{1}{2} u''(x_i)(\Delta x)^2 + \frac{1}{6} u'''(x_i)(\Delta x)^3 + \ldots, \quad (2.28a)$$

$$u(x_i - \Delta x) = u(x_i) - u'(x_i)\Delta x + \frac{1}{2} u''(x_i)(\Delta x)^2 - \frac{1}{6} u'''(x_i)(\Delta x)^3 + \ldots, \quad (2.28b)$$

which gives the second order accurate approximation for $u'(x_i)$ to be

$$u'(x_i) = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{1}{6} u'''(x_i)(\Delta x)^2 + \ldots. \quad (2.29)$$

Therefore by only using the neighbouring points $u_{i+1}$ and $u_{i-1}$ to approximate the
derivative $u'(x_i)$, an error of $O((\Delta x)^2)$ is incurred (along with higher order terms).

Errors also occur from the finite representation of continuous functions, known as
aliasing errors. These arise due to the spurious generation of modes through non-
linear operations which are not in the set of modes being represented and whose
contributions are added incorrectly to the flow field. For example, the quantities $u(x)$
and \( v(x) \) may be represented by their Fourier series

\[
\begin{align*}
    u(x) &= \sum_{m=-\infty}^{\infty} \hat{u}_m e^{imx}, \quad (2.30a) \\
    v(x) &= \sum_{n=-\infty}^{\infty} \hat{v}_n e^{inx}, \quad (2.30b)
\end{align*}
\]

with their product \( w(x) = u(x)v(x) \) given by

\[
    w(x) = \sum_{k=-\infty}^{\infty} \hat{w}_k e^{ikx}, \quad (2.31)
\]

where

\[
    \hat{w}_k = \frac{1}{2\pi} \int_{0}^{2\pi} w(x) e^{-ikx} \, dx = \sum_{m=-\infty}^{\infty} \hat{u}_m \hat{v}_{k-m}. \quad (2.32)
\]

For a discrete set of points \( x_j \) (where \( j = 0, 1, \ldots, N-1 \)), \( u_j = u(x_j) \) and \( v_j = v(x_j) \) are represented as

\[
\begin{align*}
    u_j &= \sum_{n=-N/2}^{N/2-1} \hat{u}_n e^{inx_j}, \quad (2.33a) \\
    v_j &= \sum_{m=-N/2}^{N/2-1} \hat{v}_m e^{inx_j}. \quad (2.33b)
\end{align*}
\]

However, their product is now given by

\[
    w_j = \sum_{k=-N/2}^{N/2-1} \hat{W}_k e^{ikx_j}, \quad (2.34)
\]

where

\[
    \hat{W}_k = \frac{1}{N} \sum_{j=0}^{N-1} u_j v_j e^{-ikx_j} = \sum_{m=-N/2}^{N/2-1} \hat{u}_m \hat{v}_{k-m} + \sum_{m=-N/2}^{N/2-1} \hat{u}_m \hat{v}_{k-m+N}. \quad (2.35)
\]

The first term in Equation (2.35) is just \( \hat{w}_k \) (when appropriately truncated), which is in the set of represented modes, while the second term is the aliasing error, which will add spurious contributions to any modes \( k = m + n \) that satisfy \(-N/2 \leq m + n \pm N \leq \).
$N/2 - 1$.

Finally, errors due to finite grid resolution are also introduced at scales near the grid spacing, where triadic interactions that occur between scales (because of nonlinearities in the governing equations) are not represented properly. In principle these errors will diminish as the grid resolution is increased and should be negligible in a fully resolved DNS. As stated previously in Section 2.2.1, a suitable numerical method for DNS should minimise the effects of all of these various errors for a given amount of computational effort. This aim guides much of the choice of numerical algorithm in DNS studies.

The smallest scale that needs to be resolved for a simulation to be defined as DNS is typically regarded to be the Kolmogorov scale, given by $\eta = (\nu^3/\epsilon)^{1/4}$ where $\epsilon$ is the rate of dissipation of turbulent kinetic energy. There are a few problems with this definition however. Firstly, the assumption that the Kolmogorov scale is representative of the smallest eddies in the flow is predicated upon the assumption that the dissipation rate $\epsilon$ is equal to the rate at which kinetic energy is transferred down the energy cascade to the smallest scales. For sufficiently low Reynolds numbers, or in a temporally developing flow such as a mixing layer, this is not necessarily true. Another issue pertinent to mixing layers is that of anisotropy, which makes the definition of a single Kolmogorov scale problematic. Typically in planar mixing layer configurations, the definition of length scales such as the Kolmogorov scale is restricted to the homogeneous directions in which isotropy is expected [43]. A Kolmogorov scale can also be defined in the inhomogeneous direction [3], however for highly anisotropic flows (e.g. an early time RMI mixing layer) this will not necessarily equal the value of $\eta$ defined in the homogeneous directions. It is also difficult to estimate a priori what the value of $\eta$ will be for the duration of the simulation, as well as the importance of motions smaller than $\eta$.

Given these issues, it is often sufficient to define a simulation as being DNS if the grid resolution is fine enough to accurately resolve most of the dissipation in the flow, as this will result in reliable first and second order statistics [64]. A good method for ensuring that this is the case is to check that higher-order statistics such
as the dissipation rate $\epsilon$ are sufficiently grid converged in the temporal, spatial and spectral domains. This requirement also translates to the smallest resolved length scale being of $O(\eta)$, not necessarily equal to $\eta$. Furthermore, this is still consistent with the Kolmogorov hypotheses, which imply that the characteristic size of the dissipative motions scales with $\eta$ but is not necessarily equal to $\eta$ [29]. For Schmidt numbers greater than one, it is also necessary to ensure that scalar dissipation is accurately resolved, as this will involve motions of $O(\lambda_B)$ where $\lambda_B = \eta Sc^{-1/2}$ is the Batchelor scale. In addition to requiring sufficient grid resolution at the small scales, the domain size needs to be such that the largest scales in the flow are also accurately represented. In inhomogeneous directions this will be dictated by physical constraints (e.g. mixing layer width), while in the homogeneous directions two-point correlations of the solution should decay to zero within half the domain length in order to obtain a proper statistical representation. If this is not the case then the solution is said to be ‘box-constrained’ and multiple independent realisations need to be performed, as is commonly done in experiments [121].

Flows with shock waves present an additional complication, since the thickness of the shock is typically much smaller than $\eta$, hence resolving the shock to the point where its thickness is determined by physical viscosity is usually prohibitively expensive. The conventional form of the governing equations is also likely not valid inside the shock wave, particularly for strong shocks, due to non-equilibrium effects [122]. Some calculations have been performed with fully resolved shock waves, for example the simulations of early-time RMI by Margolin and Reisner [123] or shock-turbulence interaction by Ryu and Livescu [124]. However, the typical approach when simulating such flows is to use a shock-capturing approach, where the internal structure of the shock is neglected but the jump conditions across the shock are still satisfied. With this approach, it is important to minimise the impacts of the extra numerical dissipation that is introduced in order to stably capture the shock, as discussed in Section 2.2.2.

Finally, in addition to spatial resolution requirements, sufficient temporal resolution of the smallest structures in the flow is also required. For explicit timestepping
schemes this is usually ensured by stability requirements, provided the grid resolution is sufficient. The use of implicit time-stepping or integrating factors (in periodic domains) is also common in incompressible formulations, typically for the viscous terms [64]. As with finite grid size the impact of finite time-step sizes on the solution, particularly at the smallest scales being resolved, must be negligible. In certain situations this may result in implicit time-stepping schemes no longer being cost-effective compared to explicit ones.

2.3.2 Large eddy simulation

As previously discussed, for Reynolds numbers of practical interest DNS is not a feasible approach, simply due to the prohibitive amount of computational effort needed to simulate the full range of scales present in a highly turbulent flow for any significant period of time. It is also the case that most of this effort is expended computing the evolution of scales that contain a minority of the kinetic energy in the flow; the majority is contained only in the very largest scales of motion. This is the basic motivation behind the modelling approach known as large-eddy simulation (LES), whereby the unsteady dynamics of the largest scales are explicitly computed and the influence of the smaller scales (which are presumably more universal) is modelled. Conceptually, LES consists of a low-pass filtering operation, where the flow field is decomposed into a filtered and residual component. The equations of motion for the filtered component are derived from the original governing equations and will contain contributions arising from residual motions, which are supplied by some form of closure model.

For a spatially uniform filter, the operations of filtering and differentiation commute and it is therefore straightforward to apply the filter to the governing equations. To illustrate how filtering results in additional terms requiring closure, consider the incompressible Navier–Stokes equations for a single fluid. The filtered continuity equation is

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

\[
\Rightarrow \nabla \cdot \bar{u} = 0,
\]

\[
(2.36a)
\]

\[
(2.36b)
\]
in other words the filtered velocity field $\bar{u}$ is also divergence-free. Applying the filtering operation to the momentum equation gives

$$\frac{\partial \overline{u}}{\partial t} + \nabla \cdot (\overline{uu}^t) = \nu \Delta \overline{u} - \frac{1}{\rho_0} \nabla \overline{p},$$

(2.37a)

$$\Rightarrow \frac{\partial \overline{u}}{\partial t} + \nabla \cdot (\overline{u} \overline{u}') = \nu \Delta \overline{u} - \frac{1}{\rho_0} \nabla \overline{p} - \nabla \cdot \overline{\tau^R},$$

(2.37b)

where $\overline{\tau^R} = \overline{uu'} - \overline{u} \overline{u}'$ is the residual-stress tensor that arises as a result of the quadratic nonlinearity. The filtered governing equations are closed by modelling the residual-stress tensor, for example with an eddy viscosity model.

It is important to note that the filtering operation is, in principle, independent of the grid resolution and is defined as

$$f(x,t) = \int G(r,x) f(x-r,t) \, dr$$

(2.38)

for some function $f(x,t)$. In other words, the filtering operation is a convolution of $f$ with some kernel function $G$, where $G$ depends on a characteristic filter width $\Delta$ and potentially also the grid position $x$. In practice, the ratio of the grid spacing $h$ to the filter width is fixed and a trade-off exists, for a given grid resolution, between resolving a wider range of modes versus improving the accuracy of the approximation for modes that are already resolved. If $\Delta = h$ then the residual component of the flow field may also be called the subgrid component, while the filtered component may also be called the resolved component [125]. This is the terminology used in the following sections which, although formally inappropriate when $\Delta > h$, is convenient for the purposes of the present discussion.

**Explicit subgrid modelling**

If a closure model for the residual stresses is provided, either in physical or wavenumber space, then the modelling approach is referred to as explicit subgrid modelling or explicit LES. Within explicit LES, a further distinction is made based on whether or not the error of the numerical approximation for the filtered governing equations is
negligible, similar to the requirement of negligible numerical error when conducting DNS of the full governing equations. In order to obtain grid independent solutions the filtering operation must be performed explicitly, with negligible numerical error produced when $\Delta/h \gg 1$. This approach is sometimes referred to as pure LES [125]. However, in order for the LES to generate useful results, a significant portion of the turbulent kinetic energy in the flow should be resolved. Considering homogeneous turbulence as an example, assuming a Kolmogorov $k^{-5/3}$ model spectrum and requiring that 80% of the TKE be resolved gives $k_c L_{11} = 15$ [29], where $k_c$ is the cutoff wavenumber and $L_{11}$ the integral length scale. Accurate statistics of the large scales requires that $L \approx 20 L_{11}$ [121], therefore at least 48 modes need to be resolved, requiring a minimum grid resolution of $96^3$. In addition, for negligible numerical error a filter width to grid spacing ratio of at least $\Delta/h = 4$ is required for most schemes [126], bringing the minimum required grid resolution in this example to $384^3$. If instead 90% of TKE is required to be resolved, then the grid resolution requirement now becomes at least $960^3$. Therefore, as noted by Pope [125], the optimal value of $\Delta/h$ for a given grid resolution most likely corresponds to some non-negligible amount of numerical error being retained, so as to reduce modelling error. In the limit of $\Delta = h$ the explicit filter may be dropped altogether, with the filtering instead being performed implicitly by the numerical method [127]. Despite some obvious downsides, this approach is often desirable for multicomponent flows. This is due to the fact that an explicit convolutional filter cannot satisfy positivity/boundedness of the flow variables (i.e. density, mass fractions) without also introducing aliasing errors [128].

For flow at high Reynolds number, requiring that the majority of TKE in the flow be resolved means that the filter width $\Delta$ will be located in the inertial subrange of the energy spectrum. This represents the ideal case for the application of LES, as it is in this regime that the various assumptions inherent in simple subgrid models (e.g. eddy viscosity models) are well justified and accurate estimates of the the residual quantities are available. This second point becomes increasingly valuable when estimates of the residual motions are required in models for other subgrid processes such as reactions. For cases where the filter width is not located in the inertial subrange,
such as under-resolved, transitional or laminar flow, the subgrid model can provide too much or too little dissipation, particularly if it is relatively simple in construction [29]. For laminar and transitional flow, it may be possible to obtain accurate results using DNS or more sophisticated subgrid modelling techniques. In the case of the flow being under-resolved, this is due to a lack of computing power, meaning that the Reynolds number is too high for an accurate explicit LES calculation to be performed.

In incompressible flows, as was demonstrated above, there are only a handful of terms in the filtered governing equations requiring closure; namely the residual stress tensor as well as subgrid mass/scalar fluxes in the case of multicomponent flow. A wide range of closure models exist for these terms, see the review articles of Lesieur and Métais [129] and Meneveau and Katz [130] for a summary of the most commonly used models. For a compressible flow the situation becomes more complicated, since there are additional terms produced that require closure due to there being more equations as well as variable-density effects. For example, in the energy equation there are typically three quantities requiring closure; the residual temperature flux $\tilde{T}u - \tilde{T}\tilde{u}$, the triple velocity correlation $(u \cdot u)\tilde{u} - (u \cdot \tilde{u})\tilde{u}$ and the residual viscous work $\tilde{\sigma} \cdot \tilde{u} - \tilde{\sigma} \cdot \tilde{u}$ [127]. Here $\tilde{f} = \rho\bar{f}/\bar{p}$ indicates a Favre-filtered quantity. This also does not include other terms that arise when multiple species are present.

Additional complications also occur in flows with discontinuities such as shock waves, where the combination of a subgrid model and numerical dissipation can be overly dissipative. The subgrid motion in a computational cell containing a shock is also significantly different from the case of canonical turbulence that subgrid models are typically constructed to represent, hence a common approach is to set the subgrid interaction to zero in these zones [131]. Some popular models include those of Vreman et al. [132], the stretched-vortex model [133] as well as the use of artificial fluid properties [128]. The use of DNS in deriving such models is becoming increasingly important, and is one of the main motivating factors for the present work.
Implicit subgrid modelling

The observation that, for a given grid resolution (and therefore computational effort), the optimal value of $\Delta/h$ will result in non-negligible numerical errors affecting the solution has lead to the proposal that explicit filtering and subgrid modelling be neglected altogether [41, 134]. This is particularly true of LES performed with compressible codes using some form of shock-capturing, where the dissipation provided by the numerics can be of the same order as that provided by the subgrid model [135]. In addition, pure LES computations of very high Reynolds number flows will inevitably be under-resolved, in which case the subgrid model likely provides too much dissipation due to the filter width not being located in the inertial subrange. However, this situation will improve as more computing power becomes available. Calculations that exclude the use of an explicit filter and subgrid model are referred to as implicit LES and can be used to overcome these two shortcomings and obtain accurate statistics for very high Reynolds number flows [136]. This approach is not without its own limitations however, which will be discussed below.

In principle, any sufficiently dissipative numerical method can be used to perform ILES, provided there is sufficient scale separation in the flow being simulated so that the largest scales of motion are insensitive to the specific mechanism by which energy is removed from the flow. This is achieved in the design of the problem, combined with the use of numerical methods and grid resolutions that isolate the effects of numerical dissipation to scales below the energy-containing scales in the flow. For the purposes of stability, as well as mimicking the effects of the subgrid scales, energy must be removed from the flow at the high wavenumber end by the numerics. In practice this is typically achieved by using a non-oscillatory numerical method, such as the flux-corrected transport, piecewise parabolic and Godunov finite-volume methods. When high-order schemes are used, the implicit subgrid model that is provided by the numerical dissipation is nonlinear and heavily weighted towards the smallest scales resolved by the grid, which improves the computational efficiency of the calculation. Use of these schemes also allows for discontinuities such as shock waves and material interfaces to be robustly handled in an ILES calculation. The
implicit filtering operation is also naturally anisotropic wherever there is anisotropy in the grid, which is also true of explicit LES schemes with implicit filtering.

A downside of allowing the dissipation from the subgrid model to be dictated entirely by the numerical methods is that any expected universality of the unresolved scales is not explicitly enforced. Another potentially more serious downside is the lack of any formal notion of grid independence, unlike in pure explicit LES, hence the modelling and the numerics are inseparably coupled. This means that for each grid a different flow is being computed. While methods exist for defining the effective Reynolds number (and hence viscosity) in an ILES calculation [137], it remains problematic to evaluate during the simulation itself, although this is also true of many explicit LES models. In a similar vein, when estimates of subgrid motions are required for models of other subgrid processes (such as reactions), it is only possible to use methods based on the resolved scales (see e.g. Thornber et al. [138]). The flows being solved in ILES also have the same rate of subgrid transfer for mass, momentum and energy (assuming the same numerical scheme is used for each equation) and therefore the Schmidt and Prandtl numbers are nominally equal to one [59]. However, flows of sufficiently high Reynolds number to have passed the mixing transition should be insensitive to specific values of viscosity and diffusivity [51], at least when the rate-controlling processes in the flow are determined by the resolved large scales. It is also important to remember that the primary aim of using ILES in the first place is to compute the highest possible Reynolds number flow for a given grid resolution.

Therefore, an appropriate application of ILES is in computing the high Reynolds number limit of statistical quantities that depend on the energy-containing scales, in flows where the rate-controlling processes are also determined by these scales. Free shear flows, such as RTI- and RMI-induced mixing layers, in the self-similar regime satisfy this requirement and hence ILES is expected to be effective at accurately computing integral quantities such as mix width for these flows in the high Reynolds number limit. Many of these simulations are performed as nominally inviscid, as the contributions from viscous terms to the resolved scales of motion will be negligible in comparison with numerical dissipation. In applications where quantities that depend
on the mechanism by which energy is removed from the flow need to be computed. ILES is likely not a suitable approach. This includes predominantly transitional flows and flows that have not passed the (unsteady) mixing transition, for example RMI and RTI mixing layers in the early stages of development. Therefore the ideal approach to accurately computing the complete evolution of these instabilities is perhaps a combination of DNS of the initial, laminar and transitional growth and then LES (implicit or explicit) of the late time self-similar growth.

2.3.3 Reynolds-averaged Navier–Stokes models

In situations where only limited computing power is available, or for very complicated flows with lots of other important physical processes involved (radiation, reactions etc.), it is often desirable to solve equations for the evolution of purely statistical quantities that describe the turbulent velocity (and scalar) field(s). The starting point is to decompose the velocity \( \mathbf{u}(\mathbf{x},t) = \langle \mathbf{u}(\mathbf{x},t) \rangle + \mathbf{u}'(\mathbf{x},t) \) into a mean and fluctuating component respectively. This is known as the Reynolds decomposition, and applying this decomposition to the Navier–Stokes equations results in the Reynolds-averaged Navier–Stokes (RANS) equations. In a similar manner to how the filtered equations of motion are derived in LES, applying the Reynolds decomposition and obtaining equations for the mean component results in additional terms involving the fluctuating component that require closure. As a demonstration, consider again the incompressible Navier–Stokes equations for a single fluid. Since the averaging and differentiation operations commute, these become

\[
\nabla \cdot \langle \mathbf{u} \rangle = 0, \\
\frac{\partial \langle \mathbf{u} \rangle}{\partial t} + \nabla \cdot \left( \langle \mathbf{u}\rangle\langle \mathbf{u}\rangle^t \right) = \nu \Delta \langle \mathbf{u} \rangle - \frac{1}{\rho_0} \nabla \langle p \rangle - \nabla \cdot \langle \mathbf{u}'(\mathbf{u}')^t \rangle, 
\]

where the velocity covariances \( \langle \mathbf{u}'(\mathbf{u}')^t \rangle \) are called the Reynolds stresses. This highlights how the closure problem arises; deriving a set of evolution equations for lower-order moments (i.e. the mean in this example) results in terms containing higher-order moments (i.e. the variance). In the absence of additional information, Equa-
tion (2.39) cannot be solved and is said to be unclosed. Closure is provided by modelling the Reynolds stresses (as well as other covariances that appear in variable-density/multispecies formulations), with two of the most common approaches being to determine them based on the mean rate-of-strain or to solve for them directly using additional transport equations. The first approach, known as a turbulent viscosity closure, typically also requires one or more additional transport equations to be solved, and both approaches introduce terms that must be modelled. Again DNS (as well as LES) is extremely useful for calibrating these models, since all of the terms requiring closure can be explicitly computed if the full flow field is known. This is demonstrated further in Chapter 4 and Chapter 5.
Chapter 3

Governing Equations & Numerical Methods

This chapter provides a detailed presentation of the systems of governing equations for mixtures of compressible fluids, along with how to obtain approximate solutions using finite-volume methods\textsuperscript{1}. The standard fully-conservative formulation of the governing equations typically used in studies of compressible turbulent mixing is presented, the multicomponent Navier–Stokes equations, as well as how to solve this set of equations with the Godunov-type finite-volume method that is implemented in the University of Sydney CFD code Flamenco. A novel quasi-conservative system of equations that is suitable for cases where the ratio of specific heats varies with mixture composition is also derived for binary mixtures. The existing finite-volume discretisation is then extended to solve this new set of equations and test cases are presented in one and two dimensions to demonstrate the considerable advantages it has over the conventional formulation.

3.1 The four-equation model for multiscpecies compressible flows

The governing equations for mixtures of compressible and miscible fluids have been given previously in Section 2.2.2, but will be shown again here in greater detail and for an arbitrary number of species (but with body forces neglected). The standard approach is to derive equations for the conservation of mass, momentum and total energy of the mixture, along with the conservation of mass for each species [139, 140]. In differential form these are

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (3.1a)
\]

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}\! \cdot \! \nabla + p \delta) = \nabla \cdot \mathbf{\sigma}, \quad (3.1b)
\]

\[
\frac{\partial \rho E}{\partial t} + \nabla \cdot ([\rho E + p] \mathbf{u}) = \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{u} - \mathbf{q}), \quad (3.1c)
\]

\[
\frac{\partial \rho Y_l}{\partial t} + \nabla \cdot (\rho Y_l \mathbf{u}) = \nabla \cdot \mathbf{J}_l \quad (l = 1, \ldots, N - 1). \quad (3.1d)
\]

As there are four distinct equations, this formulation is often referred to as the four-equation model. The system can also be written in terms of $N$ species mass conservation equations, as the sum of these will recover the total continuity equation (Equation (3.1a)). The total mass density of the mixture is $\rho = \sum_{l=1}^{N} \rho_l$ where $\rho_l$ is the partial mass density of species $l$. The velocity $\mathbf{u} = \sum_{l=1}^{N} Y_l \mathbf{u}_l$ is the mass-weighted mean velocity of the mixture and $Y_l = \rho_l/\rho$ and $\mathbf{u}_l$ are the mass fraction and velocity of species $l$. The difference between the mixture velocity and the velocity of each species is the diffusion velocity $V_l = \mathbf{u}_l - \mathbf{u}$, while the mass flux of species $l$ relative to $\mathbf{u}$ is

\[
\mathbf{J}_l = -\rho Y_l V_l. \quad (3.2)
\]

It is also useful to define the volume fraction $f_l$ of species $l$ in the mixture. For any volume $V$, the species contained within $V$ may be fictitiously partitioned into partial volumes $V_l$ such that the partial pressures $p_l$ and temperatures $T_l$ of the original mixture within $V$ remain unchanged in $V_l$. The volume fractions are then defined as
3.1 The four-equation model for multispecies compressible flows

\[ f_l = \frac{V_l}{V} \] and satisfy \( \rho = \sum_{l=1}^{N} \rho_l^* f_l \) where \( \rho_l^* = \frac{\rho_l V}{V_l} \) is the mass density of species \( l \) within \( V_l \). The volume-weighted mean velocity of the mixture may also be defined as \( u^{(v)} = \sum_{l=1}^{N} f_l u_l \) and is related to the mass-weighted mean velocity by

\[
u^{(v)} = \mathbf{u} + \sum_{l=1}^{N} \left( \frac{f_l}{\rho_l} \right) \mathbf{J}_l. \tag{3.3}\]

The incompressibility condition in a multicomponent fluid takes the form \( \nabla \cdot \mathbf{u}^{(v)} = 0 \) since this represents the local rate of expansion/contraction of the mixture. This is the source of the non-zero right hand side when considering the divergence of the mass-weighted velocity (i.e. Equation (2.17c)) in an incompressible mixture. Volume fractions may also be related to mass fractions by

\[
f_l = \frac{(\gamma_l - 1) Y_{c,v,l}}{\sum_{m=1}^{N} (\gamma_m - 1) Y_{c,v,m}} \tag{3.4}\]

where \( \gamma_l = c_{p,l}/c_{v,l} \) is the ratio of specific heats of species \( l \). Mole fractions may also be defined as \( X_l = c_l/c \), where \( c_l = \rho_l/W_l \) and \( c = \sum_{l=1}^{N} c_l \) (\( W_l \) being the molecular weight of species \( l \)). If the partial pressures and temperatures of all species in the mixture are equal then \( X_l = f_l \).

The total pressure is given by \( p = \sum_{l=1}^{N} p_l \), where the partial pressures \( p_l = f_l p \) each satisfy an equation of state, for example the ideal gas equation of state

\[
p_l = (\gamma_l - 1) \rho_l e_l, \tag{3.5}\]

where \( e_l \) is the specific internal energy of species \( l \). In an ideal gas, \( e_l = c_{v,l} T_l \) while the specific enthalpy is given by \( h_l = c_{p,l} T_l \). The internal energy of the mixture satisfies \( \rho e = \sum_{l=1}^{N} \rho_l Y_l e_l \) while the total energy is given by \( \rho E = \rho e + \frac{1}{2} \rho \mathbf{u} \cdot \mathbf{u} \). To close the system without any additional equations, it is assumed that the species are intimately mixed and are thus in pressure and temperature equilibrium. For an ideal gas this gives

\[
p = (\bar{\gamma} - 1) \rho e, \tag{3.6}\]
3.1 The four-equation model for multispecies compressible flows

where \( \bar{\gamma} = \frac{c_p}{c_v} \) and \( c = \sum_{i=1}^{N} c_{p,i} Y_i, c_v = \sum_{i=1}^{N} c_{v,i} Y_i \).

The specification of the system given in Equation (3.1) is completed by giving constitutive relations for the molecular transport terms; the viscous stress tensor \( \sigma \), the heat flux \( q \) and the diffusion velocities \( V_l \). These have been defined previously in Section 2.2.2 for binary mixtures but will be repeated here in greater detail. The molecular transport terms can be related to the primary variables by the Chapman–Enskog expansion [141]. To first order in the Knudsen number, the viscous stress tensor is given by

\[
\sigma = \bar{\mu} \left( \nabla u + (\nabla u)^t \right) - \left( \frac{2}{3} \bar{\mu} - \bar{\mu}_b \right) (\nabla \cdot u) \delta, \tag{3.7}
\]

and the heat flux by

\[
q = -\bar{\kappa} \nabla T + \sum_{l=1}^{N} h_l J_l + \bar{R} T \sum_{l=1}^{N} \sum_{m=1}^{N} \left( \frac{X_m D_{T,l}}{W_l D_{lm}} \right) (V_l - V_m). \tag{3.8}
\]

In Equation (3.7), \( \bar{\mu} \) and \( \bar{\mu}_b \) are the dynamic and bulk viscosities of the mixture that characterise the irreversible resistance to shear and compression/expansion respectively. For monatomic gases, kinetic theory predicts that \( \mu_b = 0 \), which is the value typically used in most simulations, including those presented here. In general however, \( \mu_b \) can often be of the same order of magnitude as \( \mu \) and including/excluding its effects can alter the local and instantaneous structure of the flow [142]. A mixture rule is needed to determine the dynamic viscosity of the flow based on its composition, with the simulations presented here using Wilke’s rule

\[
\bar{\mu} = \sum_{l=1}^{N} X_l \mu_l \left/ \sum_{m=1}^{N} X_m \phi_{nm} \right., \tag{3.9}
\]

where \( X_l \) and \( \mu_l \) are the mole fraction and viscosity of species \( l \) and \( \phi_{lm} \) is defined as

\[
\phi_{lm} = \frac{1}{\sqrt{8}} \sqrt{\frac{1}{1 + \frac{W_l}{W_m} \left( \mu_l \left/ \mu_m \right. \right)^{1/4}}} \left[ 1 + \sqrt{\frac{\mu_l}{\mu_m} \left( \frac{W_m}{W_l} \right)^{1/4}} \right]^2. \tag{3.10}
\]
In Equation (3.8), the first term represents thermal conduction with $\bar{\kappa}$ being the thermal conductivity of the mixture, calculated in an analogous manner to the mixture viscosity:

$$\bar{\kappa} = \sum_{l=1}^{N} \left[ \frac{X_l \kappa_l}{\sum_{m=1}^{N} X_m \phi_{nm}} \right],$$

(3.11)

where $\kappa_l$ is the thermal conductivity of species $l$, given by kinetic theory to be

$$\kappa_l = \mu_l \left( \frac{5 \mathcal{R}}{4 W_l^2} + c_{p,l} \right),$$

(3.12)

where $\mathcal{R}$ is the universal gas constant. The second term in Equation (3.8) is the enthalpy diffusion flux, which occurs due to changes in mixture composition from species diffusion, while the third term is the thermal diffusion term, known as the Dufour effect, and represents the energy flux due to concentration gradients. This term is typically small and is most often neglected in practical calculations [59]. $D_{T,l}$ is the thermal diffusion coefficient of species $l$, while $D_{lm}$ is the mass diffusion coefficient of species $l$ with respect to species $m$. The diffusion velocities $V_l$ are obtained by solving the following $N^2$ linear system

$$\nabla X_l = \sum_{m=1}^{N} \left( \frac{X_l X_m}{D_{lm}} \right) (V_m - V_l) + (Y_l - X_l) \left( \frac{\nabla p}{p} \right) + \ldots$$

$$+ \sum_{m=1}^{N} \left[ \frac{X_l X_m}{p D_{lm}} \left( \frac{D_{T,m}}{Y_m} - \frac{D_{T,l}}{Y_l} \right) \right] \nabla T.$$  

(3.13)

The three terms in Equation (3.13) represent mass diffusion due to concentration gradients, pressure gradients (known as baro-diffusion) and temperature gradients (known as the Soret effect). The inclusion of the last two terms is necessary for compatibility with the second law of thermodynamics [61], however these are typically neglected in practical calculations, even though they may be non-negligible at large molecular weight ratios. The inversion of Equation (3.13) is quite costly and is often replaced by the Hirschfelder and Curtiss approximation [91]. Assuming negligible
3.1 The four-equation model for multispecies compressible flows

Mass diffusion due to pressure and temperature gradients, this approximation gives

\[ \mathbf{V}_t X_l = -D_l \nabla X_l, \]  
\( (3.14) \)

where \( D_l \) is the equivalent diffusion coefficient of species \( l \) into the rest of the mixture, given by

\[ D_l = \frac{1 - Y_l}{\sum_{m \neq l} X_m / D_{ml}}. \]  
\( (3.15) \)

With this approximation for the diffusion velocities, the mass flux becomes

\[ J_l = \rho D_l \frac{W_l}{W} \nabla X_l, \]  
\( (3.16) \)

with the molecular weight of the mixture given by

\[ \frac{1}{W} = \sum_{l=1}^{N} \frac{Y_l}{W_l}. \]  
\( (3.17) \)

One drawback of using the Hirschfelder and Curtiss approximation is that global mass conservation is not maintained, since now \( \sum_{l=1}^{N} J_l \neq 0 \). This can be rectified by adding a correction velocity \( \mathbf{V}_c \) to the convective velocity \( \mathbf{u} \) in each of the species mass fraction equations. The correction velocity that ensures \( \sum_{l=1}^{N} J_l = 0 \) is

\[ \mathbf{V}_c = \sum_{l=1}^{N} D_l \frac{W_l}{W} \nabla X_l, \]  
\( (3.18) \)

so that the corrected mass flux is now

\[ J_l = \rho \left( D_l \frac{W_l}{W} \nabla X_l - Y_l \sum_{l=1}^{N} D_l \frac{W_l}{W} \nabla X_l \right). \]  
\( (3.19) \)

For binary mixtures, Equation (3.14) reduces to Fick’s law;

\[ \mathbf{V}_1 Y_1 = -D_{12} \nabla Y_1, \]  
\( (3.20) \)
3.2 Godunov-type finite-volume methods

All of the numerical methods used to solve Equation (3.1) in the Flamenco code are extensions of the Godunov finite-volume method, which itself is a conservative extension of the first-order upwind scheme for linear advection to nonlinear systems of hyperbolic conservation laws. The possibility of discontinuities such as shock waves requires the use of numerical methods that are conservative and which converge to the weak form of the governing equations. For example, the weak (or integral) form of the Euler equations is given by

\[
\frac{\partial}{\partial t} \int_V \rho \, dV + \oint_S (\rho \mathbf{u}) \cdot \mathbf{n} \, dS = 0,
\]

(3.22a)

\[
\frac{\partial}{\partial t} \int_V \rho \mathbf{u} \, dV + \oint_S (\rho \mathbf{u} \mathbf{u}^T + p \delta) \cdot \mathbf{n} \, dS = 0,
\]

(3.22b)

\[
\frac{\partial}{\partial t} \int_V \rho E \, dV + \oint_S ([\rho E + p] \mathbf{u}) \cdot \mathbf{n} \, dS = 0,
\]

(3.22c)

which leads very naturally to discretisation by a finite set of control volumes since Equation (3.22) expresses the evolution of volume-averaged quantities in terms of the fluxes through the boundary of the control volume. In one dimension with explicit timestepping, this discretisation may be expressed as

\[
U_i^{n+1} = U_i^n + \frac{\Delta t}{\Delta x} \left[ F_{i-1/2} - F_{i+1/2} \right],
\]

(3.23)

which gives the update to the discrete quantities \( U \) in cell \( i \) at time \( n \). The formulation in terms of the conserved variables \( \mathbf{U} = [\rho, \rho u, \rho E]^T \) leads to the correct jump
conditions being applied across a shock wave and hence the speed and position of the shock wave is correctly calculated. The numerical method is completed by providing an approximation for the intercell fluxes $F_{i+1/2}$ and $F_{i-1/2}$ at the boundaries between cells $i+1$ and $i$ and $i-1$ and $i$ respectively.

### 3.2.1 The first-order Godunov method

In the Godunov finite-volume method, the solution $U^n$ at time $t = t^n$ is assumed to be a piecewise-constant distribution of cell averages, given by

$$U^n_i = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} U(x, t^n) \, dx.$$  \hspace{1cm} (3.24)

The flux $F_{i+1/2}$ is calculated by solving the local Riemann problem $RP(U^n_i, U^n_{i+1})$ at the cell interface $i + 1/2$ to determine the upwind direction. For the Euler equations (and multicomponent extensions) the Riemann problem may be solved exactly, with the self-similar solution denoted by $U_{i+1/2}(\bar{x}/\bar{t})$ in terms of the local coordinates $\bar{x} = x - x_{i+1/2}$ and $\bar{t} = t - t^n$. The intercell flux is then given by

$$F_{i+1/2} = F\left(U_{i+1/2}(0)\right), \hspace{1cm} (3.25)$$

with $F = [\rho u, \rho u^2 + p, (\rho E + p)u]^t$ for the Euler equations in one dimension. The time step size must also satisfy the condition

$$\Delta t \leq \frac{\Delta x}{S_{n}^{\text{max}}}, \hspace{1cm} (3.26)$$

which is analogous to the CFL condition for linear advection. $S_{n}^{\text{max}}$ is the maximum wave speed present in the domain at time $n$, which is only known once the solution to the Riemann problem at every interface in the domain has been obtained. As already noted in Chapter 2, a common approximation is to take $S_{n}^{\text{max}} = \max(|u^n_i| + a^n_i)$ where $u^n_i$ and $a^n_i$ are the velocity and speed of sound in cell $i$ at time $n$. This introduces an element of uncertainty into the estimation of the appropriate timestep size, which in practice means that CFL coefficients of less than 1 are used to avoid this.
Some favourable properties of the Godunov finite-volume method, when used in conjunction with the exact solution of the Riemann problem, include:

1. The method is entropy satisfying and thus converges to the correct solution of the governing equations (in weak form).

2. The method is also monotone, meaning that it does not introduce any new maxima or minima for linear advection.

3. Stationary contact waves are preserved exactly.

4. When extended to multicomponent flow, the method preserves positivity of mass fractions (i.e. they remain bounded between 0 and 1).

The exact solution of the Riemann problem for the Euler equations requires an iteration to determine the pressure, which can be quite computationally expensive. This is the motivation for developing approximate Riemann solvers, which still retain most of the accuracy of the exact Riemann solver but at a fraction of the cost. Various approaches to approximating the Riemann problem are possible, and these do not come without their own downsides. For example, two classes of Riemann solvers that are relatively cheap are linearised Riemann solvers (which treat all waves as discontinuities) and incomplete Riemann solvers (which ignore linear waves). Linearised Riemann solvers (such as the Roe solver) are in general quite accurate, but are entropy violating for sonic rarefaction waves and can often fail in low-density flows. Incomplete Riemann solvers (such as the HLL solver) are very stable, but produce excessive smearing of contact waves and fail to exactly preserve stationary contact waves. This is especially problematic when simulating multicomponent flows in multiple dimensions, as it decreases the ability of the numerical method to resolve shear layers and material interfaces.

An increasingly popular approximate Riemann solver is the HLLC solver [143], which is both nonlinear and complete, as well as being robust, accurate and relatively inex-
In this method, the intercell flux $F_{i+1/2}$ is approximated by

$$
F_{i+1/2}^{HLLC} = \begin{cases} 
F_L & \text{if } 0 \leq S_L, \\
F_L^* & \text{if } S_L \leq 0 \leq S^*, \\
F_R^* & \text{if } S^* \leq 0 \leq S_R, \\
F_R & \text{if } 0 \geq S_R,
\end{cases}
$$

(3.27)

where $L, R$ refer to the left and right values in the Riemann problem and $S_L, S_R$ are the wave speeds of the left and right acoustic waves while $S^*$ is the wave speed of the intermediate contact wave. These are estimated using the pressure-based wave speed estimates of Toro [144]. Given these wave speeds, the quantities in the intermediate part of the Riemann solution, referred to as the star region, may be estimated from the left- and right-side data. The numerical flux in this region is then

$$
F_{K}^* = \begin{bmatrix} 
\rho_K^* S^* \\
\rho_K^* S^* S^* + p^* \\
S^*(\rho_K^* e_K^* + p^*)
\end{bmatrix},
$$

(3.28)

where $K=L, R$ denotes the left and right sides of the contact surface. The HLLC Riemann solver is used in all computations presented in the present work.

Easily the biggest limitation of the Godunov finite-volume method however is that it is only first-order accurate in both time and space. Indeed, any scheme that is monotone and linear (in the sense that the same differencing procedure is applied everywhere in the domain) can be at most first-order accurate [145]. Thus in order to achieve high-order accuracy, and greatly improved computational efficiency, it is necessary to remove one of these two constraints. It is highly desirable that a numerical method remain monotone, as this implies numerical stability for problems with discontinuities, therefore extension to higher order accuracy must be performed by locally modifying the scheme according to the nature of the solution.
3.2.2 Extension to higher order accuracy and multiple dimensions

Whilst there are multiple approaches to extending the first-order Godunov method, the most common method (and the one employed here) is the Monotone Upstream centred Scheme for Conservation Laws (MUSCL) approach, which is part of a more general class of variable extrapolation methods. The MUSCL approach by itself is purely an extension of the spatial order of accuracy of the Godunov method, and can be used in conjunction with fully discrete, semi-discrete and implicit timestepping methods. A semi-discrete or method of lines approach is used here, which separates the spatial and temporal discretisation and allows for a wide range of schemes to be used.

Method of lines

In the method of lines, a spatial discretisation is first assumed, such as the MUSCL approach. In this approach, high-order spatial accuracy is achieved by reconstructing a polynomial of degree $N$ from the piecewise-constant data $U^n_i$ in each cell. Roughly speaking, an $N$-th degree polynomial reconstruction leads to $(N+1)$-th order spatial accuracy. The method remains conservative by enforcing that the cell-average of this reconstructed polynomial $U(x)$ remains identical to $U^n_i$. Next, the values of $U(x)$ at the boundaries of the cell are calculated and it is these values that are used as the left and right states for the Riemann solver. For example, the boundary extrapolated values at second-order accuracy are

$$U^L_{i+1/2} = U_i + \frac{1}{2}(U_{i+1} - U_i),$$
$$U^R_{i+1/2} = U_{i+1} - \frac{1}{2}(U_{i+1} - U_i).$$

(3.29)

This process is repeated for each variable in $U^n_i$. Note that in multicomponent flows it is preferable to reconstruct the primitive variables $W = [u, p, \rho Y_1, \ldots, \rho Y_N]^T$ instead as this helps maintain uniform pressure and velocity across a material interface [146].
Monotonicity is retained by limiting the extrapolated variables such that the total variation of each solution variable, defined as

\[ TV(U^n) = \sum_{i=1}^{N_x} \left| U^n_{i+1} - U^n_i \right|, \] (3.30)

does not increase in time i.e. \( TV(U^{n+1}) \leq TV(U^n) \). The resulting scheme is referred to as being total variation diminishing (TVD). While it can only be guaranteed for the linear advection equation that a TVD scheme is monontone, it is still a very useful property to enforce when designing high-order schemes for nonlinear systems.

With the inclusion of a TVD limiter, the boundary extrapolated values from Equation (3.29) are now written as

\[
U^{L}_{i+1/2} = U_i + \frac{1}{2} \phi(r^L_i)(U_i - U_{i-1}), \\
U^{R}_{i+1/2} = U_i + \frac{1}{2} \phi(r^R_{i+1})(U_{i+2} - U_{i+1}),
\] (3.31)

where \( \phi \) is the limiter function and

\[
r^L_i = \frac{U_{i+1} - U_i}{U_i - U_{i-1}}, \quad r^R_{i+1} = \frac{U_{i+1} - U_i}{U_{i+2} - U_{i+1}}.
\] (3.32)

Many different limiters are possible; the computations in this work use the limiter of Kim and Kim [147] unless otherwise stated, defined as

\[
\phi(r^L_i) = \max(0, \min(2, 2r^L_i, \beta^L)), \\
\phi(r^R_{i+1}) = \max(0, \min(2, 2r^R_{i+1}, \beta^R)),
\] (3.33)

where

\[
\beta^L = \frac{-2/r^L_{i-1} + 11 + 24r^L_i - 3r^L_i r^L_{i+1}}{30}, \\
\beta^R = \frac{-2/r^R_{i+2} + 11 + 24r^R_{i+1} - 3r^R_{i+1} r^R_i}{30}.
\] (3.34)

The limiter and resulting reconstruction is fifth-order accurate in smooth regions of flow, while at discontinuities the spatial accuracy is reduced to first-order, which is a property shared by all TVD schemes.
Once a spatial discretisation is assumed, the governing equations are reduced to a system of ODEs

$$\frac{\partial U}{\partial t} = L(U), \quad (3.35)$$

where $$L = \left( F_{i-1/2} - F_{i+1/2} \right) / \Delta x$$ is the spatial differencing operator. This system may be approximated using conventional ODE solvers such as Runge-Kutta methods. To ensure stability, the time-stepping method used should also be TVD (since methods with backward subiterations will have the wrong upwinding). All cases here use the second-order TVD Runge-Kutta method of Gottlieb and Shu [148]:

$$U^{(1)}_i = U^n_i + \Delta t L(U^n_i),$$

$$U^{n+1}_i = \frac{1}{2} U^n_i + \frac{1}{2} U^{(1)}_i + \frac{1}{2} \Delta t L\left(U^{(1)}_i\right), \quad (3.36)$$

which satisfies the same time step size restriction as in Equation (3.26).

The extension to multiple dimensions is straightforward, at least to second-order accuracy, as the same one-dimensional algorithm may be applied in each direction. For example, in two dimensions the spatial differencing operator becomes $$L = \left( F_{i-1/2,j} - F_{i+1/2,j} \right) / \Delta x + \left( G_{i,j-1/2} - G_{i,j+1/2} \right) / \Delta y$$. Considering the $$x$$-direction, the numerical flux $$F_{i+1/2,j}$$ is now a spatial average of the physical flux $$F$$ over the $$i + 1/2$$ face of cell $$(i,j)$$ at time $$t$$ and is given by

$$F_{i+1/2,j} = \frac{1}{\Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} F\left(U_{i+1/2,j}(0, y)\right) \, dy, \quad (3.37)$$

with an analogous expression obtained for $$G_{i,j+1/2}$$. Here $$U_{i+1/2,j}(\bar{x}/\bar{t}, y)$$ refers to the solution of the one-dimensional Riemann problem in the $$x$$-direction at a point $$y$$. A second-order accurate approximation to the integral in Equation (3.37) is given by the midpoint rule, meaning that only a single Riemann problem is required to be solved at the midpoint of each cell face. Furthermore, point values $$Q_i$$ and cell averages $$\overline{Q}_i$$ of a quantity $$Q$$ are related (in 1D) by

$$Q_i = \overline{Q}_i - \frac{(\Delta x)^2}{24} Q''(x_i) - \frac{(\Delta x)^4}{1920} Q^{(4)}(x_i) + \ldots, \quad (3.38)$$
which means that values at the midpoint of each cell face may be approximated by the
average value over the face to second-order accuracy. This is relevant since the same
reconstruction method as used in one dimension but performed on multidimensional
cell-averaged data will yield the average value in the transverse direction(s) when the
variables are extrapolated to a particular interface. Thus the algorithm described so
far has fifth-order spatial accuracy in 1D (and in smooth regions of the flow) but is
formally second-order accurate in multiple dimensions and is second-order accurate
in time.

Inclusion of viscous fluxes

One big advantage of the method of lines approach is that the inclusion of viscous
terms is also relatively straightforward. By interpolating the relevant variables and
derivatives to each cell interface, a conservative finite-difference scheme may be used
to give the numerical flux due to viscous terms in each cell. For example, in one
dimension the Navier–Stokes equations may be written in vector form as

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x} [\mathbf{F}(\mathbf{U})] = \frac{\partial}{\partial x} \left[ \mathbf{F}^{(v)}(\mathbf{U}, \mathbf{U}') \right],
\]

and may be discretised according to Equation (3.23), where the numerical flux is now

\[
\mathbf{F}_{i+1/2} = \mathbf{F} \left( \mathbf{U}_{i+1/2}(0) \right) - \mathbf{F}^{(v)} \left( \mathbf{U}_{i+1/2}, \mathbf{U}'_{i+1/2} \right)
\]

In evaluating the viscous flux \( \mathbf{F}^{(v)} \), the solution variables \( \mathbf{U} \) and their derivatives \( \mathbf{U}' \)
are interpolated at the interface but no upwinding is required. This is due to the
underlying physics being approximated; the viscous terms are all diffusive in nature
and can thus be stably computed using central differencing. At second-order accuracy:

\[
\begin{align*}
U_{i+1/2} &= \frac{1}{2} (U_i + U_{i+1}), \\
U'_{i+1/2} &= U_{i+1} - U_i.
\end{align*}
\]

The inviscid flux component is computed as before, with the viscous terms neglected.
3.2.3 Low Mach correction

When simulating turbulent flow fields with significant fine-scale structure, the Mach number $M$ of these fine-scale turbulent features may be quite low. Godunov-type methods are very accurate and robust at high Mach numbers, however at low Mach numbers they add an excessive amount of numerical dissipation, which leads pressure and density fluctuations to scale as $\mathcal{O}(M)$ as $M \to 0$, rather than the theoretical scaling of $\mathcal{O}(M^2)$ [149]. Thornber et al. [150] showed that, to leading order, the irreversible rate of dissipation of kinetic energy in a Godunov scheme at low Mach number is given by

$$\epsilon = \frac{(\Delta u)^2 a}{4\Delta x} \left(1 - \frac{a\Delta t}{\Delta x}\right) + \mathcal{O}\left((\Delta u)^3\right),$$

(3.42)

which is responsible for the incorrect scaling of $p$ and $\rho$. Thornber et al. [9] proposed a simple correction to the reconstruction procedure, whereby the extrapolated velocities left and right of a cell interface are modified according to

$$u_L^* = u_L + u_R \frac{\max(M_L, M_R)}{2} \left(1 - \frac{u_R}{u_L}\right),$$

$$u_R^* = u_L + u_R \frac{\max(M_L, M_R)}{2} \left(1 - \frac{u_L}{u_R}\right).$$

(3.43)

This modification recovers the correct scaling of pressure and density fluctuations as $M \to 0$ and reverts to the standard upwind form in supersonic flows. It has been shown to significantly reduce the irreversible dissipation of kinetic energy at low Mach numbers in Godunov-type schemes, which is particularly important in compressible turbulent mixing problems. When used in conjunction with the numerical algorithm outlined above, it represents a state-of-the-art approach to simulating these types of problems [31, 138, 83, 151, 104, 152, 38].

This concludes the description of the baseline numerical method in Flamenco used to perform DNS calculations. In the next section, a novel set of governing equations for binary gas mixtures is considered. Further extensions to the numerical method within the method of lines framework are considered in Appendix C.
3.3 A five-equation model for miscible and viscous compressible mixtures

3.3.1 Introduction

It has been well documented that when using the standard four-equation model in the inviscid limit to simulate flows where the ratio of specific heats $\gamma$ varies with mixture composition, spurious pressure oscillations are generated when material interfaces are advected through the computational mesh [84]. Other types of conservative discretisations, such as the level-set method, also suffer from this error under the same conditions [153]. The primary motivation of the work presented in this section is to enable accurate, high-resolution viscous computations of compressible turbulent mixing problems where $\gamma$ varies with mixture composition; both fully resolved DNS and explicitly modelled LES. An example application is in the computation of the implosion of inertial confinement fusion capsules [154, 21]. Initially there are sharp interfaces at solid/solid or solid/gas interfaces. The very high temperatures and pressures generated by the implosion process convert all the materials to dense gaseous plasmas and at various stages of the implosion there may be both sharp and diffuse gas/gas interfaces. The need to model both sharp contact surfaces and diffuse boundaries is also a requirement in shock tube turbulent mixing experiments (e.g. [155]).

For these applications the numerical technique must be able to compute flows involving multiple gaseous species which are initially separate but become mixed as time proceeds due to various hydrodynamic instabilities. The diffuse boundary layer between components may initially be small compared to the mesh size, i.e. there is a well-defined contact surface. As the flow evolves, near-homogeneous mixing due to species diffusion may occur at a scale which is at sub-cell level at early times, then growing to the order of the mesh size at later times. When simulating these transitional, non-equilibrium flows numerically, stability and a high order of accuracy are required in order to properly capture all of the necessary physics. The purpose of this
section is to derive an advection equation which may be added to the standard four-equation model to accurately model both of these limits, including species diffusion, without spurious numerically-generated pressure oscillations.

For multiphase systems, this problem has been thoroughly studied and has prompted a number of non-conservative or quasi-conservative approaches to be proposed. Karni showed that the pressure oscillations could be eliminated, either by using a primitive variable formulation (with corrections for leading order conservation errors) [156], or a conservative formulation augmented with a non-conservative pressure evolution equation [157]. Jenny et al. [158] proposed a correction for the energy equation, rendering the computation of the conserved variables a single-fluid computation and hence reducing (but not eliminating) pressure oscillations. The same paper also gave an expression for the relative error in pressure $\epsilon_p$ generated across a contact discontinuity, propagating with constant velocity $u$, that is initially aligned with the cell interface $x_{i-\frac{1}{2}}$ and has the CFL criterion $0 < \sigma = u\Delta t/\Delta x < 1$,

$$\epsilon_p = \sigma(1 - \sigma)\frac{(T_2 - T_1)(\gamma_1 - \gamma_2)}{\sigma(\gamma_2 - 1)T_2 + (1 - \sigma)(\gamma_1 - 1)T_1},$$

where $T_l$ are the temperatures for species $l$ on either side of the contact surface, and $\gamma_l$ is the ratio of specific heats for each species.

This applies to a conservative scheme that is first-order accurate in space and time, includes a complete Riemann solver and uses the ideal gas equation of state. Hence differences in temperature and specific heat ratio across the interface, as well as the convective velocity, all contribute to the size of the pressure error. Abgrall [85] showed that such pressure errors could be eliminated by using an additional transport equation (in advection form) for a given function of the ratio of specific heats. This approach was dubbed quasi-conservative as it produces results with extremely small conservation errors. This class of algorithm was extended to a wider range of equations of state and multiple dimensions by Shyue [159] and Saurel and Abgrall [160]. A key idea behind these extensions was to have as many additional transport equations as there are parameters in the equation of state (e.g. $\gamma$ for an ideal gas), while
not requiring any additional transport equations to simulate mixtures of more than two fluids. However this results in increasing complexity of the algorithm with an increasingly complex equation of state. Other approaches for eliminating pressure oscillations have also been proposed that involve non-conservative modifications to the solution procedure rather than the addition of transport equations [153, 86, 161], however they will not be discussed in further detail here.

Shyue [159] also gave a reformulation of the $\gamma$-based model of Abgrall in terms of the four-equation volume fraction model, which consists of (in 1D) the three conservative equations for density, momentum and energy plus a non-conservative advection equation for the volume fraction of one of the species. Allaire et al. [88] and Massoni et al. [87] showed that by extending this to a five-equation model (by including the mass fraction transport equation) and providing suitable thermodynamic closure, any equation of state could be simulated whilst also maintaining pressure equilibrium across material interfaces. Massoni et al. [87] included heat conduction, and applied it to a range of multiphase problems with varying equations of state, maintaining pressure equilibrium. Murrone and Guillard presented a detailed study of the five-equation model with excellent results at low and high Mach number [162]. Their diffuse interface model, in which contacts can become smeared, is presented for inviscid, immiscible flows only.

More recent research on quasi-conservative formulations for compressible multicomponent flows has focused on extensions to high-order accuracy as well as the inclusion of viscous effects. By performing an asymptotic analysis on the equations governing multiphase flow, Perigaud and Saurel [163] derived the same five-equation model as Allaire et al. [88] and Massoni et al. [87] but including the effects of viscosity. This model neglects the effects of species diffusion however. Johnsen and Colonius [146] extended the models of Abgrall [85], Shyue [159] to high-order WENO finite-volume methods with the HLLC Riemann solver. An important result in this study was that in order to preserve pressure equilibrium across contact discontinuities, the reconstruction at cell interfaces must be performed using the primitive variables.

It was shown by Johnsen and Ham [164] that although the models of Abgrall [85],
Shyue [159] conserve total mass, momentum and energy, they do not discretely conserve the mass of each species and also generate temperature errors at material interfaces. These temperature errors are irrelevant in inviscid flows, however they become important once physical diffusion effects are added. The authors proposed adding a transport equation for species mass fraction to the model of Abgrall [85] (in conservative form, thus enforcing species mass conservation) and showed that temperature errors were prevented if the reconstruction and upwinding for both the continuity and mass fraction equations is consistent. A potential downside of this approach is that the location of the interface is not uniquely defined, although this difference is very small. Finally, Coralic and Colonius [165] applied the numerical framework of Johnsen and Colonius [146] to the five-equation model of Allaire et al. [88], with the inclusion of the effects of viscosity as in Perigaud and Saurel [163]. Species diffusion was not included however.

At very large scales of a given compressible turbulent mixing problem it may be sufficient to assume that the dissipative effects of physical mechanisms are approximated by those of the numerics (i.e. the ILES approach), however at smaller scales the effects of viscosity, thermal conduction and species diffusion become important and require explicit modelling so as to gain confidence in the results. Previously, any computation of miscible compressible turbulent mixing with species diffusion has had to use the fully conservative mass fraction model, even when the ratio of specific heats is not constant [166, 167, 138, 168]. As outlined above, this approach is likely to suffer from errors in pressure and/or temperature generated at material interfaces. These errors are important even in relatively well mixed flows as species gradients are always present in the flow and thus spurious numerically generated pressure fluctuations may be large compared to physically generated pressure fluctuations. Therefore the aim here is to derive a five-equation model incorporating both viscosity and mass diffusion, where the additional equation is employed solely to ensure that spurious pressure oscillations are not generated within a mixed cell.
3.3 A five-equation model for miscible and viscous compressible mixtures

3.3.2 Derivation of the new five-equation model

In order to model species diffusion in the presence of steep gradients in mixture composition, an additional equation is now derived which enables the preservation of pressure-constancy at contact surfaces in the sharp interface limit, and is valid for problems with viscous, thermal and species diffusion. It should be emphasised that the basic physics is the same as for the standard four-equation model. However, the integral form of the equations used for numerical integration is different, and it is this which eliminates spurious numerical pressure oscillations.

During diffusion, as mixing occurs at a molecular level, both pressure and temperature equilibrium is expected during the mixing process. Avogadro’s hypothesis is assumed to hold: gases at the same pressure and temperature have the same molecular number density [169]. As each molecule for a given species has the same mass, the number-weighted mean velocity, the volume-weighted mean velocity and the mass-weighted mean velocity for species \( l \) are all the same and denoted by \( u_l \). The evolution equation for the number density \( n_l \) is

\[
\frac{\partial n_l}{\partial t} + \nabla \cdot (n_l u_l) = 0, \tag{3.45}
\]

where \( u_l \) is now the mean velocity of each component. By summation, the equation for the evolution of total number density \( n \) is

\[
\frac{\partial n}{\partial t} + \nabla \cdot (n u^{(n)}) = 0, \tag{3.46}
\]

where \( u^{(n)} = \sum_{l=1}^{N} \frac{n_l u_l}{n} \) is the number-weighted mean velocity of the mixture. Next, the individual number density equations (3.45) are rewritten using the number fraction \( X_l = \frac{n_l}{n} \). Employing the vector identity \( \nabla \cdot (\phi F) = (\nabla \phi) \cdot F + \phi (\nabla \cdot F) \) leads to

\[
\frac{\partial n_l}{\partial t} + \nabla \cdot (n_l X_l u_l) = 0,
\]

\[
\implies n \frac{\partial X_l}{\partial t} - X_l \nabla \cdot (n_l u^{(n)}) + \nabla \cdot (n_l u_l) = 0,
\]

\[
\implies n \frac{\partial X_l}{\partial t} + (n u^{(n)}) \cdot (\nabla X_l) - \nabla \cdot (X_l n u^{(n)}) + X_l u_l \nabla n + n \nabla \cdot (X_l u_l) = 0,
\]
3.3 A five-equation model for miscible and viscous compressible mixtures

\[ \partial X_l \partial t + \mathbf{u} \cdot \nabla X_l - \nabla \cdot (X_l \mathbf{u}^{(n)}) - X_l \mathbf{u}^{(n)} \frac{\nabla n}{n} + \nabla \cdot (X_l \mathbf{u}_l) + X_l \mathbf{u}_l \frac{\nabla n}{n} = 0, \]

and therefore

\[ \frac{\partial X_l}{\partial t} + \mathbf{u}^{(n)} \cdot \nabla X_l + \nabla \cdot [X_l(\mathbf{u}_l - \mathbf{u}^{(n)})] + X_l(\mathbf{u}_l - \mathbf{u}^{(n)}) \cdot \frac{\nabla n}{n} = 0. \] (3.47)

Thus there are three terms which modify \( X_l \): advection with the number-weighted mean velocity, diffusive mixing, and pressure-temperature equilibration. According to the last term, if a parcel of fluid \( l \) moves into a region with different pressure and temperature the number fraction adjusts to the local value.

**Binary Mixtures**

For a binary mixture the terms in the number fraction equation can be specified in a simple form. If the diffusion is assumed to be Fickian then

\[ \mathbf{u}_1 - \mathbf{u}_2 = -\frac{D_{12}}{X_1 X_2} \nabla X_1, \] (3.48)

Substituting \( \mathbf{u}_2 = \frac{\mathbf{u}^{(n)} - X_1 \mathbf{u}_1}{X_2} \) into Equation (3.48) implies \( X_l(\mathbf{u}_l - \mathbf{u}^{(n)}) = -D_{12} \nabla X_l \), therefore Equation (3.47) becomes

\[ \frac{\partial X_l}{\partial t} + \mathbf{u}^{(n)} \cdot \nabla X_l = \nabla \cdot (D_{12} \nabla X_l) + D_{12} \nabla X_l \cdot \frac{\nabla n}{n}. \] (3.49)

The number-weighted mean velocity of the fluid is related to the mass weighted mean velocity by

\[ \mathbf{u} = \mathbf{u}^{(n)} + \frac{\sum_{i=1}^{N} W_i X_i(\mathbf{u}_i - \mathbf{u}^{(n)})}{\sum_{i=1}^{N} W_i X_i}. \] (3.50)

Thus for two species,

\[ \mathbf{u}^{(n)} = \mathbf{u} + \frac{W_1 - W_2}{W_1 X_1 + W_2 X_2} D_{12} \nabla X_1. \] (3.51)

This form is useful as the further manipulations may result in numerical difficulties associated with dividing by number fractions or mass fractions which could be zero.
3.3 A five-equation model for miscible and viscous compressible mixtures

For binary mixtures with gradient diffusion assumed to be dominant, diffusive fluxes can be related to mass fraction gradients \[139\], and Equation (3.48) can also be written as

\[
\mathbf{u}_1 - \mathbf{u}_2 = -\frac{D_{12}}{Y_1 Y_2} \nabla Y_1. \tag{3.52}
\]

This is employed as the diffusion term for the evolution of \(\rho Y_l\). The full set of equations for compressible binary mixtures is

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \quad (3.53a) \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}^t + p\delta) &= \nabla \cdot \mathbf{\sigma}, \quad (3.53b) \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot ([\rho E + p] \mathbf{u}) &= \nabla \cdot (\mathbf{\sigma} \cdot \mathbf{u} - \mathbf{q}), \quad (3.53c) \\
\frac{\partial \rho Y_1}{\partial t} + \nabla \cdot (\rho Y_1 \mathbf{u}) &= \nabla \cdot (\rho D_{12} \nabla Y_1), \quad (3.53d) \\
\frac{\partial X_1}{\partial t} + \mathbf{u} \cdot \nabla X_1 &= \nabla \cdot (D_{12} \nabla X_1) - \mathcal{M} D_{12} \nabla X_1 \cdot \nabla \frac{n}{n}, \quad (3.53e)
\end{align*}
\]

where \(\mathcal{M} = \frac{W_1 - W_2}{W_1 X_1 + W_2 X_2}\) and \(n = p/k_b T\). Note that only the number fraction equation is in non-conservative form.

3.3.3 Integral form and spatially averaged equation of state

The new set of governing equations can be written in integral form (replacing the continuity equation with the second species mass fraction equation) as

\[
\begin{align*}
\frac{\partial}{\partial t} \int_V \rho Y_l \, dV + \oint_S (\rho Y_l \mathbf{u}) \cdot \mathbf{n} \, dS &= \oint_S (\rho D_{12} \nabla Y_l) \cdot \mathbf{n} \, dS, \\
\frac{\partial}{\partial t} \int_V \rho \mathbf{u} \, dV + \oint_S (\rho \mathbf{u} \mathbf{u}^t + p\delta) \cdot \mathbf{n} \, dS &= \oint_S \mathbf{\sigma} \cdot \mathbf{n} \, dS, \\
\frac{\partial}{\partial t} \int_V \rho E \, dV + \oint_S ([\rho E + p] \mathbf{u}) \cdot \mathbf{n} \, dS &= \oint_S (\mathbf{\sigma} \cdot \mathbf{u} - \mathbf{q}) \cdot \mathbf{n} \, dS, \\
\frac{\partial}{\partial t} \int_V X_1 \, dV + \int_V (\mathbf{u} + \mathcal{M} D_{12} \nabla X_1 - D_{12} \frac{\nabla n}{n}) \cdot \nabla X_1 \, dV &= \oint_S (D_{12} \nabla X_1) \cdot \mathbf{n} \, dS. \tag{3.54}
\end{align*}
\]
Writing $\mathbf{U} = \mathbf{u} + \mathcal{M}D_{12}\mathbf{\nabla}X_1 - D_{12}\frac{\mathbf{u}}{n}$ it is possible to write the number fraction equation as a conservative equation minus a correction term:

$$\frac{\partial}{\partial t} \int_V X_1 \, dV + \int_S (\mathbf{U}X_1) \cdot \mathbf{n} \, dS - \int_V X_1(\mathbf{\nabla} \cdot \mathbf{U}) \, dV = \int_S (D_{12}\mathbf{\nabla}X_1) \cdot \mathbf{n} \, dS \quad (3.55)$$

In the intended applications of this model, interfaces may be initially sharp (i.e. sub-cell), then become diffuse as time proceeds. Thus it is important to clarify the definition of the volume-averaged number fraction. For a computational cell,

$$\overline{X}_l = \frac{\int_V X_l \, dV}{V} \quad (3.56)$$

is the volume-averaged number fraction for species $l$. This differs from the number fraction based on the number of molecules of species $l$ in the computational cell

$$\tilde{X}_l = \frac{\int_V nX_l \, dV}{\int_V n \, dV}. \quad (3.57)$$

If there is a sharp interface within a cell, $\overline{X}_l$ is equal to the cell average of the volume fraction $z_l$ commonly employed in multiphase systems \[88, 87, 162\]. If there is homogeneous mixing within a cell, $\overline{X}_l = \tilde{X}_l$. Moreover, if pressure and temperature are uniform within a cell, then so is $n$ (according to Avogadro’s hypothesis) which also gives $\overline{X}_l = \tilde{X}_l$. However, in the most general case $\overline{X}_l$ and $\tilde{X}_l$ will not be equivalent, as volume-averaged species temperatures can vary. It is reemphasised that the purpose of using the number fraction equation is to give improved numerical accuracy; the basic physics is the same as that used in the four-equation model.

**Equation of State for a Finite Volume**

The governing equations must be closed by an equation of state for the mixture within a finite-volume. Here only mixtures of ideal gases will be considered. For cases where diffusion is negligible, or the interface is sharp relative to the mesh size, then the algorithm must robustly advect this interface without spurious numerically generated pressure waves. Here it is important to consider a volume-averaged equation of state,
Figure 3.1 – Advection of an isolated contact surface separating two miscible gas mixtures at velocity $u > 0$ and constant pressure $p$. Initial condition at time $t$ (top) and final condition at time $t + \Delta t$ (bottom).

rather than a mixture equation of state, since the latter implies a mixture in the sense of Avogadro’s hypothesis, whereas the former does not require equal species pressures and temperatures since gases may occupy separate regions of space. Following Allaire et al. [88], the system is closed by assuming that each species has the same volume-averaged pressure, however volume-averaged species temperatures may vary (referred to as isobaric closure). At first glance this appears contrary to the application of Avogadro’s hypothesis during the derivation of the system of equations, but it is a consequence of solving the integral form of the governing equations in a finite-volume framework. The fact that a flow where all species are in local pressure and temperature equilibrium can exhibit different volume-averaged species temperatures is entirely physical as will now be outlined.

The classical approach is to consider the advection of an isolated contact surface at very high Reynolds number where the effects of diffusion, viscosity and conduction may be neglected. The Riemann problem is shown schematically in Figure 3.1. At time $t = 0$, the sharp interface is perfectly aligned with the boundary between two finite volumes. The exact solution of this simple advection problem is a constant
pressure contact surface moving at velocity \( u \), and represents the simplest case of inviscid advection. The contact surface separates a left gas mixture \( L \) and right gas mixture \( R \) with properties

\[
(\rho, u, p, Y_l, X_l, T) = \begin{cases} 
(\rho_L, u, p, Y_{l,L}, X_{l,L}, T_L) \\
(\rho_R, u, p, Y_{l,R}, X_{l,R}, T_R)
\end{cases} \tag{3.58}
\]

where the velocity \( u > 0 \), the mixture pressures are equal but the compositions and temperatures are different. All species are in local pressure and temperature equilibrium. At time \( t + \Delta t \), the contact surface has swept out a volume \( V_L = u\Delta t \) of the downstream cell. This volume now contains mixture \( L \) at a temperature \( T_L \), and the remaining volume of the cell \( V_R = V - V_L \) contains mixture \( R \) at a temperature \( T_R \). The fraction of the cell volume which is occupied by mixture \( L \) and mixture \( R \) is defined as \( f_L = V_L/V \) and \( f_R = V_R/V \) respectively, thus \( f_L + f_R = 1 \). Volume-averaged number fractions \( \bar{X}_l \) can be defined in the downstream cell at \( t + \Delta t \) as:

\[
\bar{X}_l = f_L X_{l,L} + f_R X_{l,R}, \tag{3.59}
\]

with the volume-averaged internal energy given by

\[
\bar{\rho}e = f_L \sum_{l=1}^{2} \rho_L Y_{l,L} e_{l,L} + f_R \sum_{l=1}^{2} \rho_R Y_{l,R} e_{l,R}. \tag{3.60}
\]

Defining a species partial density

\[
\rho_{l,(L,R)} = \frac{p}{T_{(L,R)} \mathcal{R}_l}, \tag{3.61}
\]

and noting that each individual mixture is in local pressure and temperature equilibrium gives

\[
\rho_{l,(L,R)} = \frac{\rho_{(L,R)} Y_{l,(L,R)}}{X_{l,(L,R)}}. \tag{3.62}
\]

Given \( e_{l,(L,R)} = c_v i T_{(L,R)} \) then the volume-averaged internal energy may be written
as
\[
\bar{\rho}e = p \sum_{l=1}^{2} \frac{f_l X_{l,L} + f_R X_{l,R}}{\gamma_l - 1} = p \sum_{l=1}^{2} \frac{\bar{X}_l}{\gamma_l - 1}. \tag{3.63}
\]

The analytical solution to this problem is a constant pressure contact surface. To satisfy this condition, it is clear that the appropriate volume-averaged ratio of specific heats is given by
\[
\frac{1}{\bar{\gamma} - 1} = \sum_{l=1}^{2} \frac{\bar{X}_l}{\gamma_l - 1}. \tag{3.64}
\]

With this condition, the downstream internal energy \(\bar{\rho}e = p/(\bar{\gamma} - 1)\) and pressure in the mixed cell is maintained at the original pressure \(p\) following the advection step as required by the analytical solution. This simple analysis can be extended to more complex equations of state following analogous derivations for immiscible fluids [88, 162, 87], and illustrates the key useful property of the governing model which will hold when the equations are discretised with a complete Riemann solver. Subsequent time steps may be treated in a similar fashion by considering the advection of sub-components of mixtures each at their respective pressure and temperature equilibria.

Note that the derivation above is equivalent to specifying that the appropriate volume-averaged temperature for each species is \(T_l = p\bar{X}_l/R_l\bar{\rho}Y_l\). In the limit of an infinitely small cell then \(T_l = T\) as expected from the assumptions underlying the governing equations. Assuming constant specific heats for each species such that \(T_l = c_l/c_v_l\), the volume-averaged species temperatures \(\bar{T}_l\) are mass-weighted averages of the initial temperatures \(T_{l,R}\). Enforcing temperature equilibrium (as is done in the four-equation model) would change the volume-averaged number fractions \(\bar{X}_l\), which would give a different \(\bar{\gamma}\) for the cell and give rise to a change in pressure if \(\gamma_1\) and \(\gamma_2\) are different. Hence homogenising a mixed cell will, in general, give a non-physical change in pressure at the contact. The isobaric closure proposed above is designed to correct this problem, where even if the species mixtures are initially in local pressure and temperature equilibrium, the analytical cell-averaged species temperatures can be expected to differ following an advection step. The above closure is only possible with the addition of the transport equation for \(X_l\).
3.3 A five-equation model for miscible and viscous compressible mixtures

3.3.4 Numerical discretisation

The following section details the implementation of the governing equations within Flamenco. The code already has an existing implementation of the inviscid volume fraction model of Allaire et al. [88], which has been well documented in previous publications [104, 38]. Given that the inviscid part of the governing model proposed here has the same mathematical form as the model of Allaire et al. [88], the discretisation is performed in an analogous fashion.

The Jacobian for the two-species system given in Equation (3.53), written in one dimension in terms of the primitive variables $W = [\rho Y_1, \rho Y_2, u, P, X_1]^T$ is

$$A(W) = \begin{bmatrix} u & 0 & \rho Y_1 & 0 & 0 \\ 0 & u & \rho Y_2 & 0 & 0 \\ 0 & 0 & u & 1/\rho & 0 \\ 0 & 0 & \rho c^2 & u & 0 \\ 0 & 0 & 0 & 0 & U \end{bmatrix}.$$  (3.65)

where for an ideal gas the speed of sound $c^2 = \sum_{l=1}^{2} Y_l h_l / \xi$ and $\xi = \sum_{l=1}^{2} X_l / (\gamma_l - 1)$.

The eigenvectors are unchanged from those in the volume fraction model of Allaire et al. [88], however the eigenvalues become

$$\lambda_1 = \lambda_2 = u, \quad \lambda_3 = u - c, \quad \lambda_4 = u + c, \quad \lambda_5 = U.$$  (3.66)

The form of the Jacobian given in Equation (3.65) is not conventional as it depends on derivatives of the solution variables. These terms are included here on the left hand side of the system of equations for numerical reasons, namely that they modify the upwind direction of $X_1$. The Jacobian may be written solely in terms of the solution variables by applying Cattaneo’s relaxation approach [170, 171], whereby a new variable $\psi$ is introduced in place of $\frac{\partial X_1}{\partial x}$ along with a transport equation that relaxes $\psi$ towards $\frac{\partial X_1}{\partial x}$ by means of a stiff source term. This highlights one possible avenue for discretisation using arbitrarily high-order methods for hyperbolic systems [172–175]. This particular relaxation approach is not without its downsides also,
which are discussed in Appendix B.

For the present work, the number fraction equation is discretised following Abgrall [85], whereby the cell interface fluxes $F_{i+1/2}$ and $F_{i-1/2}$ for cell $i$ are computed as

\[ F_{i+1/2} = (X_i U)_{i+1/2}^{RS} - [X_1]_{i+1/2} U_{i+1/2}^{RS}, \]
\[ F_{i-1/2} = (X_i U)_{i-1/2}^{RS} - [X_1]_{i-1/2} U_{i-1/2}^{RS}, \] (3.67)

where $\ldots^{RS}$ indicates a term arising from the solution of the Riemann problem at the cell interface. The key problematic terms are the diffusion and equilibration terms, which modify the upwind direction of the advection of $X_1$ dependent on the gradients of $n$ and $X_1$ itself. These gradients are computed using second-order accurate central differences, centred on the cell interface. The required values of $M$ and $n$ are computed as the arithmetic average of the left and right reconstructed values at the interface. As an example, in one dimension with constant grid spacing $\Delta x$, $U$ is given by

\[ U_{i+1/2}^{RS} = u_{i+1/2}^{RS} + D_{12} \frac{M_L + M_R [X_1]_{i+1} - [X_1]_i}{\Delta x} - D_{12} \frac{2([n]_{i+1} - [n]_i)}{(n_L + n_R)\Delta x}, \] (3.68)

where $u_{i+1/2}^{RS}$ is gained from the solution of the classical Riemann problem. The upwind number fraction $X_1^{RS}$ required to compute the number fraction fluxes is determined by modifying the signal speed in the HLLC Riemann solver to incorporate the additional diffusion velocity, i.e. the contact surface in the Riemann problem for the number fraction is assumed to advect at a velocity $U$.

Next, the diffusion terms must be discretised in a manner which is consistent with the underlying physics. For the diffusive fluxes computed at the cell interfaces, Avogadro’s hypothesis must be enforced, i.e. the species diffusion terms were derived assuming pressure and temperature equilibrium. If pressure and temperature equilibrium is not enforced at the cell interface during the computation of the diffusive fluxes, then the resultant species densities and temperatures will be in error. Within the current algorithm, this is addressed by rewriting the mass fraction gradient in the diffusive
flux as
\[ \nabla \cdot (\rho D_{12} \nabla Y_l) = \nabla \cdot (\rho D_{12} \nabla \frac{W_l X_l}{W}). \]
\[ (3.69) \]

Finally, for explicit time integration the stable time step is chosen based on the minimum in the whole domain of the following:
\[ \Delta t = \text{CFL} \times \min \left( \frac{\Delta x}{\max_k(\lambda_k)}, \frac{\rho \Delta x}{2\mu}, \frac{\rho \Delta x^2}{2D_{12}}, \frac{\rho c_s \Delta x^2}{2\kappa} \right). \]
\[ (3.70) \]

### 3.3.5 One-dimensional test cases

Three validation cases are used, with analytical solutions available in the incompressible limit, to verify the observed order of accuracy of the key components of the algorithm. The results using the new number fraction model are compared with those of the classical four-equation model (hereon referred to as the mass fraction model) using the same reconstruction and time stepping scheme, along with results from an entirely independent Lagrange-remap algorithm which employs mass fractions to track individual species [176, 40]. This algorithm is used to provide an independent benchmark solution for non-analytical fields such as the pressure field in problems at finite Mach number.

Although the model equations and algorithm are compressible, the following test case employs incompressible analytical solutions to verify and validate each of the key terms. In many applications species diffusion occurs at a very small scale, over which the pressure is near uniform. For example, in the Richtmyer-Meshkov instability a diffuse interface between the two fluids forms after shock passage, and there is little pressure variation across this interface. Hence 1D test cases based on diffusion at a boundary between two gases at uniform pressure provide highly relevant test cases of the new model. If diffusive velocities are small compared to the sound speed, the mixing process is near incompressible and results can be checked against analytic solutions of the incompressible limit. In applications, the diffuse interface will be advected through the computational mesh and this is a more challenging situation for the numerical method. Hence, results are also given for the case where a uni-
form velocity is added to the flow. Note that the numerical results are expected to agree with the analytical results only up to the point where the difference between the numerical and analytical results is not dominated by compressibility effects. This occurs at the finest grid resolutions where the error due to the discretisation (truncation error) becomes lower than the difference due to compressibility and thus the convergence rate measured relative to the analytical solution stalls. It occurs at the same error magnitude regardless of whether the mass fraction or number fraction models are employed.

The one-dimensional problem of diffusion at a plane boundary between two gases is a useful test case for numerical implementations. For mixing between two gases at the same pressure to be an incompressible process, there should be no change in pressure when the two gases mix. This will be true for two different gases at the same temperature or for two identical gases at different temperatures. In Case 1 and Case 3 heat conduction is unimportant, while in Case 2 heat conduction is the dominant process. Case 1 and 2 are used to verify the algorithms for near-pure diffusion cases, whereas Case 3 tackles a more realistic case with both advection and diffusion. In these three one-dimensional cases viscosity is assumed to be zero, and equal diffusivities are used ($D_{kj} = D$ and $\kappa = \rho c_p D$).

**Case 1: Diffusion of an isothermal material interface between two different species**

This test case has been employed in Kokkinakis et al. [177], however here the initial conditions are described in full, along with a rigorous initialisation process which enables a formal convergence study, up to the limit of assumed incompressibility. The computation domain is $0 \leq x \leq 1$ m, and grid sizes of 32 to 4096 cells are employed. Reflective boundary conditions are used at the left and right boundaries. The two fluids have the properties $\rho_1 = 20$ kg/m$^3$, $\rho_2 = 1$ kg/m$^3$, $\gamma_1 = 2$, $\gamma_2 = 1.4$. The specific heats satisfy the requirement that $(\gamma_1 - 1)\rho_1 c_v = (\gamma_2 - 1)\rho_2 c_v$, which gives temperature equilibrium if the two fluids have the same pressure. If the initial uniform pressure is sufficiently high, the mixing process is quasi-incompressible and
the analytic solution for the number fraction distribution is given by

\[ X_1 = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{x - x_0}{\sqrt{4Dt + h_0^2}} \right) \right], \quad \mathcal{Z} = \frac{x - x_0}{\sqrt{4Dt + h_0^2}}, \tag{3.71} \]

where \( x_0 = 0.5 \text{ m}, h_0 = 0.02 \text{ m} \) and the diffusion coefficient \( D = 0.01 \text{ m}^2/\text{s} \). In the initialisation of the problem, compressibility effects are minimised by assuming that the volume weighted mean velocity is initially zero. Hence the initial mass weighted mean velocity is given by \( u = -\frac{D}{\rho} \frac{\partial \rho}{\partial x} \). Noting that a finite volume algorithm requires the cell averaged quantities,

\[ \bar{q} = \frac{1}{x_{i+1/2} - x_{i-1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x) \, dx \tag{3.72} \]

this results in the following initialisation:

\[ \rho = \frac{1}{x_{i+1/2} - x_{i-1/2}} \left[ \frac{\rho_1 + \rho_2}{2} x + \frac{\rho_1 - \rho_2}{2} \mathcal{A} \right]_{x_{i-1/2}}^{x_{i+1/2}}, \tag{3.73} \]

\[ \rho Y_1 = \frac{1}{x_{i+1/2} - x_{i-1/2}} \left[ \frac{\rho_1}{2} x - \frac{\rho_1}{2} \mathcal{A} \right]_{x_{i-1/2}}^{x_{i+1/2}}, \tag{3.74} \]

\[ \overline{X_1} = \frac{1}{x_{i+1/2} - x_{i-1/2}} \left[ \frac{1}{2} x - \frac{1}{2} \mathcal{A} \right]_{x_{i-1/2}}^{x_{i+1/2}}, \tag{3.75} \]

\[ \overline{\rho u} = \frac{1}{x_{i+1/2} - x_{i-1/2}} \left[ -D \left( \frac{\rho_2 - \rho_1}{2} \right) \text{erf} \left( \mathcal{Z} \right) \right]_{x_{i-1/2}}^{x_{i+1/2}}, \tag{3.76} \]

\[ \mathcal{A} = (x - x_0) \text{erf} \left( \mathcal{Z} \right) + \frac{\sqrt{4Dt + h_0^2}}{\sqrt{\pi}} e^{-\mathcal{Z}^2}. \tag{3.77} \]

For the standard test case, the initial uniform pressure is \( p_0 = 10000 \text{ Pa} \). The peak initial Mach number, based on the mass-weighted mean velocity is then \( M = 0.019 \). In order to show the effect of compressibility, calculations are also performed with \( p_0 = 10 \text{ Pa} \). The initial Mach number is then \( M = 0.6 \). For \( p_0 = 10000 \text{ Pa} \), the flow is near-incompressible with pressure and temperature remaining approximately constant, thus the incompressible analytical solution may be employed as a reference solution to demonstrate the scheme’s order of accuracy. Note that for this test case,
3.3 A five-equation model for miscible and viscous compressible mixtures

Table 3.1 – Case 1 convergence rates for the number fraction model.

<table>
<thead>
<tr>
<th>( N_x )</th>
<th>( L^1 )</th>
<th>( L^2 )</th>
<th>( L^\infty )</th>
<th>( O(L^1) )</th>
<th>( O(L^2) )</th>
<th>( O(L^\infty) )</th>
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<td>-</td>
<td>-</td>
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Table 3.2 – Case 1 convergence rates for the mass fraction model.

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<th>( L^2 )</th>
<th>( L^\infty )</th>
<th>( O(L^1) )</th>
<th>( O(L^2) )</th>
<th>( O(L^\infty) )</th>
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the \( u^{(n)} \cdot \nabla X_1 \) term in the number fraction equation (Equation (3.51)) is essential, but the \( \nabla n/n \) term vanishes.

Table 3.1 and 3.2 document the \( L^1 \), \( L^2 \) and \( L^\infty \) errors in the simulated volume fraction profile at \( t = 0.5 \) s for the number fraction and mass fraction formulations compared to the incompressible analytical solution, along with the observed convergence rates. Figure 3.2 plots the error norms as a function of number of cells \( N_x \) for the mass fraction and number fraction models. There are several important points to make. Firstly, the results produced here demonstrate that a formal convergence at approximately second order accuracy is achieved. Convergence to the analytical solution stalls at error norms of \( \approx 10^{-5} \rightarrow 10^{-6} \) as here the effects of compressibility are no longer negligible, thus the incompressible analytical solution is not the exact solution to this (marginally) compressible problem. Secondly, for a given grid resolution, the number fraction model has a substantially lower actual error, on the order of one third of the errors for the mass fraction formulation. Thus for a constant error, the
number fraction equations may be run on a mesh of nearly 1/2 the number of points at the coarser resolutions.

The results are plotted for grid resolutions up to \( N_x = 2048 \) for both the mass fraction and number fraction models in Figure 3.3. The non-analytical pressure and temperature fields are also shown in these figures, where it can be seen that the number fraction model has substantially lower pressure fluctuations for a given grid resolution. For example, at a grid resolution of 32 points the pressure fluctuation is less than 4 Pa in the number fraction model compared to 18 Pa in the mass fraction model. This is due to the better treatment of the equation of state in the mixed
Figure 3.3 – Comparison of variables across all grid resolutions for Case 1 with the mass fraction model results on the left and the number fraction model results on the right.
Case 1 comparison of non-analytical field variables for the mass fraction (MF) and number fraction (NF) models in Flamenco (2048 cells) as well as the results from the Lagrange-remap code (2048 cells).

Figure 3.4 – Case 1 comparison of non-analytical field variables for the mass fraction (MF) and number fraction (NF) models in Flamenco (2048 cells) as well as the results from the Lagrange-remap code (2048 cells).

cells. Figure 3.4 shows the converged solutions for the pressure and temperature fields. Both are extremely challenging to resolve since \( t = 0.5 \) s represents greater than 30 periodic reflections of extremely small acoustic waves in the domain. Here a comparison is plotted at the finest grid resolution with the results from the Lagrange-remap algorithm as a cross-check. The temperature field in the number fraction model is substantially steeper at \( x \approx 0.65 \) m, which is thought to be a feature of the governing equations.

For the calculations with \( p_0 = 10 \) Pa, there is no analytical solution as the density distribution varies slightly from the analytical solution, hence Figure 3.5 plots the comparison between the mass fraction, number fraction and Lagrange-remap results. The key result here is that all models converge to the same solution using 256 cells.

Case 2: Diffusion of a contact surface between two identical species at different temperatures

The computational domain for this case is again \( 0 \leq x \leq 1 \) m, and grid sizes from 32 to 4096 cells are employed. Reflective boundary conditions are used at the left and right boundaries. The two fluids have the properties \( \rho_1 = 20 \) kg/m\(^3\), \( \rho_2 = 1 \)
3.3 A five-equation model for miscible and viscous compressible mixtures

kg/m³, γ₁ = γ₂ = 5/3. The specific heats satisfy the requirement that \( c_v^1 = c_v^2 \), and \( D = 0.01 \text{ m}^2/\text{s} \). A uniform initial pressure is achieved by specifying that \( T_2 = 20T_1 \). As in Case 1, \( p_0 = 10000 \text{ Pa} \) and the solution is run to \( t = 0.5 \text{ s} \). As the heat diffusivity is constant, the error function solution for the density distribution is again applicable for the quasi-incompressible case. The initial density and mass fraction distributions are the same as in Case 1, implying that the initial number fractions are different. Thus the initial cell averages \( \rho, \rho Y_1 \) and \( \rho \pi \) are the same as Case 1. The initial distribution (and incompressible analytical solution) of \( X_1 \) is equal now to \( Y_1 \).
3.3 A five-equation model for miscible and viscous compressible mixtures

Table 3.3 – Case 2 convergence rates for the number fraction model.

<table>
<thead>
<tr>
<th>( N_x )</th>
<th>( L^1 )</th>
<th>( L^2 )</th>
<th>( L^\infty )</th>
<th>( \mathcal{O}(L^1) )</th>
<th>( \mathcal{O}(L^2) )</th>
<th>( \mathcal{O}(L^\infty) )</th>
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<td>32</td>
<td>3.8913e-03</td>
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<td>2.0614</td>
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<td>-0.0396</td>
<td>0.1613</td>
<td>0.8452</td>
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Table 3.4 – Case 2 convergence rates for the mass fraction model.

<table>
<thead>
<tr>
<th>( N_x )</th>
<th>( L^1 )</th>
<th>( L^2 )</th>
<th>( L^\infty )</th>
<th>( \mathcal{O}(L^1) )</th>
<th>( \mathcal{O}(L^2) )</th>
<th>( \mathcal{O}(L^\infty) )</th>
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</thead>
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<td>-</td>
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<td>2048</td>
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<td>-0.6492</td>
<td>-0.8416</td>
<td>-0.0077</td>
</tr>
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</table>

and is given by

\[
X_1 = \frac{\rho_1 [1 - \text{erf}(Z)]}{(\rho_1 + \rho_2) + (\rho_1 - \rho_2)\text{erf}(Z)}.
\]  

(3.78)

This function does not have an exact anti-derivative, so the initial conditions for \( X_1 \) are computed by a five-point Gaussian quadrature scheme. In the incompressible limit, the density and mass fraction distributions are the same as for the uniform temperature case. However, number fractions are different; the cold gas now expands when it mixes with the hot gas. In the number fraction equation, the term \( u^{(n)} \cdot \nabla X_1 \approx 0 \) but the \( \nabla n/n \) term is now essential.

Table 3.3 and 3.4 document the \( L^1 \), \( L^2 \) and \( L^\infty \) errors in the simulated volume fraction profile at \( t = 0.5 \) s for the number fraction and mass fraction models compared to the incompressible analytical solution, along with the observed convergence rates. Figure 3.6 plots the error norms as a function of number of cells \( N_x \) for the mass fraction and number fraction models. As this case includes two species with the
same thermodynamic properties (i.e. $\gamma_1 = \gamma_2$), then the differences between the mass and number fraction formulations should be lower. This is indeed the case, and both algorithms converge at the expected order of accuracy up to the point where compressibility impacts the agreement with the incompressible solution. As with Case 1, the errors with the mass fraction model increase at 4096 points which confirms this hypothesis. The number fraction model again has lower error at a given grid resolution, however the differences are not as substantial as the previous case. This is to be expected as the principal errors in the mass fraction approach are generated when the ratio of specific heats varies with mixture composition.
3.3 A five-equation model for miscible and viscous compressible mixtures

![Graphs of density, velocity, pressure, and temperature](image)

Figure 3.7 – Comparison of variables across all grid resolutions for Case 2 with the mass fraction model results on the left and the number fraction model results on the right.
Figure 3.8 – Case 2 comparison of non-analytical fields for the mass fraction (MF) and number fraction (NF) models in Flamenco (512 cells) as well as the results from the Lagrange-remap code (256 cells).

Figure 3.7 plots the spatial variation of flow properties for both the mass fraction and number fraction models, demonstrating that for a specific grid resolution there are only slight variations in the solutions. Figure 3.8 compares with the Lagrange-remap formulation for 256 cells, showing good agreement for the temperature distribution. The pressure distributions are similar but are not converged (between algorithms) at this mesh resolution. Again, in this case the acoustic waves have travelled about 70 times the domain width by \( t = 0.5 \) s.

Case 3: Advection and diffusion of an isothermal material interface between two different species

As highlighted in the introduction, the key errors in the mass fraction model appear when a material interface between two species with different values of \( \gamma \) is advected through the computational mesh. Thus Case 3 is a periodic version of Case 1, with a mean advection velocity of 4 m/s. This ensures that at \( t = 0.5 \) s, the initially diffuse interface returns exactly to the original position \( x_0 \). The computation domain is now \( 0 \leq x \leq 2 \) m, and grid sizes from 32 to 4096 are employed. Periodic boundary conditions are used at the left and right boundaries. The two fluids have the same
3.3 A five-equation model for miscible and viscous compressible mixtures

Table 3.5 – Case 3 convergence rates for the number fraction model.

<table>
<thead>
<tr>
<th>(N_x)</th>
<th>(L^1)</th>
<th>(L^2)</th>
<th>(L^\infty)</th>
<th>(O(L^1))</th>
<th>(O(L^2))</th>
<th>(O(L^\infty))</th>
</tr>
</thead>
<tbody>
<tr>
<td>64</td>
<td>3.8866e-03</td>
<td>3.9599e-03</td>
<td>6.9897e-03</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>256</td>
<td>8.8780e-05</td>
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<tr>
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<td>0.3780</td>
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Table 3.6 – Case 3 convergence rates for the mass fraction model.

<table>
<thead>
<tr>
<th>(N_x)</th>
<th>(L^1)</th>
<th>(L^2)</th>
<th>(L^\infty)</th>
<th>(O(L^1))</th>
<th>(O(L^2))</th>
<th>(O(L^\infty))</th>
</tr>
</thead>
<tbody>
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<td>-</td>
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<tr>
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</tr>
<tr>
<td>256</td>
<td>3.4366e-03</td>
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<td>9.2933e-03</td>
<td>2.0191</td>
<td>2.0200</td>
<td>1.9996</td>
</tr>
<tr>
<td>512</td>
<td>8.7023e-04</td>
<td>1.1486e-03</td>
<td>2.3790e-03</td>
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<td>1.9890</td>
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</tr>
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<td>3.5851e-05</td>
<td>1.9900</td>
<td>1.9971</td>
<td>2.0480</td>
</tr>
</tbody>
</table>

properties as Case 1, namely \(\rho_1 = 20\ \text{kg/m}^3\), \(\rho_2 = 1\ \text{kg/m}^3\), \(\gamma_1 = 2\), \(\gamma_2 = 1.4\). The specific heats satisfy the requirement that \((\gamma_1 - 1)\rho_1 c_{v1} = (\gamma_2 - 1)\rho_2 c_{v2}\), which gives temperature equilibrium if the two fluids have the same pressure. For \(0 \leq x \leq 1\ \text{m}\), the analytical solution for the number fraction distribution is given by

\[ X_1 = \frac{1}{2} \left[ 1 - \text{erf}(Z) \right], \quad Z = \frac{x - x_0}{\sqrt{4Dt + h_0^2}} \]

where \(x_0 = 0.5\ \text{m}\). The number fraction profile is then mirrored about \(x = 1\ \text{m}\), thus for \(1 \leq x \leq 2\ \text{m}\) the number fraction distribution is given by

\[ X_1 = \frac{1}{2} \left[ 1 + \text{erf}(Y) \right], \quad Y = \frac{x - x_1}{\sqrt{4Dt + h_0^2}} \]

where \(x_1 = 1.5\ \text{m}\), \(h_0 = 0.02\ \text{m}\) and the diffusion coefficient \(D = 0.01\ \text{m}^2/\text{s}\). The initial cell averaged quantities are gained by simply mirroring the expressions detailed for Case 1 about \(x = 1\ \text{m}\).
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Table 3.5 and 3.6 document the $L^1$, $L^2$ and $L^\infty$ errors in the simulated volume fraction profile at $t = 0.5$ s for the number fraction and mass fraction models compared to the incompressible analytical solution, along with the observed convergence rates. Figure 3.9 plots the error norms as a function of number of cells $N_x$ for the mass fraction and number fraction models. Once again, the error norms show approximate second-order accuracy for both sets of governing equations. However, there is an enormous difference in the absolute error; with the number fraction model giving results that are at least one order of magnitude more accurate for this problem at a given grid resolution. This highlights perfectly the key motivation for the development of this

Figure 3.9 – Plot of Case 3 convergence rates, comparing the mass fraction (MF) and number fraction (NF) models.
model. In practical computations of mixing problems there is usually very little possibility to resolve the diffuse interface between two gases with as many points as is possible in one dimension here. Thus, the results of the 64 or 128 cell grids are most representative of practical computations of mixing flows with turbulent fluctuations. This result implies that for a fixed error in a three dimensional problem the new number fraction model may be run on a mesh almost 4 times smaller in each direction, or 64 times smaller overall. Assuming a CFL restriction on the time step size this translates to a potential computational saving on the order of $200\times$ in three dimensions (compensating for the additional computational expense in the number fraction formulation compared to the mass fraction formulation).

Figure 3.10 plots the density, velocity, pressure and temperature distributions at $t = 0.5$ s for both models for $0 \leq x \leq 1$ m (i.e. one half of the periodic solution). The errors in mass-weighted velocity, pressure and temperature when using the mass fraction model are substantial. Figure 3.11 compares the non-analytical fields from the three algorithms at a lower grid resolution (128 cells), highlighting the substantial improvement gained using the number fraction model at realistic resolutions for a three dimensional computation. Note that the large mass fraction errors are present in both the Eulerian and Lagrange remap mass fraction model implementations. This case demonstrates that for miscible mixing of gases with differing $\gamma$, the single pressure and temperature closure in the mass fraction model greatly impacts the accuracy of the scheme. Allowing volume-averaged species temperatures to vary results in a substantially more accurate numerical solution for the same computational effort.

3.3.6 Two-dimensional test case

To demonstrate the applicability of the new algorithm to compressible mixing problems, Case 4 undertakes direct numerical simulations of a two-dimensional single-mode Richtmyer-Meshkov instability triggered by a shock wave passing from air to SF$_6$. The setup for this case is adapted from that proposed by Tritschler et al. [166]. The purpose of this case is to illustrate the advantage of using the proposed number
Figure 3.10 – Comparison of variables across all grid resolutions for Case 3 with the mass fraction model results on the left and the number fraction model results on the right.
3.3 A five-equation model for miscible and viscous compressible mixtures

Fraction model in a more practical setting, since there is widespread use of air-SF$_6$ combinations in shock-induced turbulence experiments [178–181].

To conduct an accurate simulation, the initial conditions must be very well resolved. Here, a single mode perturbation of wavelength 0.5 mm and initial amplitude 0.025 mm is computed. The initial diffuse layer thickness is 0.1 mm, sufficiently low to prevent substantial damping of the initially imparted impulse. The initial background state of the unshocked gases is $p_0 = 23000$ Pa and $T = 298$ K. For simplicity a fixed viscosity $\mu = 2.243 \times 10^{-5}$ Pa-s is specified [4], along with $Sc = 1$ and $Pr = 1$. Note that inviscid computations have also been run to represent the high Reynolds number limit. Air is assumed to have $\gamma_{air} = 1.4$, and $\gamma_{SF6} = 1.1$, while the molecular weights are $W_{air} = 28.964$ g/mol and $W_{SF6} = 146.057$ g/mol [166]. The shock Mach number is 1.5, and the shock has an initial offset of 1 mm from the mean interface position. The interface diffuses slightly prior to shock interaction, increasing the integral width by 2.7% at the time of shock interaction in the cases incorporating viscosity, diffusion and conduction. All results are scaled by the modal wavelength $\lambda$ and the Richtmyer velocity (Equation (2.4)).

The details of the initial conditions for this two-dimensional problem are derived as
follows. The incompressible limit of mixing by species diffusion gives the following non-zero divergence of velocity \[59\]:

\[ \nabla \cdot u = -\nabla \cdot \left( \frac{D}{\rho} \nabla \rho \right), \]

with the diffusion coefficient is given by

\[ D = \frac{\mu}{\rho Sc} \]

In 2D this becomes

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \frac{2\mu}{Sc \rho^3} \left( \left( \frac{\partial \rho}{\partial x} \right)^2 + \left( \frac{\partial \rho}{\partial y} \right)^2 \right) - \frac{\mu}{Sc \rho^2} \left( \frac{\partial^2 \rho}{\partial x^2} + \frac{\partial^2 \rho}{\partial y^2} \right). \]

Now, let

\[ \frac{\partial u}{\partial x} = \frac{2\mu}{Sc \rho^3} \left( \frac{\partial \rho}{\partial x} \right)^2 - \frac{\mu}{Sc \rho^2} \frac{\partial^2 \rho}{\partial x^2}, \quad \frac{\partial v}{\partial y} = \frac{2\mu}{Sc \rho^3} \left( \frac{\partial \rho}{\partial y} \right)^2 - \frac{\mu}{Sc \rho^2} \frac{\partial^2 \rho}{\partial y^2}, \]

and integrate to give

\[ u = -\frac{\mu}{Sc \rho^2} \frac{\partial \rho}{\partial x}, \quad v = -\frac{\mu}{Sc \rho^2} \frac{\partial \rho}{\partial y}. \]

Finally, taking cell averages gives

\[ \bar{u}_i = \frac{\mu}{Sc \Delta x \Delta y} \int_{y_{i-\frac{1}{2}}}^{y_{i+\frac{1}{2}}} \left( \frac{1}{\rho(x_{i+\frac{1}{2}}, y)} - \frac{1}{\rho(x_{i-\frac{1}{2}}, y)} \right) dy, \tag{3.81} \]

\[ \bar{v}_i = \frac{\mu}{Sc \Delta x \Delta y} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left( \frac{1}{\rho(x, y_{i+\frac{1}{2}})} - \frac{1}{\rho(x, y_{i-\frac{1}{2}})} \right) dx, \tag{3.82} \]

where \( \rho(x, y) = \rho_1 X_1(x, y) + \rho_2 (1 - X_1(x, y)) \) and

\[ X_1(x, y) = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{F(x, y) \sqrt{\pi}}{h_0} \right) \right]. \tag{3.83} \]

Equation (3.81) and (3.82) are calculated numerically using a 5-point Gaussian quadra-
3.3 A five-equation model for miscible and viscous compressible mixtures

Figure 3.12 – Density (top) and temperature (bottom) contours for the single mode RM instability between air and SF$_6$. For each image, the left panel is a computation using the mass fraction model and the right is the same computation but using the number fraction model.

Figure 3.12 shows visualisations of inviscid and viscous computations with the number fraction and mass fraction models. In this problem, the inviscid computations highlight the worst of the numerical errors in the mass fraction model, where temperature errors of several hundred Kelvin appear across the layer. The inviscid computation clearly shows the benefit of the number fraction approach for inviscid advection when $\gamma_1 \neq \gamma_2$. The addition of viscosity, diffusion and thermal conductivity reduces the error in the mass fraction model results, such that both models converge to the same solution as expected. The converged solutions are visualised in Figure 3.12 (a) and (c) and are identical for both models. However, the spurious temperatures produced in the inviscid component of the mass fraction model are expected to impact on the convergence of the solution, as highlighted in the previous periodic advection case.
3.3 A five-equation model for miscible and viscous compressible mixtures

Here, three quantitative measures are employed to explore this. These common measures of the time evolution of the layer are the integral mixing width $W$, molecular mixing fraction $\Theta$ and the mixing parameter $\Xi$ \cite{41, 40, 182, 183, 31}, defined as

\[
W = \int \langle f_1 \rangle \langle f_2 \rangle \, dx, \quad \Theta = \frac{\int \langle f_1 f_2 \rangle \, dx}{\int \langle f_1 \rangle \langle f_2 \rangle \, dx}, \quad \Xi = \frac{\int \langle \min(f_1, f_2) \rangle \, dx}{\int \min(\langle f_1 \rangle, \langle f_2 \rangle) \, dx}. \tag{3.84}
\]

These quantities are plotted in Figure 3.13 for the mass fraction and number fraction models at the finest grid resolution, showing that the respective quantities have converged to the same solution regardless of model. There are slight differences in the inviscid solution, however the general trend is that the inviscid case has lower width at late times, and lower mixing parameters.

Figure 3.14 plots $W$, $\Theta$ and $\Xi$ for cross-sectional resolutions from $N_y = 32$ to $N_y = 512$ cells per wavelength for the mass fraction and number fraction models. Firstly, the integral width $W$ converges at $N_y = 128$ for both schemes. Rather surprisingly, the mass fraction model appears to converge faster. The mixing parameters $\Theta$ and $\Xi$ follow the expected trends, with the number fraction model converging at $N_y = 64$ while the mass fraction model varies substantially until $N_y = 256$. Thus the observations of errors in the prediction of $\Theta$ and $\Xi$ are as expected from the previous cases, but not for $W$. Figure 3.15 plots the $x$ variation of the planar averages $\langle X_1 \rangle \langle X_2 \rangle$ and $\langle X_1 X_2 \rangle$ (which are equivalent to volume fraction planar averages) for the mass fraction model and number fraction model both at the converged grid resolution ($N_y = 512$) and at an intermediate resolution ($N_y = 128$). The integral width is the
Figure 3.14 – Comparison of mixing measures across all grid resolutions for Case 4 with the mass fraction model results on the left and the number fraction model results on the right.
area under the curve given by $\langle X_1 \rangle \langle X_2 \rangle$. From this figure it can be seen that the mass fraction model has larger errors in $\langle X_1 \rangle \langle X_2 \rangle$ than the number fraction model, however those errors are approximately equal on both sides of the mixing layer. Thus although the integral width appears to converge faster for the mass fraction model, it is simply that the errors are cancelling each other.

Turning to $\langle X_1 X_2 \rangle$, the integral of which is equivalent to the numerator in the $\Theta$ equation, there is a very large error when using the mass fraction model compared to the number fraction model at $N_y = 128$. Overall, the solution of the number fraction model at $N_y = 64$ has an equivalent error to the mass fraction model at $N_y = 256$, computed using an identical variable reconstruction, Riemann solver and discretisation of the viscous terms. This represents an enormous computational saving for equivalent error, a factor of $16 \times$ fewer points in 2D along with a factor of $4 \times$ fewer time steps. Even with an observed (unoptimised) increase in computational cost of 25–50%, the computations are on the order of 40× faster for equivalent accuracy.

For three-dimensional flows the gain would be expected to be greater than 100×. This clearly demonstrates the superiority of the newly proposed number fraction formulation of the governing equations. This formulation is directly applicable to DNS (as undertaken here) as well as LES with an explicit subgrid model.
3.4 Conclusions

This chapter has presented a new number fraction based five-equation model for miscible fluids incorporating viscosity, species diffusivity and thermal conduction. An equation is solved for the variable \( \bar{X} \) which reduces to the usual definition of volume fraction when there is a sharp interface in a computational cell and to the species number fraction if there is homogeneous mixing within the cell. A numerical scheme has been derived to solve these equations which is second-order accurate in space and time and respects the underlying physics. Four test cases have been proposed, and computations have been run using both the standard mass fraction model and the newly proposed number fraction model. These test cases were designed such that they validate and verify all key terms in the governing equations.

Three of the cases have analytical solutions in the incompressible limit which were used to compute the observed order of accuracy. The discretisation of the number fraction and mass fraction models were both demonstrated to be second-order accurate in space. This was shown to be valid up to the point at which compressibility effects became important. The first two cases are relatively straightforward for both models, having either constant temperature or constant ratio of specific heats. The third test case was designed to be more challenging and consisted of a diffusing contact surface between fluids of different thermodynamic properties moving with a mean velocity. Although both models converge at second-order accuracy, the number fraction model is approximately one order of magnitude more accurate for a given grid resolution. The final test case was of a commonly employed gas combination in experiments of shock-induced turbulent mixing. A shock wave impinges on a two-dimensional perturbed interface between air and SF\(_6\), triggering the growth of the Richtmyer-Meshkov instability. In this test case, the number fraction model is approximately converged on all measures at \( 128^2 \) cross-sectional grid resolution, whereas the mass fraction model is not converged until at least \( 512^2 \) points. This represents a computational saving of approximately \( 40\times \) for the equivalent accuracy.

Based on these results, the new number fraction model is clearly superior to the stan-
standard mass fraction approach for the computation of compressible turbulent mixing problems of miscible fluids with distinct thermodynamics properties. Further examples are presented in Appendix A for other commonly employed gas combinations. This formulation is readily applicable to both direct numerical simulation as well as explicit large eddy simulation, however the model still has some undesirable aspects that should be rectified in future work. One such disadvantage is that the model is not hyperbolic and is therefore difficult to discretise at arbitrarily high-order accuracy. As a first step towards a unified hyperbolic model for viscous, compressible mixtures, the four-equation model is reformulated as a fully in the framework of thermodynamically compatible first-order systems in Appendix B. It is anticipated that this approach could also be applied to the five-equation model.
Chapter 4

Direct Numerical Simulation of the Narrowband Richtmyer–Meshkov Instability

4.1 Introduction

In most applications involving the Richtmyer–Meshkov instability quantitative experimental data is difficult to obtain, therefore gaining an understanding of the underlying physics relies to a considerable extent upon the use of numerical simulation. Furthermore, given the broad range of scales involved in these phenomena, as well as the fact that often other physics must be considered such as radiation or chemical/nuclear reactions, it is currently necessary to model the effects of mixing and turbulence to some degree in order to maintain computational tractability. This motivates the use of high-fidelity simulation techniques such as large eddy simulation (LES) and direct numerical simulation (DNS) for fundamental problems with the purpose of increasing the understanding of turbulent mixing and guiding the development of reduced-order modelling techniques and sub-grid models. Previous numerical studies of this instability have demonstrated the ability of LES algorithms to predict mixing at late time due to turbulent stirring in the high Reynolds number
limit [40, 95, 31, 184, 4, 82, 185, 45]. In the largest such study to date (known as the \( \theta \)-group collaboration), Thornber et al. [30] showed that good agreement is obtained for various integral measures such as the mixing layer width, mixedness and total fluctuating kinetic energy across eight independent algorithms. In a follow-up paper, Thornber et al. [105] computed the transport equation budgets for the mean momentum, mean heavy fluid mass fraction, heavy fluid mass fraction variance, and specific turbulent kinetic energy to provide useful benchmark data for the development of closure models for these quantities.

However, there is still a lack of understanding with regards to the behaviour of the mixing layer during transition, where the turbulence is not fully developed and the energy-containing scales grow under the influence of viscous and diffusive dissipation. In this regime the use of LES, with either implicit or modelled subgrid terms, is not necessarily well justified and indeed this is where the algorithms in the \( \theta \)-group collaboration showed the greatest disagreement. Also with regards to ICF, recent simulations have indicated that the capsule hot spot is very viscous due to the high temperatures involved, hence the assumption of turbulent conditions in the hot spot is likely incorrect as small-scale mixing should be viscously damped [186]. It is also possible that ablator material is spread through the hotspot via molecular diffusion [21].

This motivates the exploration of the effects of these dissipative processes on the evolution of RMI at early time through direct numerical simulation of the governing equations. In particular, the use of DNS is crucial in determining how key flow quantities vary with Reynolds number so as to help identify the conditions that give rise to fully developed turbulence, as well as to provide useful data on how the mixing layer evolves under conditions that inhibit turbulence to some degree. An additional complication when analysing this transitional behaviour in RMI is that the outer-scale Reynolds number of the layer is not constant but depends on the growth rate (see Section 4.3), which in turn depends on the initial conditions [31]. Thus it is possible for a mixing layer to become fully turbulent (i.e. the energy-containing scales decouple from the dissipation range) only briefly before decaying to some sub-
critical state if the Reynolds number is decreasing in time. This behaviour is not observed in the evolution of other interfacial instabilities such as Kelvin–Helmholtz or Rayleigh–Taylor instabilities, both of which have an outer-scale Reynolds number that increases steadily with time. Therefore the usefulness of DNS in studying RMI is not merely confined to early-time growth and transitional behaviour but also late-time decay and slowly developing mixing layers.

Previous published direct numerical simulations of RMI include a study by Olson and Greenough [92], as well as the studies of Tritschler et al. [187, 166]. In Olson and Greenough [92], single-shock RMI in air and sulphur hexafluoride (SF$_6$) initiated by a Mach 1.18 shock was analysed using two different numerical methods. A maximum grid resolution of $1024 \times 512^2$ was considered, with an initial perturbation similar to that used in the present study. The initial Reynolds numbers, based on the post-shock velocity and fastest growing wavelength, were 1200 and 7200 in air and SF$_6$ respectively. Using the methodology outlined in [30], and which is also used in the present study (see Section 4.6.1), this is equivalent to a Reynolds number of 817 based on the initial mixing width growth rate $\dot{W}_0$ and mean initial wavelength $\lambda$. Similarly in Tritschler et al. [166], RMI initiated by a Mach 1.05/1.2/1.5 shock was simulated, also in air and SF$_6$. A deterministic initial perturbation was used, the maximum grid resolution considered was $1024 \times 512^2$ and the initial Reynolds number based on $\dot{W}_0$ and $\lambda$ was 739.

The transition to fully developed turbulence of a turbulent mixing layer evolving from RMI was investigated in shock tube experiments by Weber et al. [186], using a broadband initial condition imposed on an interface between helium and argon and either a $M = 1.6$ or $M = 2.2$ shock Mach number. In that study the authors found an approximate $k^{-5/3}$ inertial range in the scalar variance spectra as well as sufficient separation in the Batchelor and Taylor length scales and final outer-scale Reynolds numbers of $5.7 \times 10^4$ and $7.2 \times 10^4$ respectively. This suggests that the turbulence had reached a fully developed state by the latest time considered. Mohaghar et al. [188] also performed shock tube experiments using nitrogen and carbon dioxide with both single-mode and broadband initial conditions and a $M = 1.55$ shock. For both initial
4.1 Introduction

conditions the outer-scale Reynolds number was found to be greater than $1 \times 10^4$ and the ratio of Liepmann–Taylor to inner-viscous length scales greater than 1, which is a sufficient criterion for fully developed turbulence in stationary flows [51]. A scaling of close to $k^{-5/3}$ was also found in the inertial range of the turbulent kinetic energy spectra. In Mohaghar et al. [189], results for a second shock Mach number of $M = 1.9$ were added and the time-dependent mixing transition criterion of Zhou et al. [52] was evaluated, showing that the ratio of diffusion layer to inner-viscous length scales was greater than 1 only after reshock had occurred in the $M = 1.55$ case and just prior to reshock in the $M = 1.9$ case.

Lombardini et al. [184] investigated the Mach number dependence of transition to fully developed turbulence in RMI by performing large eddy simulations with Mach numbers ranging from $M = 1.05$ to $M = 5$. For these simulations the effects of the unresolved scales of motion were explicitly modelled using the stretched-vortex model of Misra and Pullin [133]. A deterministic initial condition was used with a radial power spectrum consisting of a Gaussian profile in wavenumber space. The profile was centred at a dominant wavenumber, with a suitably determined variance such that the extent of the Gaussian profile is contained in the resolved range of annular wavenumbers. The flow was observed to only partially return to isotropy in the turbulent kinetic energy components at late time and fully developed turbulence, characterised by a $k^{-5/3}$ inertial range in the kinetic energy spectra, was found to occur for Taylor microscale Reynolds numbers of $Re_\lambda \gtrsim 250$. It should be noted that this estimate for $Re_\lambda$ is based on the kinetic energy dissipation rate, the majority of which was modelled, not resolved.

In Tritschler et al. [166], direct numerical simulations of RMI-induced turbulence with $M = 1.05$ to $M = 1.5$ were used to determine the critical Taylor microscale Reynolds number for fully developed turbulence to be somewhere in the range of $35 \leq Re_\lambda \leq 80$, substantially lower than previous estimates. A deterministic initial condition was also used, consisting of a dominant single mode perturbation with a multimode perturbation imposed on top of this whose coefficients approximately obey a Gaussian distribution. The decay rates of turbulent kinetic energy, as well as proba-
bility density functions of the velocity and its longitudinal and transverse derivatives, were determined to be in good agreement with values for decaying isotropic turbulence.

So far the majority of experimental and numerical studies focused on transition to fully developed turbulence due to RMI have explored the effects of Mach number on the temporal development of the flow. Outside of the effects of compressibility however, the variation in time-dependent transitional behaviour of the mixing layer is actually due to the variation in Reynolds number (which increases with increasing shock Mach number), hence it is valuable to explore this parameter space directly as has been done previously for homogeneous turbulence. Direct numerical simulation is the ideal tool for this, as it allows for unparalleled levels of insight into the behaviour of quantities that are typically quite hard to obtain experimentally. This is the main focus of this chapter; to explore the Reynolds number dependence of turbulent mixing induced by RMI using direct numerical simulations, with the aim of using the results to infer the behaviour at higher Reynolds numbers.

One aspect of the simulations presented here that makes them particularly challenging, at least from the point of view of achieving a sustained level of turbulence, is the fact that the Reynolds number decreases with time. This challenge also applies to RMI experiments and is due to the dependence of the growth rate exponent $\theta$ on initial conditions [31]. As is illustrated in Section 4.5, if the layer width grows as $\sim t^\theta$ then the Reynolds number based on this width evolves as $\sim t^{2\theta-1}$. For the class of initial conditions presented here, it is expected that $\theta \leq 1/3$ and hence the Reynolds number decreases with time. This is contrasted with simulations/experiments of the Rayleigh–Taylor instability where the layer width grows as $\sim t^2$ and hence the associated Reynolds number grows as $\sim t^3$, which makes it easier to obtain fully developed turbulence.

Given the intention of studying the Reynolds number dependence of transitional behaviour in RMI, it is desirable to use a well-defined and well understood initial condition. It is also desirable to start with the simplest possible problem and then gradually introduce additional levels of complexity once the previous level has been
well understood. The aim of this Chapter is therefore twofold. Firstly, it presents a thorough assessment of grid convergence for this specific initial condition. Given that this case was formulated to help understand and compare the performance of individual algorithms, the results presented here should serve as a useful guide in estimating the grid resolution requirements in other DNS studies of RMI, either with different numerical algorithms, or different initial conditions. Secondly, this same methodology is used to perform a comprehensive study of the Reynolds number dependence of many key quantities of interest in the early time evolution and transition to turbulence of an RMI-induced mixing layer. Comparisons are also drawn, where appropriate, between the current DNS and previous ILES results for this case using the same numerical algorithm. This clearly demonstrates the impact of finite Reynolds number, how far the current results are from the expected high Reynolds number limit, and indicates specifically in which quantities the effects of viscous dissipation and molecular diffusion are important.

The layout of this chapter is as follows. Section 4.2 details the initial condition, domain size and boundary conditions as well as diagnostic quantities. Section 4.3 details how grid convergence is assessed for DNS at a given Reynolds number. Preliminary results as well as comparisons with previous ILES results are presented in Section 4.5 including visualisations, integral mix measures and power spectra and comparisons between DNS and ILES\(^1\). More detailed results including the Reynolds number dependence of various statistics of the velocity and scalar fields, as well as the evolution of key length scales and Reynolds numbers, are given in Section 4.6. In Section 4.7 these are used to evaluate the mixing transition criterion for unsteady flows and assess how close the turbulence in the flow is to becoming fully developed\(^2\). Finally, Section 4.8 gives a conclusion of the main findings, as well as the direction of future work on this problem.

\(^1\)The work presented in Sections 4.3 and 4.5 of this chapter has been published in Groom, M., Thornber, B. (2019). Direct numerical simulation of the multimode narrowband Richtmyer–Meshkov instability. *Computers & Fluids*, 194, 104309.

\(^2\)The work presented in Sections 4.6 and 4.7 of this chapter has been accepted for publication in the *Journal of Fluid Mechanics* in an article titled ‘Reynolds number dependence of turbulence induced by the Richtmyer–Meshkov instability using direct numerical simulations’ by Groom, M. and Thornber, B.
4.2 Problem description

4.2.1 Computational approach

The equations solved are the compressible multicomponent Navier-Stokes equations, given in Section 3.1, which govern the behaviour of mixtures of miscible gases. The governing equations are solved using the University of Sydney code Flamenco, which has been extended to include a DNS capability and is described in full in Section 3.2. Further extensions to the numerical method were assessed in Appendix C, however based on the findings from the 2D test cases considered there the baseline spatial and temporal discretisation of the four-equation model, as well as the original low Mach correction of Thornber et al. [9], is used for all of the simulations presented in this chapter.

4.2.2 Initial condition

The initial condition used for all simulations here is identical to that of the $\theta$-group collaboration by Thornber et al. [30]. Two test cases were utilised in that study, referred to as the standard problem and the quarter-scale problem, which used the same computational domain size but with the initial length scales reduced by a factor of four. This allowed for simulations to be run to much later dimensionless times while still being able to obtain grid converged results for the various integral measures of interest. Since the focus of the present study is on the Reynolds number dependence at relatively early dimensionless times, the starting point for the current setup is the standard test case from Thornber et al. [30]. This maximises the Reynolds numbers at which grid converged DNS solutions may be obtained while still allowing for the simulations to be run up until the onset of late-time behaviour. A summary of how grid convergence is assessed in DNS of this initial condition is given in Section 4.3. Using the methodology presented in that section, the results for all simulations given in this chapter may be considered to be sufficiently converged and independent of the grid resolution used.
A brief description of the initial condition will now be given. The setup consists of two quiescent gases separated by a material interface and with a shock wave initialised in the heavy gas travelling towards the interface. The material interface is given a surface perturbation, defined in Fourier space as a power spectrum of the form

\[ P(k) = \begin{cases} 
C, & k_{\text{min}} < k < k_{\text{max}}, \\
0, & \text{otherwise},
\end{cases} \tag{4.1} \]

where \( k = \sqrt{k_y^2 + k_z^2} \) is the radial wave number. The specific perturbation used in this study is a narrowband perturbation containing length scales ranging from \( \lambda_{\text{min}} = L/8 \) m to \( \lambda_{\text{max}} = L/4 \) m where \( L = 2\pi \) m is the cross section of the computational domain. Setting \( C = \lambda_{\text{min}}/10 \) ensures that all modes are initially growing in the linear regime. The amplitudes and phases of each mode are defined using a set of random numbers that are constant across all grid resolutions and cases, thus allowing for a grid convergence study to be performed for each case. The interface is also initially diffuse for this same reason, with the profile given by an error function with characteristic initial thickness \( \delta = L/32 \) m. The volume fractions \( f_1 \) and \( f_2 = 1 - f_1 \) are computed as

\[ f_1(x, y, z) = \frac{1}{2} \text{erfc} \left( \frac{\sqrt{\pi} |x - S(y, z)|}{\delta} \right), \tag{4.2} \]
where \( S(y, z) = x_0 + A(y, z) \), with \( A(y, z) \) being the amplitude perturbation satisfying the specified power spectrum and \( x_0 \) the mean position of the interface. For present purposes it is sufficient to state that \( A(y, z) \) is given by

\[
A(y, z) = \sum_{m,n=0}^{N_k} \left[ a_{mn} \cos(mk_0 y) \cos(nk_0 z) + b_{mn} \cos(mk_0 y) \sin(nk_0 z) \right. \\
+ \left. c_{mn} \sin(mk_0 y) \cos(nk_0 z) + d_{mn} \sin(mk_0 y) \sin(nk_0 z) \right],
\]

where \( N_k = k_{max} L / (2\pi) \), \( k_0 = 2\pi / L \) m\(^{-1}\) and the coefficients \( a_{mn} \ldots d_{mn} \) are selected from a Gaussian distribution and scaled such that the overall standard deviation of the perturbation is \( 0.1\lambda_{min} \). For full details on the derivation of the surface perturbation see Section 5.2.2, as well as Thornber et al. [31, 30]. A visualisation of the initial perturbation is shown in Figure 4.1.

A Cartesian domain of dimensions \( x \times y \times z = 2.8\pi \times 2\pi \times 2\pi \) m\(^3\) is used for all simulations presented here. Periodic boundary conditions are used in the \( y \) and \( z \) directions, while in the \( x \) direction outflow boundary conditions are imposed very far away from the test section so as to minimise spurious reflections from outgoing waves impacting the flow field. The initial mean positions of the shock wave and the interface are \( x_s = 3.0 \) m and \( x_0 = 3.5 \) m respectively, as shown in Figure 4.2, and the initial pressure of both (unshocked) fluids is \( p = 1.0 \times 10^5 \) Pa. The shock Mach number is 1.8439, equivalent to a four-fold pressure increase, the initial densities of
Table 4.1 – The molecular weight $W$ (g/mol), ratio of specific heats $\gamma$ and Prandtl and Schmidt numbers of fluid 1 (heavy) and fluid 2 (light).

<table>
<thead>
<tr>
<th>Property</th>
<th>Heavy fluid</th>
<th>Light fluid</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W_l$</td>
<td>90</td>
<td>30</td>
</tr>
<tr>
<td>$\gamma_l$</td>
<td>5/3</td>
<td>5/3</td>
</tr>
<tr>
<td>$Pr_l$</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>$Sc_l$</td>
<td>1.0</td>
<td>1.0</td>
</tr>
</tbody>
</table>

the heavy and light fluids are $\rho_1 = 3.0$ kg/m$^3$ and $\rho_2 = 1.0$ kg/m$^3$ and the post-shock densities are $\rho_1^+ = 5.22$ kg/m$^3$ and $\rho_2^+ = 1.80$ kg/m$^3$ respectively. This gives a post-shock Atwood number of $At^+ = 0.487$. The variation in density and mass fraction across the interface is computed using $\rho = \rho_1 f_1 + \rho_2 (1 - f_1)$ and $\rho Y_1 = \rho_1 f_1$ with $f_1$ given by Equation (4.2).

The evolution of the interface is solved in the post-shock frame of reference by applying a factor of $\Delta u = -291.575$ m/s to the initial velocities of the shocked and unshocked fluids. In order to be suitable for DNS, the velocity field must be modified so as to include an initial diffusion velocity at the interface [110]. This is performed by considering the incompressible limit of a binary mixture [59], which specifies that

$$\nabla \cdot u = -\nabla \cdot \left( \frac{D}{\rho} \nabla \rho \right).$$

(4.4)

To improve the quality of the initial condition, three-point Gaussian quadrature is used in each direction to accurately compute the cell averages required by the finite-volume algorithm. The dynamic viscosity $\mu$ is used to set the initial Reynolds number $Re_0$, described in Section 4.6, while all other thermodynamic properties of both fluids are given in Table 4.1.

4.2.3 Implicit large eddy simulations

A brief overview of the previous implicit large eddy simulations performed of this initial condition is also given here in order to aid comparison with the present set of results. In Thornber et al. [30], ILES computations were performed to explore the high
4.2 Problem description

Reynolds number limit of key integral quantities in the self-similar regime. Several assumptions are made when justifying the use of ILES as being representative of this high Reynolds number limit. Firstly, it is assumed that there is sufficient separation between the integral length scales and the grid scale such that the growth of the integral length scales is independent of the exact dissipation mechanism. This is addressed in the formulation of the problem, where a sufficient amount of the high wavenumber end of the spectrum is resolved by the grid at all times.

It is also assumed that the species are intimately mixed at the subgrid level, such that scalar dissipation rates are well represented and are insensitive to the actual values of viscosity and diffusivity. This may be understood as an assumption that the turbulence in the flow is fully developed in the sense of Dimotakis [51]. Since the effects of physical viscosity and diffusivity on the resolved scales are assumed to be zero, the simulations are nominally inviscid. However, it must be noted that numerical dissipation acts to dissipate kinetic energy and that the equation of state for mixed cells assumes intimate mixing at a sub-grid scale. At early times, when the layer is still non-turbulent and highly corrugated and strained, particular care must be taken in interpreting ILES results as the flow is not yet turbulent. This is because the thickness of contact surfaces and thus the amount of mixing are impacted by physical diffusion.

Once the flow has transitioned to fully developed turbulence however, integral properties of the mixing layer such as width, mixing fractions, turbulent kinetic energy and kinetic energy spectra are considered to be well resolved and an accurate representation of the high Reynolds number limit for this particular flow. At early time it would be expected that quantities dependent on the small scale properties of the layer would differ between the ILES and DNS, yet as the layer transitions to turbulent and becomes well mixed, both ILES and DNS are expected to agree. Any disagreement is important as it gives a sense of how far current DNS results are from passing through the mixing transition observed for many other turbulent flows, beyond which point these statistics should become insensitive to the Reynolds number. A similar comparison of DNS and ILES results has been made in Youngs [36] for various flows
driven by Rayleigh–Taylor instability, showing that both approaches give very similar results for the degree of molecular mixing at late time. The main conclusions from that paper were that if the high Reynolds number behaviour of the global properties of the mixing zone are of primary interest then ILES results are able to estimate these accurately and with substantially less computational effort. However, if the effects of finite Reynolds number and/or small-scale properties of the mixing zone are desired then DNS (or explicitly modelled LES) is essential.

4.3 Assessing grid convergence

4.3.1 Quantities of interest

To assess the extent of grid convergence, various integral measures are used as well as domain integrated values of some important quantities that are indicative of the fidelity of the numerical simulation at large and small scales. The time dependent integral mixing width $W$ is given by

$$W(t) = \int \langle f_1 \rangle \langle f_2 \rangle \, dx$$

(4.5)

where $\langle \ldots \rangle$ denotes a $y$-$z$ plane average. Similarly the molecular mixing fraction $\Theta$ and mixing parameter $\Xi$ are given by

$$\Theta(t) = \frac{\int \langle f_1 f_2 \rangle \, dx}{\int \langle f_1 \rangle \langle f_2 \rangle \, dx}, \quad \Xi(t) = \frac{\int \langle \min(f_1, f_2) \rangle \, dx}{\int \min(\langle f_1 \rangle, \langle f_2 \rangle) \, dx}.$$  

(4.6)

A third integral mixing measure is also computed, the recently proposed normalised mixed mass \[190\]:

$$\Psi(t) = \frac{\int \langle \rho Y_1 Y_2 \rangle \, dx}{\int \langle \rho \rangle \langle Y_1 \rangle \langle Y_2 \rangle \, dx}.$$  

(4.7)

At the end of the simulation the integral width is less than 10% of the domain size, thus the integral measures should be close to statistically converged and not constrained by the choice of domain size \[121\]. The Favre-averaged total fluctuating
kinetic energy is given by

\[ TKE(t) = \iiint \frac{1}{2} \rho u''_i u''_i \, dx \, dy \, dz, \quad (4.8) \]

where \( u''_i = u_i - \bar{u}_i \) and \( \bar{u}_i = \bar{u}_i/\bar{p} \) is a Favre average. The TKE contained in the \( i = 1, i = 2 \) and \( i = 3 \) directions is denoted by TKX, TKY and TKZ respectively. Similarly, the domain-integrated instantaneous enstrophy \( \Omega \) and scalar dissipation rate \( \chi \) are given by

\[ \Omega(t) = \iiint \rho \omega_1 \omega_1 \, dx \, dy \, dz, \quad \chi(t) = \iiint D_{12} \frac{\partial Y_1}{\partial x_i} \frac{\partial Y_1}{\partial x_i} \, dx \, dy \, dz, \quad (4.9) \]

where \( \omega_i \) is the vorticity in direction \( i \).

The dissipation rate of turbulent kinetic energy is calculated according to Equation (4.21), and the Taylor and Kolmogorov length scales are given in Equation (4.41) and (4.43) respectively. Similarly, a transverse Taylor-scale Reynolds number is defined at the mixing layer centre plane as in Equation (4.42), while a Reynolds number based on the integral width \( W \) is also considered, defined as

\[ Re_W = \frac{W \bar{W}}{\langle \nu \rangle}, \quad (4.10) \]

with \( \langle \nu \rangle \) also calculated at the mixing layer centre plane. Finally, radial power spectra of turbulent kinetic energy, enstrophy and scalar dissipation rate are also calculated in the same manner as in Equation (4.27).

4.4 Grid convergence

Simulations using the initial condition described in Section 4.2.2 were computed from \( t = 0 \) s to \( t = 0.5 \) s using successively refined grid resolutions of \( 90 \times 64^2 \), \( 180 \times 128^2 \), \( 360 \times 256^2 \) and \( 720 \times 512^2 \). In order to demonstrate that the results on the \( 720 \times 512^2 \) grid were suitably converged at early time, a higher grid resolution of \( 1440 \times 1024^2 \) was simulated up to \( t = 0.1 \) s. The methods used for determining grid convergence
4.4 Grid convergence

will be discussed in this section. All quantities presented in the following sections are non-dimensionalised as described in Section 4.6.1. Note that in this section and Section 4.5, the diffuse interface correction factor $\psi$ given in Equation (4.14) is not applied when calculating $\tilde{W}_0$. Therefore the initial growth rate is $\tilde{W}_0 = 12.649 \text{ m/s}$, the same as that in the $\theta$-group study, and the initial Reynolds number is $Re_0 = 457$. This is the same case as the $Re_0 = 348$ case referred to in the later sections, just with a different non-dimensionalisation so as to allow a simpler comparison with the ILES results.

Visualisations of the solution at dimensionless times $\tau = 1.23$ and $\tau = 6.15$ are given in Figure 4.3 showing red bubbles rising into the heavy fluid and blue spikes penetrating into the light fluid. At the end time the mixing layer is still largely laminar with a relatively narrow range of modes, as would be expected for this Reynolds number range, and for the most part the interface has retained a coherent structure. The ability of the numerical algorithm to resolve gradients across the stretched, corrugated layer at early time is the limiting factor in achieving a completely grid-independent solution for this case. At later times increased mixing leads to a decrease in mean gradients and hence the resolution requirements are not as severe.

Two domain-integrated dissipative measures of the DNS data, enstrophy and scalar dissipation rate, are plotted in Figure 4.4. Grid convergence in these measures is harder to obtain than for lower order statistics [92], as this is heavily reliant on the fidelity of the numerical algorithm, in particular how well gradients in the flow field have been captured. Very good agreement is observed for the two finest grid resolutions across all points in time, which gives a good indication that the flow field has been suitably resolved. Figure 4.4 also shows that the early time transitional period is the most challenging to fully resolve, which is when the layer is thinnest with respect to the computational grid.

A more demanding measure is the spectral convergence of these quantities at a given point in time in addition to the domain integrated values. Figure 4.5 shows the power spectra of enstrophy and scalar dissipation rate at time $\tau = 1.23$ and $\tau = 6.15$. Both quantities are grid converged for wavenumbers up to at least $k \approx 100$. 
Figure 4.3 – Contours of volume fraction $f_1$ between the isosurfaces $f_1 = 0.1$ (blue) and $f_1 = 0.9$ (red), for the $720 \times 512^2$ grid. The left and right images show the spike and bubble sides of the mixing layer respectively.
Figure 4.4 – Time histories of enstrophy and scalar dissipation rate. Shown are data for the $180 \times 128^2$ grid (green), $360 \times 256^2$ grid (blue), $720 \times 512^2$ grid (black + circles) and $1440 \times 1024^2$ grid (magenta).

throughout the entire simulation, and both display a lack of an inertial range. At the two times considered the (non-dimensionalised) Kolmogorov microscale is calculated to be 0.0283 and 0.0624 respectively, equivalent to a wavenumber of $k = 222$ and $k = 101$, thus the Kolmogorov microscale is less than the Nyquist frequency for both times. There is a turnup at the high wavenumber end for the higher grid resolutions at late times, where the power is five to six orders of magnitude lower than the peak. This turnup effect is only observed on grids where the solution is well resolved, being isolated to the far dissipation range of the spectrum (i.e. greater than the Kolmogorov microscale). The most likely source is the reduction of numerical dissipation at low Mach, which is no longer sufficient to remove energy from the very highest modes, however the impact on the spectral range up to the Kolmogorov scale is minimal (it could be filtered out as is commonly done at high wavenumbers when using spectral methods). Comparisons between the spectra for the $720 \times 512^2$ and $1440 \times 1024^2$ grids at time $\tau = 1.23$ (or alternatively the $360 \times 256^2$ and $720 \times 512^2$ grids at time $\tau = 6.15$) show that when the grid resolution is doubled, the dissipation range beyond the Kolmogorov microscale is resolved with no impact on the spectrum at the larger scales. This gives a good indication of the overall fidelity of the numerical method,
with discretisation errors being isolated to the highest wavenumbers.

The full temporal evolution of the Kolmogorov microscale, as well as the Taylor microscale, is shown in Figure 4.6. Perhaps counter-intuitively, the Taylor microscale is observed to be harder to converge than the Kolmogorov microscale, however both are considered well converged on the $720 \times 512^2$ grid across all points in time. With the exception of the very first data point, which is sampled during the interaction of the shock and the interface, $\lambda_K \geq 0.0127$ and is therefore above the finest grid resolution of $\Delta x = 0.0122$ m for all subsequent times. Thus it can be concluded that
4.5 Preliminary results and comparisons with ILES

The solution on the $720 \times 512^2$ grid qualifies as DNS [64]. The DNS of Tritschler et al. [166] achieved a similar level of resolution, with the Kolmogorov microscale calculated to be between 5 µm and 92 µm on a grid spacing of $\Delta x = 19.5$ µm. It should be noted that the validity of the Kolmogorov microscale as being representative of the smallest scales is questionable prior to the flow being fully developed, and as such it is better to focus on the degree to which the results are independent of numerical dissipation (i.e. a grid-converged solution for the quantities of interest for this study).

4.5 Preliminary results and comparisons with ILES

This section will present a comparison of results between the current DNS and ILES of the same initial condition as presented in the $\theta$-group collaboration [30]. The ILES results on a grid resolution of $720 \times 512^2$ (using the same numerical algorithm for the inviscid flux) are included in the plots below for comparison. In order to facilitate comparisons with prior DNS in the literature, in particular prior DNS studies of RMI, the temporal variation in Taylor microscale Reynolds number $Re_T$ is given in Figure 4.7. The Reynolds number based on integral width, $Re_W$, is also presented, showing...
that it is of similar magnitude. Indeed, at early time both $Re_T$ and $Re_W$ reach a maximum of 49.8 and 48.6 respectively, after which they both decay to final values of 11.3 and 6.5.

All of the statistics presented here should exhibit some dependence on Reynolds number, at least up until some transitional Reynolds number and necessary time to transition is reached [51, 53]. Establishing whether a high Reynolds number limit exists, and whether the results from resolved simulations at lower Reynolds numbers can point to it, is of crucial importance for further understanding the nature of the mixing transition in RMI induced flows. For the initial condition considered here the flow is becoming more well resolved at late time and therefore it is only necessary to use very high grid resolutions at early times to fully capture the flow behaviour. This decreasing resolution requirement at late time can be explained by considering the variation in Reynolds number throughout the simulation. Assuming the mixing layer at late time can be described by a single length scale such as the integral width $W$, then given a Reynolds number for the layer defined as $Re = \bar{W}W/\nu$ it is
4.5 Preliminary results and comparisons with ILES

It is straightforward to show that if the late-time growth obeys a power law $W \propto t^\theta$ then

$$Re \propto \frac{\theta t^{\theta-1} t^\theta}{\nu} = \frac{\theta t^{2\theta-1}}{\nu}. \quad (4.11)$$

This implies that the Reynolds number either decreases with time if $\theta < \frac{1}{2}$ or increases with time if $\theta > \frac{1}{2}$. For the current narrowband perturbation the growth rate exponent $\theta$ is 0.2185 (similar to the ILES where $\theta = 0.2203$) and hence the Reynolds number is expected to decrease at late time, which is indeed the case as shown in Figure 4.7. This is also consistent with the observation of decreasing resolution requirements for DNS as time progresses, which suggests for the possibility of varying the mesh resolution during the simulation so as to achieve a higher Reynolds number while still remaining fully resolved throughout in future computations.

### 4.5.1 Integral measures

The temporal evolution of integral width and the various mixing fractions is given in Figure 4.8. There is little difference in the integral width predicted by the current DNS versus that of the ILES, particularly at early time. This indicates that the largest scales are still evolving mostly independently of the dissipation mechanism in the present DNS at this given Reynolds number. This trend is expected to eventually no longer hold as the Reynolds number is further decreased \[38\]. The end time (non-dimensional) integral width is 0.6676 for the DNS compared to 0.6628 for the ILES, a difference of 0.72%. This corresponds to a visual width of $\delta = 5.28$ and $\delta = 5.24$ respectively, where $\delta$ is defined in Equation (4.39).

The end time values of the mixing fractions $\Theta$, $\Xi$ and $\Psi$ are 0.8064, 0.8073 and 0.8048 respectively for the DNS, compared to 0.7945, 0.7915 and 0.7968 for the ILES. This equates to an average difference of 1.48% across all three metrics. Note that at the initial time, $\Theta$, $\Xi$ and $\Psi$ are not equal to 1 since the layer does not begin in a purely homogeneous state due to the initial perturbation and is therefore not perfectly mixed (i.e. $\langle f_1 f_2 \rangle \neq \langle f_1 \rangle \langle f_2 \rangle$). The slightly larger values of $W$, $\Theta$, $\Xi$ and $\Psi$ for the DNS compared to the ILES are caused by extra spreading of the layer due to molecular
4.5 Preliminary results and comparisons with ILES

Figure 4.8 – Time histories of integral width and mixing parameters comparing the DNS and ILES results. Shown are DNS data for the $180 \times 128^2$ grid (green), $360 \times 256^2$ grid (blue), $720 \times 512^2$ grid (black + circles), $1440 \times 1024^2$ grid (magenta) and ILES data on a $720 \times 512^2$ grid (grey dashed).

diffusion at early time and inhibition of turbulence. It is also interesting to note the degree of similarity of the late time values of the mixing fractions between the DNS and ILES (in particular the agreement in $\Psi$ at late time), despite the inhibition of fine-scale turbulent motions in the DNS. This indicates that at late time the mixing is dominated by large scale motions, which are very similar for the the DNS and ILES. Examining the early time behaviour of $W$ and $\Theta$ in Figure 4.9 shows the initial com-
pression of the layer due to the shock, which corresponds to a minimum in $W$ and a maximum in $\Theta$. At a slightly later time $\Theta$ obtains a minimum value, which corresponds to when the interface is most highly stretched. For the DNS, this stretching of the interface due to the initial impulse is balanced by molecular diffusion due to gradients across the interface as well as the onset of any secondary instabilities. As a result, the value and temporal location of minimum mix is conjectured to be a function of the initial Reynolds number. The values of $\Theta$ and $\Xi$ at this point are 0.2221 and 0.2148 respectively, both occurring at a time of $\tau = 0.2126$, which is earlier than the time of maximum scalar dissipation rate. For the ILES, the stretching due to the initial impulse is balanced purely by secondary instabilities and the implicit sub-grid model, with the minimum in $\Theta$ and $\Xi$ of 0.1616 and 0.1572 occurring slightly later at $\tau = 0.2274$ and $\tau = 0.2268$ respectively. Whether this is an accurate estimate of the high Reynolds number limit is unclear, since at this time the evolution of the large scales may not be independent of the dissipation mechanism. At the very least this value represents the inviscid limit for a given grid resolution and algorithm.
4.5.2 Turbulent kinetic energy

An integral measure of turbulent kinetic energy may be compared between the DNS and ILES since in the high Reynolds limit it depends only on the large scales and as such will converge in a similar manner to the integral width. Comparing the temporal evolution of total fluctuating kinetic energy (TKE) in Figure 4.10, the DNS results show a higher decay rate of $\tau^{-1.41}$, compared to a rate of $\tau^{-1.25}$ for the ILES. The decay rate of $-1.41$ for the DNS is very close to the theoretical value of $-10/7$ for homogeneous decaying turbulence (assuming a $k^4$ Batchelor form for the large scales [121]), however this is likely just a coincidence given that the decay rate of TKE does not match the value that can be calculated from the observed growth of the integral width assuming self-similarity [31]. Nor does it correspond with the observed decay rate of enstrophy as shown in Figure 4.4, which should scale in the same manner as the dissipation rate. In addition, the low Reynolds number, short time scale and anisotropy of the mixing layer (see below) indicate that instead it is far more likely that the increased decay rate is simply due to the additional dissipation and a lack of scale separation.

Figure 4.10 also contains the evolution of the individual components of TKE. All components of TKE are reduced in magnitude compared to the ILES results, however the $x$-component of turbulent kinetic energy has a smaller reduction than in the $y$ and $z$ directions, indicating that there is an increase in anisotropy with increased viscous dissipation. This suggests that viscosity has suppressed secondary instabilities which transfer kinetic energy from the $x$ direction to the $y$ and $z$ directions. This reduced transfer of energy to the perpendicular directions in the DNS can be quantified by considering the ratio of turbulent kinetic energy components $TKR = (2 \times TKX)/(TKY + TKZ)$ as well as the ratio of Taylor microscale Reynolds numbers $Re_{T,x}/Re_T$.

Figure 4.11 shows the temporal evolution of both of these ratios for the DNS and ILES (note that although $Re_T$ cannot be defined for the ILES, the ratio is a valid quantity as $\langle \nu \rangle$ cancels). A peak in these ratios (ignoring the initial compression) occurs at a time of $\tau = 0.1845$, slightly before the observed minimum in mixing parameters.
At the latest time, the ratio of turbulent kinetic energy components is 1.692 for the DNS compared to 1.423 for the ILES, while the ratio of Taylor microscale Reynolds numbers is 1.508 and 1.318 for the DNS and ILES respectively. Thus both metrics show that there is still a significant amount of anisotropy in the flow at the latest time considered. Although this anisotropy is still decreasing (with the DNS results also approaching those of the ILES), an analysis of the quarter-scale case data from the $\theta$-group collaboration, given in Appendix D, shows that persistent anisotropy still remains at much later non-dimensional times. This is also in good agreement with

**Figure 4.10** – Time histories of turbulent kinetic energy components comparing the DNS and ILES results. Shown are DNS data for the $180 \times 128^2$ grid (green), $360 \times 256^2$ grid (blue), $720 \times 512^2$ grid (black + circles), $1440 \times 1024^2$ grid (magenta) and ILES data on a $720 \times 512^2$ grid (grey dashed).
4.5 Preliminary results and comparisons with ILES

The wavenumber dependence of turbulent kinetic energy is examined by computing the 2D radial power spectra, shown in Figure 4.12. Power spectra of both the in-plane \((E_v + w)\) and the out-of-plane \((E_u)\) components are shown. The turbulent kinetic energy spectra for the DNS show no signs of an inertial range, indicating that a significant separation of scales is not present. When comparing with the ILES results it is clear that the reduction in TKE is due to viscous suppression of the higher wavenumbers; the large scales are in good agreement. In particular, this agreement is stronger for the \(E_u\) spectra than the \(E_v + w\) spectra, again showing that the suppression of secondary instabilities reduces the transfer of energy from the \(x\) direction to the \(y\) and \(z\) directions in accordance with Figure 4.10. This is also the mechanism behind the increased levels of anisotropy observed in the DNS compared to the ILES.

The excellent agreement in the large scales between the DNS and ILES gives support to the assumption that the growth of the integral length scale is independent of the mechanism of dissipation [30], one of the key tenets of the ILES philosophy. A \(k^{-3/2}\)
inertial range is present in the ILES data across at least half a decade, consistent with the theory of Zhou [191] and previous simulations [31, 121]. It is anticipated that as the Reynolds number increases the agreement between the DNS and ILES results will extend to higher and higher wavenumbers, ultimately resulting in the development of an inertial range once some critical Reynolds number is reached. The spectra also show that the Reynolds number is decreasing at late-time as the energy contained at high wavenumbers is decreasing, in line with the argument made at the beginning of this section.

4.6 Reynolds number dependence

4.6.1 Non-dimensionalisation

All of the quantities presented in the following sections (as well as the preceding ones) are non-dimensionalised as follows. All velocities are normalised by the initial growth rate of integral width $W_0$, given by linear theory. By relating the integral width to the initial variance of the perturbation, Thornber et al. [30] showed that the estimated initial growth rate is given by

$$W_0 = 0.564 \bar{k} At^+ \sigma_0^+ \Delta u,$$

(4.12)

where $\bar{k}$ is a weighted average wavenumber and $\sigma_0^+$ is the post-shock standard deviation of the perturbation, given by

$$\bar{k} = \frac{\int_0^\infty k^2 P(k) \, dk}{\sqrt{\int_0^\infty P(k) \, dk}},$$

(4.13a)

$$\sigma_0^+ = \left(1 - \frac{\Delta u}{U_*}\right) \sqrt{\int_0^\infty P(k) \, dk}.$$

(4.13b)
For the current problem, $\bar{k} = \sqrt{7/12k_{\text{max}}} \text{ m}^{-1}$ and the shock velocity is $U_s = 434.61$ m/s. Following Youngs and Thornber [48], to account for the initial diffuse interface a correction factor $\psi$ is applied to Equation (4.12) of the form

$$\psi = 1 + \sqrt{\frac{2}{\pi}} \delta^+,$$  

(4.14)

where $\delta^+ = C\delta^-$ is the post-shock characteristic thickness of the interface, $\delta^-$ is the
pre-shock thickness and \( \overline{C} = (\rho_1^- + \rho_2^-)/(\rho_1^+ + \rho_2^+) \) is the mean compression rate. For
the present set of DNS cases, \( \delta^- \) will be slightly larger than the initial characteristic
thickness \( \delta_0 \) due to diffusion prior to shock arrival. To account for this, \( \delta^- \) is calculated
assuming the diffusion occurs purely in \( x \)-direction, i.e.
\[
\delta^- = \sqrt{4Dt_0 + \delta_0^2},
\]
where \( t_0 = 0.0011 \) s is the time taken for the shock to reach the interface and \( \delta_0 = \lambda_{\text{min}}/(4\sqrt{\pi}) \). Therefore the initial growth rate \( \dot{W}_0 = 0.564\bar{\lambda}At^+\sigma_0^+ \Delta u/\psi \) ranges from
9.468 m/s to 9.665 m/s for all cases considered here.

All length scales are non-dimensionalised by \( \bar{\lambda} = 2\pi/k = 1.0283 \) m, while the mean
post-shock density \( \overline{\rho} = 3.51 \) kg/m\(^3\) is used to non-dimensionalise mass in all relevant
quantities. For example, the dimensionless time is defined as \( \tau = t\dot{W}_0/\bar{\lambda} \). Based on
these reference values, the initial Reynolds number of each case is defined as
\[
Re_0 = \frac{\overline{\rho}^+\dot{W}_0\bar{\lambda}}{\mu}.
\]
Using the initial condition described in Section 4.2.2, a series of simulations are per-
formed, each with a different value of \( \mu \) and hence \( Re_0 \). The values of \( \mu \) used are
\( \mu = 0.8, 0.6, 0.4, 0.3, 0.2, 0.1 \) and 0.05 Pa-s, which correspond to initial Reynolds
numbers \( Re_0 = 43, 57, 86, 115, 174, 348 \) and 697. For each simulation, grid con-
vergence is assessed using the methodology outlined in Section 4.3. For example,
the \( Re_0 = 174, Re_0 = 348 \) and \( Re_0 = 697 \) cases are found to be suitably converged
on grids of \( 360 \times 256^2, 720 \times 512^2 \) and \( 1440 \times 1024^2 \) cells respectively. Figure 4.13
shows the temporal evolution of domain integrated enstrophy and scalar dissipation
rate for the \( Re_0 = 697 \) case computed on various grid resolutions. The solutions for
both of these quantities are clearly converging with each successive doubling of the
grid resolution, with a sufficiently small difference observed between the \( 720 \times 512^2 \)
and \( 1440 \times 1024^2 \) grids. The differences between the solutions obtained on the two
finest grids are greatest at early time when the layer is being thinned and stretched,
resulting in large gradients across the interface.
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Power spectra of $\Omega$ and $\chi$ are presented in Figure 4.14, taken at time $\tau = 0.470$ corresponding to the peak scalar dissipation rate. There is excellent agreement across all grid resolutions for the low wavenumber end of the spectra ($k \leq 10$), while for the two highest grid resolutions the results are converged up to at least $k \leq 128$ for the enstrophy spectra and $k \leq 100$ for the scalar dissipation rate spectra. This represents the least converged region of the entire solution; for later times the scalar dissipation rate spectra are converged up to at least $k \leq 128$ also. These results should be compared with similar ones presented in Olson and Greenough [92] and Tritschler et al. [166] for DNS of Richtmyer–Meshkov flows. Similar levels of convergence are obtained for all of the other cases presented in this section.

All simulations are calculated to a final time of $t = 0.5$ s, at which point the most extreme spikes are approaching the domain boundary. An additional simulation with $Re_0 = 1395$ is also performed to a final time of $t = 0.1$ s, using a domain of size $1.4\pi \times 2\pi \times 2\pi$ and grids of up to $1440 \times 2048^2$ cells. Figure 4.15 shows visualisations of the solution at $\tau = 0.94$ for the $Re_0 = 174$ and $Re_0 = 697$ cases. Bubbles of light fluid can be seen flowing into the heavy fluid on the upper side of the mixing layer, while heavy spikes are penetrating into the light fluid on the lower side. When
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Figure 4.14 – Power spectra at time $\tau = 0.470$. Results are shown for grid resolutions of $180 \times 128^2$ (dotted lines), $360 \times 256^2$ (dashed lines), $720 \times 512^2$ (solid lines) and $1440 \times 1024^2$ (circles)

comparing between the two cases, it can be observed that the effects of Reynolds number are more apparent at the spike side than the bubble side of the mixing layer. Whereas the structure of the bubble front is largely the same between the two cases, there is substantially more fine scale detail in the spikes for the $Re_0 = 697$ case. Thus it appears that the transition to fully developed turbulence begins preferentially on the spike side, likely due to the higher velocity and stronger gradients of the spikes feeding the growth of secondary shear layer instabilities at a faster rate. The following sections will explore this transitional behaviour further through an analysis of the variation with Reynolds number in the velocity and scalar fields.

4.6.2 Mixing measures & growth rates

It is reasonably well established that multimode RMI will evolve into a turbulent mixing layer whose width is proportional to $t^\theta$, however there are still differences in the exact value of $\theta$ reported in the literature [18]. Thornber et al. [31] showed that these discrepancies can be at least partially explained by dependence on initial conditions, and for narrowband perturbations where the instability growth is due to non-linear
4.6 Reynolds number dependence

(a) $Re_0 = 174$

(b) $Re_0 = 697$

Figure 4.15 – Contours of volume fraction $f_1$ at time $\tau = 0.94$, bounded by the isosurfaces $f_1 = 0.1$ (black) and $f_1 = 0.9$ (white).

coupling/backscatter from the energetic modes a value of $\theta = 0.26$ was obtained from numerical simulations. This was found to be in good agreement with the experimental measurements of Dimonte and Schneider [47] which gave $\theta = 0.25 \pm 0.05$. However, Thornber [121] showed that the value of $\theta$ is sensitive to the length of dimensionless time a simulation (or experiment) is run for and gave an updated value of $\theta = 0.275$. Similarly, in the recent $\theta$-group collaboration using eight independent algorithms [30], a value of $\theta = 0.219$ was obtained for the standard narrowband case, while the quarter-scale version of that case that was run to much later dimensionless time gave $\theta = 0.291$.

Elbaz and Shvarts [46] gave a theoretical argument that for incompressible and immiscible fluids, the bubble front should reach a self-similar state once at least 3-4 mode coupling generations have occurred, with $\theta_b = 1/3$. Soulard et al. [45] applied an eddy damped quasinormal Markovianized (EDQNM) closure to RM turbulence in the low Atwood number limit and also obtained $\theta = 1/3$ for narrowband perturbations with a constant initial power spectrum. This is quite close to the results of Reese et al. [192], who found $\theta = 0.34 \pm 0.01$ in vertical shock tube experiments (after adjusting the
concentration field to remove large-scale structures from the mixing layer). Experiments in air and SF$_6$ conducted by Prasad et al. [193] examining late-time behaviour found that $0.26 \leq \theta \leq 0.33$, roughly spanning the range of different values from simulations of narrowband perturbations. Recently, Youngs and Thornber [48] modified a Buoyancy-Drag model based on results from the $\theta$-group study to account for initial conditions. This analysis also provided a new method for estimating the asymptotic value of $\theta$ at late-time and found that $0.32 \leq \theta \leq 0.36$, in excellent agreement with the theoretical and experimental results mentioned above.

One area on which little data has been published is the effects of Reynolds number on $\theta$, which can be discerned using data taken from the present set of DNS results. A caveat must first be made; the results presented here are for comparatively early dimensionless times and should not be interpreted as representative of any late-time self-similar state. A commonly used quantity for estimating $\theta$ is the integral width, given by Equation (4.5). Another quantity, that may be considered to be a more direct measure of the mixing layer evolution, is the mixed mass [190], which is given by

$$M = \int \langle \rho Y_1 Y_2 \rangle \, dx. \quad (4.17)$$

An important feature of the mixed mass is that it is a conserved quantity. Figure 4.16 shows the evolution in time of $W$ and $M$, with both quantities exhibiting a non-trivial variation with Reynolds number. At the latest time considered, $W$ is smallest for the $Re_0 = 43$ case and largest for the $Re_0 = 174$ case. This ordering can be explained by the variation that occurs in dissipation of kinetic energy due to viscous action and dissipation due to turbulence as the Reynolds number is increased. For low Reynolds numbers, such as $Re_0 = 43$ and $Re_0 = 57$ (not shown), the growth in $W$ is damped by viscous dissipation, in other words the largest scales are evolving under the influence of viscosity. At Reynolds numbers even lower than those presented here another regime is possible, whereby the growth in $W$ is dominated by the diffusion velocity (and hence grows as $\sim t^{1/2}$). For high Reynolds numbers $W$ grows independently of viscous effects, and the growth rate is instead damped by turbulent dissipation. This is beginning to occur in the two highest $Re_0$ cases, where comparisons with the ILES
data from Thornber et al. [30] in Section 4.5 show that \( W \) is tending towards the high Reynolds number limit. The \( Re_0 = 174 \) case is representative of an intermediate regime where damping due to viscous dissipation has reduced but the amount of turbulence in the flow is still relatively low, thus the damping on the growth of \( W \) is lowest.

A different variation with Reynolds number is observed for \( M \), where at the latest time considered the \( Re_0 = 697 \) case has the lowest amount of mixed mass, followed by the \( Re_0 = 43 \) case, while the \( Re_0 = 86 \) case has the highest amount of mixed mass. At early times \( M \) decreases with increasing \( Re_0 \), which can be explained in terms of increasing levels of molecular diffusion leading to greater mixing. As the simulations progress however, the amount of mixed mass in the \( Re_0 = 43 \) case is eventually overtaken by that in the \( Re_0 = 86 \) case, which in turn is overtaken by the \( Re_0 = 115 \) case (not shown). This is most likely due to a combination of two factors that influence the rate at which molecular mixing occurs; the steepness of gradients across the interface and the interfacial surface area. As mixing progresses in the lowest \( Re_0 \) cases, the gradients across the interface (which control the rate of
molecular diffusion) are reduced and hence the mixing rate slows. When combined with the fact that there is less interfacial surface area (i.e. the area across which molecular diffusion can occur) due to inhibition of turbulence, this explains why the amount of mixed mass in these cases is eventually overtaken by that in the higher Reynolds number cases. Indeed, this trend could be expected to continue if the simulations were run to later times, where eventually the highest $Re_0$ case would be expected to obtain the highest amount of mixed mass.

Using nonlinear regression to fit a function of the form $W = \beta (\tau - \tau_0)^\theta$ allows the exponent $\theta$ to be obtained for each case, with the fit performed from $\tau = 2.3$ to $\tau = 4.7$. In order of ascending $Re_0$, the calculated values are $\theta = 0.172$, $\theta = 0.163$, $\theta = 0.178$, $\theta = 0.197$, $\theta = 0.215$, $\theta = 0.214$ and $\theta = 0.214$. These values should be compared to the value of $\theta = 0.219$ that was obtained from ILES simulations of the same initial condition [30]. There is a clear trend of increasing values of $\theta$ with increasing $Re_0$, although the variation is only 25% at most. The same procedure is also performed for the mixed mass $M$, for which the corresponding values of $\theta$ are $\theta = 0.189$, $\theta = 0.186$, $\theta = 0.195$, $\theta = 0.198$, $\theta = 0.204$, $\theta = 0.219$ and $\theta = 0.214$. These values are not significantly different from those calculated using $W$, except at the lowest Reynolds numbers considered. At even lower Reynolds numbers than those in the present study, it is likely that the calculated values of $\theta$ using $W$ and $M$ would begin to differ more substantially.

Following Krivets et al. [6], the evolution of integral width can be decomposed into bubble and spike widths as

$$W_b = \int_{-\infty}^{x_c} \langle f_1 \rangle \langle f_2 \rangle \, dx,$$

(4.18a)

$$W_s = \int_{x_c}^{\infty} \langle f_1 \rangle \langle f_2 \rangle \, dx,$$

(4.18b)

where the mixing layer centre $x_c$ is defined as the $x$ position of equal mixed volumes [38], given by

$$\int_{-\infty}^{x_c} \langle f_2 \rangle \, dx = \int_{x_c}^{\infty} \langle f_1 \rangle \, dx.$$  

(4.19)
4.6 Reynolds number dependence

Figure 4.17 shows the evolution in time of $W_b$ and $W_s$, as well as the ratio $W_s/W_b$. There is a clear asymmetry in the width of the spikes compared to the width of the bubbles, as well as a clear trend that this asymmetry increases with increasing $Re_0$. This is likely due to there being less viscous drag on the spikes at higher Reynolds number, allowing them to attain a higher velocity. The asymmetry between $W_s$ and $W_b$ is greatest at early time, after which it decreases gradually over the course of the simulation. A key consideration is whether the ratio $W_s/W_b$ approaches a constant value, which implies that $\theta_b = \theta_s$. In all of the simulations this appears to be occurring, although they do not run to late enough dimensionless time to show this definitively. Youngs and Thornber [49] showed that the ratio of bubble and spike heights approaches a constant at late time using ILES of a very similar problem, hence it is also expected this is the case for $W_s/W_b$.

At low Reynolds numbers the late time value $r$ of this ratio is substantially smaller, and the variation of $r$ with $Re_0$ can be estimated by fitting a curve to the end time data of each simulation. Assuming a function of the form $r = 1 + A/[1 + \exp(-BRe_0 + C)]$, the parameters $A$, $B$ and $C$ were found using nonlinear regression to be 0.283, 0.036 and 25.5 respectively. This gives the high Reynolds number limit of $r$ to be 1.283. It should be noted that the values of these parameters are not equal to those that would be obtained at much later dimensionless time, and they likely do not capture the correct behaviour as $Re_0 \to 0$. There is also very likely a dependence of the bubble-spike asymmetry, both the early-time peak and the late-time asymptote, on other key parameters such as the Atwood and Mach numbers. This should be especially true at early times and would therefore make for an interesting extension of the current work.

Figure 4.18 shows the evolution in time of the molecular mixing fraction $\Theta$ and the normalised mixed mass $\Psi$, with both quantities displaying a clear trend of a more heterogeneous mixture with increasing Reynolds number. After the initial compression by the shock, at which point the mixing layer is highly homogeneous, the interface is rapidly stretched by instability growth due to the impulsive acceleration. This stretching of the interface, combined with the increasing amplitude of each mode,
leads to a rapid increase in the heterogeneity of the mixing layer. This is soon balanced by molecular diffusion due to gradients across the interface as well as the onset of secondary instabilities, leading to a minimum in both $\Theta$ and $\Psi$. The value of this minimum varies between 0.449 and 0.161 as $Re_0$ is increased for $\Theta$ and between 0.438 and 0.153 for $\Psi$. Thus this value, and to a lesser degree the temporal location, is observed to depend on the initial Reynolds number. There is also evidence that a high Reynolds number limit exists, for example the distance between the $Re_0 = 1395$ and $Re_0 = 697$ minima is less than that between the $Re_0 = 697$ and $Re_0 = 348$ minima. The convergence also appears to be more rapid for $\Psi$ than for $\Theta$. The variation of the minimum values of $\Theta$ and $\Psi$ with initial Reynolds number $Re_0$ is shown in Figure 4.19. Also shown are lines of best fit to the data, obtained using nonlinear regression with a functional form of $f = A + \sqrt{B/(Re_0 - C)}$. The optimal parameters are $A = 0.10$, $B = 5.34$ and $C = -0.60$ for $\Theta_{\text{min}}$ and $A = 0.098$, $B = 3.96$ and $C = 8.95$ for $\Psi_{\text{min}}$. As before, the correct behaviour as $Re_0 \to 0$ is not captured, however the high Reynolds number limit for both quantities may be estimated and is given by the coefficient $A$.

Beyond the point of minimum mix, both $\Theta$ and $\Psi$ start to increase and by the end of the simulation both quantities are close to obtaining an asymptotic value, which is also observed to be a function of the initial Reynolds number. A simple Richardson

**Figure 4.17** – Temporal evolution of integral spike and bubble widths as well as the ratio of spike and bubble widths. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).
extrapolation of the end time values of $\Theta$ and $\Psi$ for the $Re_0 = 174$, $Re_0 = 348$ and $Re_0 = 697$ cases gives estimates of 0.765 and 0.772 for the high Reynolds number limit. These are slightly lower than the values obtained with ILES for this problem. At much later dimensionless times $\Theta$ and $\Psi$ have been shown to gradually decay as self-similarity is approached [30], however this phenomenon may only occur for sufficiently high Reynolds number turbulence.

**4.6.3 Reynolds number effects**

**Velocity field**

The observed Reynolds number dependence in Section 4.6.2 motivates a systematic study of Reynolds number effects in both the velocity and scalar fields. The first quantity considered is the turbulent kinetic energy, defined as

$$\overline{E_k^u} = \frac{1}{2} u''_i u''_i,$$  \hspace{1cm} (4.20)
where $\psi'' = \psi - \tilde{\psi}$ indicates a fluctuating quantity and $\tilde{\psi} = \frac{\bar{\psi}}{\rho}$ is a Favre average. A plane average taken over the statistically homogeneous directions is used to calculate the ensemble average $\bar{\psi}$ of a quantity $\psi$. The dissipation rate of the Favre-averaged turbulent kinetic energy is given by

$$\tilde{\epsilon}'' = \frac{2\bar{\mu}}{\rho} \left( \tilde{s}''_{ij} \tilde{s}''_{ij} - \frac{1}{3} \tilde{\theta}''^2 \right),$$

(4.21)

where $s''_{ij} = \frac{1}{2} \left( \frac{\partial u''_i}{\partial x_j} + \frac{\partial u''_j}{\partial x_i} \right)$ is the fluctuating strain rate tensor and $\theta'' = \frac{\partial u''_l}{\partial x_l}$.[194].

Figure 4.20 shows the evolution in time of $\tilde{E}''_k$ and $\tilde{\epsilon}''$ at the mixing layer centre plane $x_c$, given by Equation (2.6). Both quantities exhibit a decay in time as the kinetic energy initially deposited by the shock wave is converted into internal energy by irreversible processes. The initial amount of turbulent kinetic energy is also essentially the same for all cases, with only very small differences observed due to slightly different values of $\delta^-$. The dissipation rate is initially highest for the $Re_0 = 43$ case and lowest for the $Re_0 = 1395$ case, and at all times considered there is more turbulent kinetic energy in the flow for increasing $Re_0$. The turbulent kinetic energy is also monotonically decreasing in time for all cases, as is the dissipation rate in all cases except for the $Re_0 = 1395$ case, which exhibits a maximum at time $\tau = 0.224$. At
late times the dissipation rate increases with increasing $Re_0$ due to the presence of more turbulent structures in the mixing layer. Beyond the initial transient stage, the turbulent kinetic energy decays as $\bar{E}''_k \sim t^{-n}$. Using linear regression, the decay rate $n$ is found to be 2.20, 2.00 1.83, 1.76, 1.68, 1.59 and 1.51 in order of lowest to highest initial Reynolds number (excluding $Re_0 = 1395$). Similarly, the dissipation rate is expected to decay as $\bar{\epsilon}'' \sim t^{-(n+1)}$ with the actual decay rates found to be 3.24, 2.97, 2.80, 2.73, 2.66, 2.67 and 2.40, in good agreement with the measured values of $n$.

Figures 4.21 and 4.22 show the spatial distribution across the layer of $\bar{E}''_k$ and $\bar{\epsilon}''$ at three different points in time. The $x$-coordinate is normalised by the integral width $W$ and is centred about $x_c$. To give some context to the figures, the locations at which $\langle f_1 \rangle = 0.99$ and $\langle f_1 \rangle = 0.01$ (i.e. the 99% bubble and spike heights) range between $(x - x_c)/W = -2.8$ to $-3.0$ and $(x - x_c)/W = 4.9$ to 5.1 respectively throughout the simulation. At the earliest time shown, the turbulent kinetic energy profile is biased towards the spike side of the layer, with the peak occurring at a distance of about two integral widths from the layer centre in all cases. This is also observed for the dissipation rate. As time progresses, the profiles become more symmetric about...
The spatial distribution of turbulent kinetic energy in the $x$-direction is shown in Figure 4.21 for different Reynolds numbers. For $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

$x_c$, although there is a persistent bias towards the spike side, indicating that more turbulent fluctuations are occurring there. The difference between the profiles of the highest and lowest $Re_0$ cases also increases throughout the simulation, particularly at the very fringes of the spike side of the layer. Indeed, at the latest time considered, there is a substantially higher amount of turbulent kinetic energy (as well as a larger dissipation rate) in this region for the $Re_0 = 348$ and $Re_0 = 697$ cases than in any of the lower Reynolds number cases. This suggests that there are spikes penetrating deep into the light fluid at these Reynolds numbers, and which break down more rapidly at lower Reynolds numbers. In fact, the spikes in the $Re_0 = 348$ case actually penetrate further. This is because of a lower amount of turbulent dissipation inhibiting their growth, as was previously mentioned in Section 4.6.2. A similar phenomenon can also be observed in Thornber et al. [30] for the ILES codes with greater numerical dissipation.

Two other important quantities for modelling variable-density turbulence are the Reynolds stress tensor, given by

$$R_{ij} = \rho u'_i u'_j,$$  \hspace{1cm} (4.22)
as well as the turbulent mass flux, given by

\[ a_i = \frac{\rho' u'_i}{\bar{\rho}} \]

which appears as a production term in many Reynolds stress closure models \[195\]. Figure 4.23 shows the spatial distribution of the principal component of the Reynolds stress tensor in the \( x \)-direction (i.e. in the direction normal to the mixing layer). Since isotropy is expected in the homogeneous directions, Figure 4.24 shows the average of the principal components of the Reynolds stress tensor in these directions (i.e. the transverse directions). Similar trends to those found for the turbulent kinetic energy are observed for both quantities, with the peak normal and transverse Reynolds stress occurring at very similar \( x \)-locations at all times. Reese et al. \[192\] observed the Reynolds stress profiles to peak at approximately the same non-dimensional distance from the mixing layer centre (assuming the layer thickness \( h \approx 6W \)) and found that the mean density-velocity correlation \( \langle \rho \rangle \langle u'_i u'_j \rangle \) was the main contributing term. At the latest time, the normal Reynolds stress at the fringes of the spike side is much higher than the corresponding transverse Reynolds stress, indicating that the spikes that escape the main mixing layer are highly anisotropic.

Figure 4.25 shows the spatial distribution of the \( x \)-component of turbulent mass flux. Based on the choice of coordinates, positive fluctuations in density correspond
Figure 4.23 – Spatial distribution of the normal Reynolds stress $R_{11}$ in the $x$-direction. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

Figure 4.24 – Spatial distribution of the average of the transverse Reynolds stresses $R_{22}$ and $R_{33}$ in the $x$-direction. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

to positive fluctuations in velocity (i.e. towards the light gas side) and negative fluctuations in density correspond to velocity fluctuations in the opposite direction, hence $a_1$ is always positive. The profiles of turbulent mass flux are initially less skewed than those of the Reynolds stresses, and at late time the peak turbulent mass flux occurs closer to the centre of the mixing layer. Reese et al. [192] and Mohaghar et al. [188, 189] also observed that the peak in turbulent mass flux approaches the mixing layer centre (prior to reshock), with an initial bias towards the spike side of the layer. Interesting behaviour is observed at $\tau = 0.939$, whereby the largest turbulent mass flux occurs for the $Re_0 = 86$ and $Re_0 = 174$ cases rather than for higher Reynolds
4.6 Reynolds number dependence

Figure 4.25 – Spatial distribution of the $x$-component of turbulent mass flux velocity in the $x$-direction. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

numbers. At later times the profiles for the higher $Re_0$ cases are no longer monotonic, which was also observed in the experiments of Reese et al. [192] and Mohaghar et al. [188, 189] and was found to be due to nonlinear acoustic effects and bubble/spike development. There is also comparatively less turbulent mass flux located at the fringes of the spike side of the layer at late time, where the peaks in turbulent kinetic energy were observed. This indicates that although these ejected spikes are quite energetic, they contain relatively little ejected material.

Figures 4.23 and 4.24 also indicate that there is a significant amount of anisotropy present in the flow, particularly at early times. This can be quantified more precisely using the Reynolds stress anisotropy tensor, defined as

$$b_{ij} = \frac{\langle \rho u_i'^{\prime} u_j'' \rangle}{\langle \rho u_l'^{\prime} u_l'' \rangle} - \frac{1}{3} \delta_{ij}. \tag{4.24}$$

This tensor, specifically the $x$-direction principal component $b_{11}$ for this particular flow, is a measure of anisotropy in the energy-containing scales of the flow field. An analogous tensor may be defined using the principal components of the dissipation rate tensor [42], which gives a measure of the anisotropy in the dissipative scales. This tensor, referred as the dissipation rate anisotropy tensor, is defined as

$$d_{ij} = \frac{\epsilon_{ij}}{\epsilon_{ll}} - \frac{1}{3} \delta_{ij}, \tag{4.25}$$
where $\epsilon_{ij}$ is defined by taking the $ij$ entries of the contraction of the strain-rate tensor and square of the velocity divergence in Equation (4.21). Figure 4.26 shows the evolution in time of $b_{11}$ and $d_{11}$ at the mixing layer centre plane. For both quantities, the anisotropy is greatest during shock passage and rapidly decreases afterwards. A small rise in anisotropy occurs just after the initial drop, prior to the point of minimum mix in $\Theta$ and $\Psi$, and is observed for all cases. From this point in time onwards the level of anisotropy gradually decays, however here there is a noticeable difference in behaviour for different values of $Re_0$, with lower levels of persistent anisotropy (in the Reynolds stresses) observed for higher Reynolds numbers. This is consistent with the notion of increasing levels of turbulence leading to increased isotropisation of the flow field. At the latest time considered, $b_{11} = 0.30$ for $Re_0 = 43$ and 0.091 for $Re_0 = 697$. These values can also be expressed as a ratio of normal to transverse Reynolds stresses, or equivalently turbulent kinetic energy components, using the relation

$$\frac{2R_{11}}{R_{22} + R_{33}} = \frac{2b_{11} + 2/3}{2/3 - b_{11}}. \quad (4.26)$$

Therefore these late-time values of $b_{11}$ are equivalent to there being $3.45 \times$ and $1.47 \times$ more turbulent kinetic energy in the shock perpendicular direction. In terms of the dissipation rate anisotropy, there is a clear trend of isotropy being approached as time progresses and $Re_0$ is increased. This is notably different from results that were presented for this quantity in Livescu and Ristorcelli [42] for homogeneous RTI, where persistent anisotropy at the small scales was observed. This was determined to be due to cancellation of viscous dissipation and nonlinear transfer in the turbulent kinetic energy budget, such that buoyancy production remains important at these scales. For RMI there is no continuous forcing, just impulsive acceleration followed by pure decay, hence it is not surprising that isotropy is approached at these scales.

The spatial distribution of $b_{11}$ and $d_{11}$ in the inhomogeneous direction is plotted in Figures 4.27 and 4.28. At early time ($\tau = 0.187$), just after shock passage, there is significant anisotropy across the mixing layer in the energy-containing scales for all initial Reynolds numbers. The anisotropy in the dissipative scales is less at this time, with the spike side of the layer (1-2 integral widths from the centre plane)
4.6 Reynolds number dependence

Figure 4.26 – Temporal evolution of the $x$-direction principal component of the Reynolds stress and dissipation rate anisotropy tensors at the mixing layer centre plane. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

approaching isotropy for the $Re_0 = 697$ case. For both measures the anisotropy is highest at the very fringes of the spike side of the layer. A similar observation was made by Mohaghar et al. [188] for the $M = 1.55$ experiment, however for the $M = 1.9$ experiment reported in Mohaghar et al. [189] the peak in streamwise anisotropy was found to occur at the fringes of the bubble side of the layer (although significant levels of anisotropy were still present in the spikes). As time progresses, the differences between cases become more pronounced, particularly on the spike side where the higher $Re_0$ cases are substantially less anisotropic. This is because of the isotropisation that occurs due to increasingly turbulent flow. There is also a clear trend of isotropy being approached in the core of the mixing layer with increasing $Re_0$, especially at the dissipative scales. For the higher $Re_0$ cases, the distribution of $b_{11}$ is reasonably symmetric at the bubble and spike sides of the layer by the end of the simulation, however for the lower $Re_0$ cases significantly more anisotropy remains at the spike side.

Finally, the distribution of turbulent kinetic energy is examined in spectral space.
Radial power spectra for each component of the turbulent kinetic energy per unit volume are calculated at the mixing layer centre plane as

$$E_i^{(e)}(k) = \hat{\psi}_i^\dagger \hat{\psi}_i,$$  \hspace{1cm} (4.27)

where $\psi_i = \sqrt{\bar{u}''_i}$, $k = \sqrt{k_y^2 + k_z^2}$ is the radial wavenumber in the $y$-$z$ plane at $x = x_c$, $\hat{\psi}$ denotes the 2D Fourier transform taken over this plane and $(\ldots)^\dagger$ is the complex conjugate of this transform. As isotropy is expected in the homogeneous directions,
4.6 Reynolds number dependence

Figure 4.29 – Power spectra of the average transverse turbulent kinetic energy per unit volume taken at the mixing layer centre plane. Shown are data for $Re_0 = 43$ (dotted black lines), $Re_0 = 86$ (dashed black lines), $Re_0 = 174$ (white circles), $Re_0 = 348$ (grey circles), $Re_0 = 697$ (black circles) and $Re_0 = 1395$ (solid grey lines).

The spectra $E^{(v)}_y$ and $E^{(v)}_z$ are averaged to give a single transverse spectrum $E^{(v)}_{yz}$. This spectrum is shown in Figure 4.29 for each case at three different times, while the spectra of the normal component $E^{(v)}_x$ is shown in Figure 4.30. There is an extremely similar distribution of energy at the large scales across all cases at time $\tau = 0.187$, particularly for the normal component. This is in agreement with the observations made for Figure 4.20 at early time. Substantially more energy is contained at the small scales as $Re_0$ is increased, however this represents a small fraction of the total turbulent kinetic energy in the flow. By the end of the simulation there are much greater differences in the energy contained in the large scales between cases, while the differences at the small scales are even greater than at earlier times.

The $E^{(v)}_{yz}$ spectra at time $\tau = 0.187$ indicate the presence of a power law scaling of the intermediate wavenumbers for the higher $Re_0$ cases, spanning roughly half a decade. The slope is close to a Kolmogorov $k^{-5/3}$ scaling, with the spectra for the $Re_0 = 697$ and $Re_0 = 1395$ cases observed to scale as $k^{-1.78}$ and $k^{-1.65}$ respectively when measured over the range of wavenumbers $8 \leq k \leq 30$. Tritschler et al. [166] also observed a power law scaling in the turbulent kinetic energy spectra from their DNS at early time (shortly after shock passage) over a similar span of wavenumbers with a scaling close to $k^{-5/3}$. A visualisation of the mixing layer at time $\tau = 0.187$ is given in Figure 4.31 in the form of a simulated density Schlieren. The density Schlieren
used is similar to that in Schilling et al. [196] and is defined by

\[ \Phi = \exp \left( -f(Y_1) \frac{|\nabla \rho|}{\max |\nabla \rho|} \right), \tag{4.28} \]

where \( f(Y_1) = 30 \) for \( Y_1 > 0.5 \) and \( 90 \) otherwise. Therefore \( \Phi \) varies between \( 0 \) and \( 1 \), with values closer to 0 indicating stronger density gradients.

Figure 4.31 shows density gradients calculated in the \( x-y \) plane located at \( z = 0 \), with the structure of the mixing layer clearly visible. Although it is already strongly nonlinear at this time, the mixing layer is clearly not turbulent. There are also a lot of acoustic waves present in the density Schlieren, which are generated by the corrugation and subsequent straightening of the shock wave. To investigate the effect these acoustic waves have on the turbulent kinetic energy spectra, the vector field \( \psi_{yz} = \sqrt{\rho} [v''', w''']^t = \sqrt{\rho} u_{yz}''' \) is decomposed into its solenoidal and dilatational components as

\[ \psi_{yz} = \nabla \phi + \nabla \times \xi. \tag{4.29} \]

A further distinction is made between dilatation due to compressibility effects and dilatation due to variable-density mixing in the incompressible limit. This is performed by using the relation in Equation (4.4) to calculate the divergence of \( \psi_{yz} \) in
Figure 4.31 – Simulated density Schlieren in the $x$-$y$ plane located at $z = 0$ for the $\text{Re}_0 = 1395$ case at time $\tau = 0.187$. The major ticks on both axes correspond to a grid spacing of $\Delta x = \Delta y = 1 \text{ m}$.

the incompressible limit as

$$\nabla \cdot \psi_{yz} = \frac{D}{\sqrt{\rho}} \left( \frac{\nabla \rho \cdot \nabla \rho}{\rho} - \nabla^2 \rho \right) + \frac{1}{2\sqrt{\rho}} \nabla \rho \cdot u_{yz}'' = g; \quad (4.30)$$

and further decomposing $\phi$ into $\phi = \zeta + \alpha$ where $\nabla^2 \alpha = g$. In spectral space, the Fourier transform of the total dilatational component $\nabla \phi$ is calculated as

$$\mathcal{F}\{\nabla \phi\} = \frac{k \cdot \hat{\psi}_{yz}}{|k|^2}k, \quad (4.31)$$

which gives the solenoidal component $\mathcal{F}\{\nabla \times \xi\} = \hat{\psi}_{yz} - \mathcal{F}\{\nabla \phi\}$. The compressible component is calculated as

$$\mathcal{F}\{\nabla \zeta\} = \frac{k \cdot \hat{\psi}_{yz} + i\hat{g}}{|k|^2}k. \quad (4.32)$$

These components are used to calculate the solenoidal, total dilatational and compressible turbulent kinetic energy, denoted as $E_{yz}^{(s)}$, $E_{yz}^{(d)}$ and $E_{yz}^{(c)}$ respectively. The
solenoidal, total dilatational and compressible turbulent kinetic energy for the $Re_0 = 697$ case are plotted in Figure 4.32 (results for the $Re_0 = 1395$ case are shown later in Figure 4.45), alongside the total transverse turbulent kinetic energy $E^{(c)}_{yz}$. At time $\tau = 0.187$ it can be seen that there is a significant contribution from the total dilatational component to the overall energy spectrum in the intermediate wavenumber range, which is almost entirely due to compressibility effects. At later times the spectrum is dominated by the solenoidal component at all but the lowest wavenumbers.

This shows that care must be taken when interpreting spectra at early times in RMI flows, as there are significant acoustic effects that are present in the energy-containing scales and to a lesser degree the inertial scales too. These effects are the dominant source of dilatation in the flow, except at the highest wavenumbers, and can significantly alter the shape of the spectrum compared to a fully incompressible flow. In particular, they can lead to the appearance of an inertial range when in fact one does not exist. The procedure detailed in Section 4.7.1 shows how to give more precise estimates of the scaling of any inertial range that may form in the energy spectra, as well as when it is appropriate to do so.

Figure 4.32 – Decomposition of the average transverse turbulent kinetic energy per unit volume (black circles) in the $Re_0 = 697$ case into solenoidal (solid grey lines), total dilatational (dashed black lines) and compressible (dashed grey lines) components.
Scalar field

The variance of the heavy fluid mass fraction is denoted by $\bar{Y}_1^{''2}$, with its corresponding dissipation rate given by

$$\bar{\chi}'' = D \left( \frac{\partial Y''_1}{\partial x_j} \right)^2.$$  \hspace{1cm} (4.33)

Figure 4.33 shows the evolution in time of $\bar{Y}_1^{''2}$ and $\bar{\chi}''$ at the mixing layer centre plane. A maximum in the scalar variance is observed for all cases and occurs at approximately the same time as the minimum in the mixing measures $\Theta$ and $\Psi$. The value of this maximum also increases as $Re_0$ is increased, indeed at all points in time a higher value of $Re_0$ corresponds to a higher scalar variance. A maximum in the scalar dissipation rate is also observed, however the relation between this maximum and the maximum in scalar variance changes as $Re_0$ is varied. For low $Re_0$, the maximum in scalar dissipation rate occurs prior to the maximum in scalar variance, with these cases having the greatest scalar dissipation rate at early time. As $Re_0$ is increased, the location of the maximum scalar dissipation rate shifts later and later in time so that for the higher $Re_0$ cases this maximum occurs later than the maximum scalar variance. In the $Re_0 = 1395$ case, the maximum in $\bar{\chi}''$ occurs slightly later than the maximum in $\bar{\epsilon}''$ (see Figure 4.20), at a time of $\tau = 0.326$. It also appears that a high Reynolds number limit should exist in the value and location of this maximum, although it is not able to be estimated from the current data as no clear pattern of convergence is present.

Figures 4.34 and 4.35 show the spatial distribution of $\bar{Y}_1^{''2}$ and $\bar{\chi}''$ across the layer. Similar trends to those observed for the spatial distribution of turbulent kinetic energy and dissipation rate are also seen here. The peaks in scalar variance and scalar dissipation rate are also biased towards the spike side of the layer, however they occur closer to the mixing layer centre. There is also less variation in the data, particularly for the scalar dissipation rate at later times. Very little scalar variance/dissipation rate is located at the fringes of the spike side of the layer at late time. This is consistent with the earlier observations for turbulent mass flux that very little material is ejected far away from the main layer.
An interesting phenomenon is observed in the scalar dissipation rate data at the latest time considered, with multiple distinct peaks forming across the layer at higher Reynolds numbers. This is not seen in the turbulent kinetic energy or dissipation rate plots. To investigate the cause of these peaks, contours of heavy fluid mass fraction at time $\tau = 4.70$ are plotted in Figure 4.36 for $Re_0 = 86$ and $Re_0 = 697$. Non-dimensional coordinates are used in these plots for ease of comparison with Figure 4.35. Examining the $Re_0 = 697$ mass fraction field in Figure 4.36, it can be seen that the peaks in $\tilde{\chi}''$ at $(x - x_c)/W = 0, 0.75$ and 2 correspond to regions of much sharper gradients than in the $Re_0 = 86$ case. These gradients occur across areas of fluid that has been stirred but not yet molecularly mixed.

Another useful measure of mixing, and an important quantity for modelling, is the density-specific volume correlation, given by

$$b = -\left\langle \rho' \left( \frac{1}{\rho} \right)' \right\rangle. \quad (4.34)$$

The density-specific volume correlation controls the production of turbulent mass flux,
which in turn is responsible for production of turbulent kinetic energy. Furthermore, a value of $b = 0$ corresponds to complete mixing and $b > 0$ indicates an increasingly heterogeneous mixture. Figure 4.37 shows the spatial distribution of $b$ across the layer. In all cases $b$ is decreasing as time progresses, indicating the layer is becoming increasingly mixed. The profiles at early times are also skewed towards the bubble side of the layer, which shows that the two fluids are least mixed in this region. This is consistent with the spatial profiles of $Y_1''$ and $\chi''$ which show that mixing occurs more rapidly on the spike side of the layer at early time. At intermediate times the mixing is more uniformly distributed across the layer at low Reynolds numbers than
4.6 Reynolds number dependence

Figure 4.36 – Contours of mass fraction $Y_1$ in the $x$-$y$ plane located at $z = 0$ at time $\tau = 4.70$. Note that $\bar{x} = x - x_c$.

at high Reynolds numbers, while towards the end of the simulation, the region of least mixed fluid has shifted to the centre of the layer. Weber et al. [186] observed the density-specific volume correlation to be biased towards the bubble side of the layer, although this was less pronounced in the higher Mach number experiment. Reese et al. [192] found the profiles of $b$ to be more symmetric, with a peak close to the mixing layer centre, while Mohaghar et al. [188, 189] observed a bias towards the bubble side, particularly for the higher Mach number case. The profiles of $b$ in the present set of simulations also become increasingly less monotonic as time progresses, which is consistent with similar observations that were made for the turbulent mass flux.

Normalised dissipation rates

To conclude this section, the normalised dissipation rate $C_\epsilon$ and normalised scalar dissipation rate $C_\chi$ are examined to assess the degree to which they are independent
of the Reynolds number of the flow. Following Donzis et al. [197], the normalised dissipation rates are defined as

\[
C_\epsilon = \frac{\langle \epsilon \rangle}{u'\langle \theta' \rangle} \quad \text{(4.35a)}
\]

\[
C_\chi = \frac{\langle \chi \rangle}{L_u \langle \phi' \rangle^{-2} u'} \quad \text{(4.35b)}
\]

Here the dissipation rates \( \tilde{\epsilon}' \) and \( \tilde{\chi}' \), evaluated at the mixing layer centre plane, are used in place of \( \langle \epsilon \rangle \) and \( \langle \chi \rangle \). The RMS velocity \( u' \) is calculated from the turbulent kinetic energy at the mixing layer centre as

\[
u' = \frac{2}{3} \frac{E_k}{k},
\]

while the scalar variance \( \langle \phi'^2 \rangle \) is given by that of the heavy fluid mass fraction \( \tilde{Y}_1'^2 \).

Finally the integral length \( \Lambda \), calculated using the radial power spectrum of turbulent kinetic energy per unit volume (taken at the mixing layer centre), is used for the characteristic length scale \( L_u \). This is calculated as

\[
\Lambda = \frac{3\pi}{4} \int_0^\infty \frac{E^{(v)}}{k} \frac{d\tilde{\epsilon}}{d\tilde{\chi}}.
\]
Note that if the power spectrum of turbulent kinetic energy per unit mass is used instead, the resulting integral length is very similar for this flow [121]. Figure 4.38 shows the evolution in time of both $C_\epsilon$ and $C_\chi$ at the mixing layer centre plane. As the current flow under investigation is unsteady, it is not surprising that both quantities are varying with time, especially while the flow is still in the relatively early stages of development. That both quantities are increasing with time is also in agreement with the fact that the outer-scale Reynolds number decreases with time, as shown in Section 4.7.1. Of interest is whether this variation becomes independent of Reynolds number at any point in time, a necessary (but not sufficient) criterion for a flow to be classified as fully turbulent. Examining Figure 4.38 it can be seen that a high Reynolds number limit is being approached with each increase in $Re_0$, for the timescale considered, but has not yet been reached. The data are slightly closer to collapsing for the normalised scalar dissipation rate; at the latest time considered there is a 22% difference between $Re_0 = 348$ and $Re_0 = 697$ for $C_\chi$ compared to a 32% difference for $C_\epsilon$. For the higher $Re_0$ cases the curves of both $C_\epsilon$ and $C_\chi$ are becoming constant. This behaviour at late time was also observed by Yoffe and McComb [198] for $C_\epsilon$ in simulations of decaying homogeneous isotropic turbulence (HIT), as well as by Zhou and Cabot [39] in DNS of RTI. Note that in the latter study, $C_\epsilon$ is decreasing with time since the Reynolds number is increasing.

The variation with Reynolds number is shown more precisely in Figure 4.39, which plots $C_\epsilon$ and $C_\chi$ against the Taylor microscale Reynolds number $Re_\lambda$ (given by Equation (4.42)) for each simulation at four different times. The resulting curves at each time instant follow the same functional form as those produced by isotropic turbulence [199], but their asymptotic value increases as the simulation progresses. By late time the curves have nearly collapsed, indicating that their high Reynolds number asymptote is also close to becoming independent of time. Nonlinear regression can be used to fit the expected functional form of $C_\epsilon$ and $C_\chi$ to the data and extract this asymptotic value. Following Donzis et al. [197], a function is used of the form

$$f = A(1 + \sqrt{1 + (B / Re_\lambda)^2}).$$

(4.38)
Fitting this function to the $\tau = 4.70$ data gives $A = 0.77$, $B = 27$ for $C_\epsilon$ and $A = 0.33$, $B = 20$ for $C_\chi$. The lower value of $B$ in the curve fit to the normalised scalar dissipation rate data indicates that the asymptotic value of $C_\chi$ is attained faster than that of $C_\epsilon$. This is in agreement with the observations made in section 4.6.3, as well as those for homogeneous passive scalar turbulence at $Sc = 1$ [197]. The asymptotic values of $C_\epsilon$ and $C_\chi$ are equal to $2A$, implying that the high Reynolds number limit of these quantities is 1.54 and 0.66 respectively.

Zhou and Cabot [39] split $C_\epsilon$ into normal and transverse components and found values in the range 0.3-0.4 and 0.5-0.6 respectively at the latest time considered, both of which are substantially lower than the estimate of the high Reynolds number limit given here for RMI. This is analogous to the difference in asymptotic value observed between forced and freely decaying HIT [200]. Yoffe and McComb [198] showed that this difference can be rectified by using values of $C_\epsilon$ at a specified onset time, taken to be either the time of maximum dissipation rate (if it exists) or the time of maximum inertial transfer rate. This onset time typically occurs much earlier than the point at which $C_\epsilon$ becomes time-independent, and estimates of the high Reynolds number limit
using this criterion were virtually identical to those obtained in the forced, stationary case. Using the time of maximum dissipation rate in the $Re_0 = 1395$ case as an approximation of the onset time criterion for all cases, the high Reynolds number limit at this time ($\tau = 0.224$) is found to be 0.28, which is a plausible asymptotic value for the normal component of $C_\epsilon$ in RTI. A more rigorous comparison would involve performing the same split of $C_\epsilon$ (and other key quantities) into normal and transverse components as in Zhou and Cabot [39], which will be performed in future work.

4.7 Assessment of the mixing transition criterion

4.7.1 Mixing transition

All of the results presented in the previous sections have been calculated from simulations which are, in reality, at quite modest Reynolds numbers compared to the actual flows observed in experiments or nature. Given this fact it is natural to ask, particu-
larly for those quantities that do not depend predominantly on the large scales, how representative are these results compared to those that would be obtained at higher Reynolds numbers? In particular, it is useful to know when extrapolating results to higher Reynolds numbers whether the amount of turbulence present in the flow is approaching levels that would be considered fully developed in the sense proposed by Kolmogorov [201]. This is helpful for determining how close the current results are to any high Reynolds number limits that exist for quantities that are known/expected to exhibit universal, asymptotic behaviour once turbulence has fully developed. This section investigates the evolution of various key length scales and Reynolds numbers that are commonly used to characterise turbulent flows. The \( Re_0 = 174 \), \( Re_0 = 348 \) and \( Re_0 = 697 \) cases are used for the analysis in this section, along with the additional \( Re_0 = 1395 \) case that was run up until time \( \tau = 0.939 \).

**Length scales and Reynolds numbers**

In turbulent flows, a number of statistics are used to characterise the typical spatial scales at which energy is generated, transferred and dissipated in the flow. The largest of these is the outer length scale \( \delta \), which for RMI and RTI induced flows is identified as the visual width \( H \) [182], given by

\[
H = x (\langle f_1 \rangle = 0.01) - x (\langle f_1 \rangle = 0.99). \tag{4.39}
\]

This is representative of the largest dynamical motions in the flow. Given the definition of \( H \), an outer-scale Reynolds number may also be defined,

\[
Re_H = \frac{H \dot{H}}{\nu}, \tag{4.40}
\]

where \( \dot{H} \) is the time derivative of the outer length scale and \( \nu \) is the average kinematic viscosity across the layer (from \( x (\langle f_1 \rangle = 0.99) \) to \( x (\langle f_1 \rangle = 0.01) \)). The next largest length scale to consider is the integral length \( \Lambda \), already defined in Equation (4.37), which characterises the distance over which the fluctuating velocity field is correlated. Related to \( \Lambda \) is the Taylor microscale \( \lambda \), which is obtained from the curvature of the
fluctuating velocity autocorrelation, or equivalently from the variance of fluctuating velocity and its derivatives. Although there is no clear physical interpretation for $\lambda$, it may be considered to be representative of scales located in some part of the inertial range for fully developed turbulence. To account for anisotropy, directional Taylor microscales may be defined for direction $i$ as

$$\lambda_i = \left[ \frac{\langle u_i'^2 \rangle}{\langle (\partial u_i''/\partial x_i)^2 \rangle} \right]^{1/2},$$

where plane averages are taken at the mixing layer centre plane. Since isotropy is expected in the transverse directions, a single transverse Taylor microscale is defined as $\lambda_{yz} = (\lambda_y + \lambda_z)/2$ [3]. Similarly, a transverse Taylor-scale Reynolds number is defined at the mixing layer centre plane as $Re_{\lambda_{yz}} = (Re_{\lambda_y} + Re_{\lambda_z})/2$, where

$$Re_{\lambda_i} = \frac{\langle u_i'^2 \rangle}{\langle \nu \rangle \sqrt{\langle (\partial u_i''/\partial x_i)^2 \rangle}}.$$

Finally, the Kolmogorov microscale $\eta$ characterises the scale at which dynamical motions in the flow are strongly affected by viscosity and is given by

$$\eta = \left( \frac{\langle \nu \rangle^3}{\langle \epsilon'' \rangle} \right)^{1/4}.$$

The temporal evolution of the visual width, integral length and Taylor and Kolmogorov microscales is shown in Figure 4.40, from which a clear trend of increasing scale separation with increasing $Re_0$ can be observed. Comparing results across the three simulations, there is only a small difference in the outer scale (mostly at late time), whereas the integral length, Taylor microscale and Kolmogorov microscale all decrease uniformly in time with increasing $Re_0$. In addition to this observed decrease in each of these individual length scales, the relative distance between each length scale for a given $Re_0$ is also increasing. This is consistent with the notion that the mixing layer is becoming progressively more turbulent as the damping of fine-scale motions due to viscosity is reduced, as observed in Figure 4.15. Tritschler et al. [166] also observed a similar increase in the separation of scales but by varying the initial
Mach number $M_0$ of the problem rather than the initial Reynolds number. This is because, for a fixed initial perturbation, decreasing the viscosity $\nu$ and increasing the interface velocity jump $\Delta u$ (through increasing $M_0$) have approximately the same effect on the level of turbulence that subsequently develops. In Section 4.1 it was shown that the highest Mach number case of Tritschler et al. [166] corresponds to an initial Reynolds number $Re_0 = 739$ (ignoring any correction factor for the initial diffuse interface).

Figure 4.41 shows the temporal evolution of the outer-scale and Taylor-scale Reynolds numbers. Dimotakis [51] proposed, based on experimental evidence, that fully developed turbulent flow requires $Re_\delta \geq 1\ldots 2 \times 10^4$, or equivalently $Re_\lambda \geq 100\ldots 140$, in order for it to be sustained. Hence both Reynolds numbers are important parameters for assessing the transition to fully developed turbulence. From Figure 4.41 it can be seen that for the $Re_0 = 697$ case a peak outer-scale Reynolds number of $Re_H = 6.57 \times 10^3$ is obtained shortly after shock passage, before decaying to a value of $Re_H = 926$ at the latest time. It is worth noting that, for a compressible simulation, the visual width $H$ is easily contaminated by small acoustic waves and imperfect boundary conditions. Hence when calculating $Re_H$, which requires the derivative of $H$, these small fluctuations get amplified resulting in a rather noisy signal.

For the Taylor-scale Reynolds number, a peak value of $Re_\lambda = 121$ is observed in the $Re_0 = 697$ case, at an earlier time than the peak in $Re_H$. This is very similar to the
value of $Re_{\lambda}$ that Tritschler et al. [166] observed shortly after shock passage for their $M_0 = 1.5$ case. By the end of the simulation $Re_{\lambda}$ has decayed to a value of 27.6 in the $Re_0 = 913$ case, which is very close to the value of 26 obtained by Tritschler et al. [166] at the end of the estimated period of uncoupled length scales for the $M_0 = 1.5$ case. It is important to note that the drop in Taylor microscale Reynolds number occurs very rapidly across all three cases, at around the same time that the peak in outer-scale Reynolds number occurs. Thus the peak value of $Re_{\lambda}$ is not sustained for very long, but conversely the subsequent decay is quite gradual.

Therefore in the $Re_0 = 697$ case, the requirement of $Re_\delta \geq 1.2 \times 10^4$ for fully developed turbulence is not met at any point of the simulation, while the equivalent requirement that $Re_{\lambda} \geq 100$–$140$ is met only very briefly. In the lower $Re_0$ cases, neither requirements are met at any point. However, given that there is little change in $H$ between simulations, the additional $Re_0 = 1395$ case should achieve $Re_H \geq 10^4$ for at least a small fraction of time. This is confirmed in Figure 4.42, which shows the evolution of both the length scales and Reynolds numbers up until a time of $\tau = 0.939$ for this additional case. Between approximately $\tau = 0.1$ and $\tau = 0.4$ the outer scale Reynolds number for this case is greater than $1 \times 10^4$, while the Taylor-scale Reynolds number is also greater than 100 up until a time of about $\tau = 0.5$. This indicates that there should be significant levels of turbulence within the mixing layer at this time.

A contour plot of the scalar field at $\tau = 0.939$ for this case is given in Figure 4.43 and
shows a relatively wide range of scales have been produced. Pronounced RM bubbles and spikes produced by the initial impulse are also still visible however, suggesting that the flow is not yet fully developed.

**Mixing transition criterion**

A key idea introduced by Dimotakis [51] to quantify the transition to fully developed turbulence, known as the mixing transition, is to refine the bounds on the second similarity hypothesis of Kolmogorov [201]. This may be stated as the requirement that

\[ \eta \ll l \ll \delta, \]  

for some intermediate scale \( l \), in order for the dynamics in the range of scales of size \( l \) to be uncoupled from those of the large scales while also evolving independently of viscous effects. By considering the thickness of a laminar vorticity layer growing over spatial extent \( \delta \) and using an estimate of \( k_V \eta \approx 1/8 \) for the beginning of the dissipation range in various high Reynolds number flows [202], Dimotakis [51] refined...
the criterion given in Equation (4.44) to be
\[ \eta < \lambda_V < l < \lambda_L < \delta. \] (4.45)

Here \( \lambda_V \approx 50\eta \) is referred to as the inner-viscous scale while \( \lambda_L = C_{lam}\lambda \) is the Liepmann–Taylor scale, with \( C_{lam} \approx 5 \) a weakly flow-dependent constant. An important conclusion of this analysis is that by requiring \( \lambda_L/\lambda_V \geq 1 \), the critical outer-scale Reynolds number for fully developed turbulence must be \( Re_\delta \gtrsim 10^4 \), which is in good agreement with the critical values of \( 1\text{--}2 \times 10^4 \) observed in experiments.

Crucially however, this criterion is only strictly valid for stationary flows. For time-dependent flows, Zhou et al. [52] showed that an additional length scale \( \lambda_D \) characterising the growth rate of shear-generated vorticity must be considered. The temporal development of such a scale, referred to as the diffusion layer scale, is given by
\[ \lambda_D = C_{lam}(\nu\bar{t})^{1/2}, \] (4.46)
where \( C_{lam} \) is the Liepmann–Taylor growth constant and \( \bar{t} = t - t_0 \). It is important
to note that Equation (4.46) only describes the late-time behaviour; the virtual time origin has been neglected [203], which implies $\lambda_D = 0$ at $\bar{t} = 0$. This may be rectified by providing an estimate for the virtual time origin, or equivalently the initial momentum thickness of the shear layer. Here the post-shock integral width $W_0^+$ is used as an estimate for the initial momentum thickness, which gives $\lambda_D = C_{lam}(\nu \bar{t})^{1/2} + W_0^+$.

Following Zhou et al. [52], the lower bound of the energy containing scales in an unsteady flow is given by the minimum of $\lambda_D$ and $\lambda_L$, therefore the condition for fully developed turbulence becomes

$$\min(\lambda_L, \lambda_D) > \lambda_V.$$  \hspace{1cm} (4.47)

Qualitatively, the mixing transition criterion for unsteady flows may be expressed as saying that an additional amount of time is required in the presence of a sufficient Reynolds number in order to generate the range of scales that produces a mixing transition. In particular, the hypothesis is that uncoupled fluctuations develop within laminar boundary layers created by viscous diffusion at locations of significant shear. Therefore transition to turbulence occurs once these viscous layers grow for a long enough time such that their extent exceeds the inner-viscous scale [204]. The temporal evolution of the Liepmann–Taylor and inner-viscous scales at the mixing layer centre plane for the four highest $Re_0$ cases is shown in Figure 4.44, along with the diffusion layer length scale for the $Re_0 = 1395$ case. Since $\lambda_D$ is trivial to calculate, it has been plotted up until the end time of $\tau = 4.70$ for the rest of the simulations. The Liepmann–Taylor scale is almost independent of $Re_0$ at early time, due to each case having the same amount of kinetic energy imparted by the shock. Subsequent differences in $\lambda_L$ are due to the fact that as $Re_0$ is increased, the fluctuating velocity gradients increase at a faster rate than the turbulent kinetic energy. Meanwhile for each successive doubling of $Re_0$, the inner-viscous scale is reduced by a factor of close to 1.4 at early time. In the high Reynolds number limit this factor is expected to approach $2^{3/4} \approx 1.7$ according to Equation (4.43), assuming that the dissipation rate becomes independent of $\nu$ (which is halved each time $Re_0$ is doubled).
Figure 4.44 – Liepmann–Taylor (black lines) and inner-viscous (grey lines) length scales vs. time. Results are shown for \( \text{Re}_0 = 174 \) (dotted lines), \( \text{Re}_0 = 348 \) (dashed lines), \( \text{Re}_0 = 697 \) (dash-dotted lines) and \( \text{Re}_0 = 1395 \) (solid lines). Also shown is the estimated diffusion layer length scale (circles) for the \( \text{Re}_0 = 1395 \) case.

Figure 4.44 shows that for \( \text{Re}_0 = 348 \) there exists a period of time from the beginning of the simulation to approximately \( \tau = 2.5 \) during which \( \lambda_L \geq \lambda_V \), due to the observations given above. For the \( \text{Re}_0 = 697 \) case this period has extended to the end time of the simulation and the separation of scales has increased, while for the \( \text{Re}_0 = 1395 \) case the two scales have separated even further. However, it can also be seen that \( \lambda_D < \lambda_V \) for the entirety of the simulation, from which it can be concluded that the turbulence in the flow has not yet passed the mixing transition. Figure 4.45 shows the turbulent kinetic energy spectra for the \( \text{Re}_0 = 1395 \) case at times \( \tau = 0.187 \) and \( \tau = 0.939 \), annotated with the wavenumbers corresponding to the Liepmann–Taylor and inner-viscous length scales. These scales are intended to represent the smallest of the energy containing scales and the largest of the dissipative scales respectively, and qualitatively this appears to be true when examining the spectrum. The slope of the narrow inertial range that is formed between these two scales is also measured; at \( \tau = 0.187 \) the turbulent kinetic energy scales as \( k^{-1.59} \) while at \( \tau = 0.939 \) the scaling
4.7 Assessment of the mixing transition criterion

Figure 4.45 – Decomposition of the average transverse turbulent kinetic energy per unit volume (solid black lines) in the \(Re_0 = 1395\) case into solenoidal (solid grey lines), dilatational (dashed black lines) and compressible (dashed grey lines) components. Also shown are the wavenumbers corresponding to the Liepmann–Taylor (squares) and inner-viscous (diamonds) length scales, as well as the \(k^{−5/3}\) fiducial.

is \(k^{−1.47}\). As was the case for the lower Reynolds number cases, care must be taken when interpreting the early-time spectra, which contain a significant acoustic component that influences the slope. If the slope is measured purely from the solenoidal component, the resulting scaling is \(k^{−0.93}\) instead. At the later time of \(τ = 0.939\), the contribution from the acoustic component to the overall kinetic energy has substantially diminished; the scaling measured from the solenoidal spectra is \(k^{−1.44}\). This scaling of the inertial range is very close to the \(k^{−3/2}\) scaling that has been observed in ILES computations of this case and which is predicted by the theoretical analysis of Zhou [191], rather than the \(k^{−5/3}\) scaling for canonical turbulence. Admittedly the slope has only been measured over a small number of data points, therefore higher Reynolds number cases that have passed the mixing transition would be needed to verify these findings.

While the present set of simulations do not allow for an explicit evaluation of the Reynolds number at which the mixing transition will occur, they can still be used to infer this by considering the variation in length scales with \(Re_λ\) at a given time.
This is shown in Figure 4.46 for a time of \( \tau = 0.939 \), from which it can be seen that the inner-viscous scale is smaller than the Liepmann–Taylor scale for \( Re_\lambda \gtrsim 25 \) and is approaching the diffusion layer length scale as \( Re_\lambda \) is further increased. The ratio of \( \lambda_V/\lambda_D \) is also shown in Figure 4.46 at time \( \tau = 0.939 \). By using a curve fitting procedure similar to the one performed for \( C_\epsilon \) and \( C_\chi \), the Reynolds number at which this ratio equals one can be estimated. The choice of an appropriate functional form is guided by considering how \( \lambda_V \) and \( \lambda_D \) vary with Reynolds number. Both \( \lambda_V \) and \( \lambda_D \) can be related to the outer-scale Reynolds number by

\[
\lambda_V \approx 50\eta \propto Re_\delta^{-3/4},
\]

\[
\lambda_D = C_{lam}(\nu t)^{1/2} \propto Re_\delta^{-1/2},
\]

which can be combined with the relation \( Re_\delta = 3/20Re_\lambda^2 \) for isotropic turbulence to derive that \( \lambda_V/\lambda_D \propto Re_\lambda^{-1/2} \). Thus the curve that is fit to the data is chosen to be of the form

\[
f = \sqrt{\frac{B}{Re_\lambda + C}}. \tag{4.49}
\]

The curve of best fit is also shown in Figure 4.46, for which the parameters are \( B = 364, C = 4.90 \). Therefore the critical Taylor-scale Reynolds number at which \( \lambda_V/\lambda_D = 1 \) is estimated to be \( Re_\lambda = 359 \) at time \( \tau = 0.939 \).

The curve-fitting procedure is repeated for a range of times between \( \tau = 0.187 \) and \( \tau = 4.70 \), with the estimated critical Taylor-scale Reynolds number at each time also plotted in Figure 4.46. It can be seen that at very early times the required Taylor-scale Reynolds number for fully developed turbulence is very high, for example at \( \tau = 0.187 \) it is estimated to be \( Re_\lambda = 1068 \). A caveat must be made here; it is expected that \( Re_\lambda \to \infty \) for some time \( \tau > \tau_0 \) since a finite amount of time is required for the initial energy injected at the driving scales to pass down to smaller and smaller scales via nonlinear transfer and form an inertial range. This process is not explicitly represented in Equation (4.47), therefore the estimated critical Taylor-scale Reynolds number may not be accurate as \( \tau \to \tau_0 \). Nonetheless it will still be extremely large, which is sufficient for the purposes of this study. Of much greater
interest is the behaviour at late time; at the latest time considered it is estimated that flows with $Re_\lambda = 225$ or greater will be fully developed. This is slightly less than the criteria of $Re_\lambda \gtrsim 250$ for fully developed turbulence derived by Lombardini et al. [184], but is significantly greater than the estimate of $35 \leq Re_\lambda \leq 80$ given by Tritschler et al. [166]. The corresponding critical outer-scale Reynolds number is approximately $8 \times$ that of the $Re_0 = 697$ case at this time, which suggests that a case with $Re_0 = 5576$ would begin to pass the mixing transition. Such a case is also likely currently achievable using a substantial portion of the computational resources on one of the world’s top supercomputers. The critical Taylor-scale Reynolds number curve also has an approximate $t^{-1}$ dependence (based on a curve fit to the data) and asymptotically approaches a value of $Re_\lambda = 174$ as $t \to \infty$, which is reasonably close to the $Re_\lambda \geq 100–140$ requirement for stationary flows. Furthermore, as was observed in Figure 4.41, the outer-scale and Taylor-scale Reynolds numbers also decrease in time, beyond some initial peak shortly after shock passage, implying that the mixing transition criterion may only be satisfied temporarily. Such a phenomenon does not occur in turbulence induced by the Rayleigh–Taylor instability, for which the Reynolds number increases as $Re_H \propto t^3$, and reflects a fundamental difficulty in attaining sufficiently high Reynolds numbers for universal behaviour to be observed in experiments or simulations of the Richtmyer–Meshkov instability.

An additional point to note is that flows just satisfying the time-dependent mixing transition criterion, such as the projected $Re_0 = 5576$ case, will not necessarily capture all of the physics of the energy-containing scales that are present at higher Reynolds numbers as there is still some interaction with the dissipation range. Zhou [53] showed that in order for there to be complete decoupling of the energy-containing and dissipation scales the mode with wavenumber $k_Z = 2k_L$, where $k_L$ is the wavenumber of the Liepmann–Taylor scale, must lie within the inertial range. This argument is then used to define the minimum state Reynolds number as the lowest Reynolds number for which the dynamics of the energy-containing scales are completely independent of the dissipation mechanism in the flow and which requires that $k_v = k_Z = 2k_L$ (where $k_v$ is the wavenumber of the inner-viscous scale). This definition, along with the defi-
4.8 Conclusions

This chapter has investigated the effects of initial Reynolds number $Re_0$ on a turbulent mixing layer induced by RMI evolving from narrowband initial conditions using a series of direct numerical simulations. Grid converged solutions were clearly demonstrated by considering the temporal evolution of enstrophy and scalar dissipation rate as well as their power spectra. Satisfactory convergence in these quantities was also shown to be consistent with the Kolmogorov scale being resolved on the finest grid for the entire duration of the simulation.
By comparing the results of the \( Re_0 = 457 \) case with those of an implicit large eddy simulation of the same initial condition a detailed account of the early time transitional behaviour, and insight into the high Reynolds number limit, can be made as follows. After compression of the interface by the shock wave at \( \tau \approx 0.01 \), a minimum in the integral width \( W \) and maximum in the mixing fractions \( \Theta \) and \( \Xi \) occurs at \( \tau = 0.0300 \) corresponding to the point of peak compression. The anisotropy of the layer, as measured by the ratios of components of turbulent kinetic energy as well as directional Taylor microscale Reynolds numbers, has an initial peak at the time of compression before declining and then peaking again at a time of \( \tau = 0.1845 \) in both the DNS and ILES. This is followed shortly thereafter by a minimum in \( \Theta \) and \( \Xi \), at time \( \tau = 0.2126 \) in the DNS and at \( \tau = 0.2268 \) and \( \tau = 0.2274 \) in the ILES. The enstrophy in the DNS decays monotonically throughout the simulation after the shock interaction, while the scalar dissipation rate exhibits a maximum at \( \tau = 0.4931 \), beyond which it also decays monotonically. The maximum in scalar dissipation rate is indicative of the time when energy coupling to the highest modes has occurred and the flow is becoming damped at these scales. Late time decay rates for turbulent kinetic energy, enstrophy and scalar dissipation rate were calculated, with the TKE found to be decaying at a faster rate at late time in the DNS than in the ILES. Examination of the power spectra at various points in time showed that this increased decay is confined to the high wavenumber portion of the spectrum, at low wavenumbers there is good agreement between the DNS and ILES results (prior to the start of the inertial range in the ILES spectrum).

After the initial shock passage the turbulence in the layer is freely decaying, with the outer-scale Reynolds number obtaining its maximum value at very early time, after which it continually decreases for each of the simulations. An analysis of various mixing measures showed that there was little variation in the integral width for the range of \( Re_0 \) considered here, while lower \( Re_0 \) cases have more mixed mass at early times. At later times the amount of mixed mass in these cases is overtaken by that of higher \( Re_0 \) cases due to a larger interfacial surface area and steeper gradients. A clear trend of increasing growth rate exponent \( \theta \) was also observed with increasing
4.8 Conclusions

$Re_0$, although the overall variation was only 25%. By decomposing the integral width into separate bubble and spike widths it was shown that the ratio of these two widths approaches a constant value at late time, implying that they eventually both grow with equal exponent $\theta$. Both the molecular mixing fraction and the normalised mixed mass showed a dependence on $Re_0$, in particular the point of minimum mix which was estimated to be $\Theta_{\min} = 0.10$ and $\Psi_{\min} = 0.098$. The late time asymptotic value of these two quantities also varied with $Re_0$, with the data observed to be approaching a high Reynolds number limit of 0.765 and 0.772 respectively.

A detailed analysis of the Reynolds number dependence of various statistics of the velocity and scalar fields was also presented. The decay rates of turbulent kinetic energy and its dissipation rate were shown to decrease with increasing $Re_0$. The spatial distribution of both of these quantities was also shown to be biased towards the spike side of the layer. Significant levels of anisotropy were observed in the Reynolds stresses, with the lower $Re_0$ cases having the greatest degree of anisotropy. Less anisotropy were observed at the dissipative scales, as measured by the dissipation rate anisotropy tensor, with the higher $Re_0$ cases approaching isotropy in this measure as the simulation progressed. For both measures the anisotropy was found to be highest at the very fringes of the spike side of the layer, where some energetic spikes had escaped the main layer. An analysis of the turbulent kinetic energy spectra showed that the distribution of energy at the largest scales was extremely similar across all cases, while substantially more energy is contained in the small scales as $Re_0$ is increased. The spectra were also decomposed into solenoidal, total dilatational and purely compressible components, which showed that at early time the energy at low to intermediate wavenumbers is dominated by compressible modes. At later times the solenoidal component begins to dominate the overall energy spectrum, indicating that the mixing layer is approaching incompressible flow.

For the scalar variance and scalar dissipation rate, similar trends to the turbulent kinetic energy and dissipation rate were observed. There was found to be less variation with $Re_0$ however, particularly for the scalar dissipation rate at later times. The spatial distribution of density-specific volume correlation was also analysed, showing
that the two fluids are less mixed on the bubble side of the layer. This is consistent with the observation that mixing occurs more rapidly on the spike side of the layer, particularly at early times. The Reynolds number dependence of the normalised dissipation rate $C_\epsilon$ and scalar dissipation rate $C_\chi$ was assessed, showing that a high Reynolds number limit is being approached. At early times the asymptotic values of $C_\epsilon$ and $C_\chi$ vs. Reynolds number vary significantly as the flow continues to develop, while at late times the curves have collapsed. Fitting an appropriate functional form to the data showed that the asymptotic value of $C_\chi$ is attained faster than that of $C_\epsilon$, in agreement with similar observations made for homogeneous passive scalar turbulence at $Sc = 1$.

Finally, an evaluation of the mixing transition was performed, showing that although the highest $Re_0$ case satisfies the criteria of Dimotakis [51] for fully developed stationary turbulence, it does not meet the additional requirement of Zhou et al. [52] for unsteady flows and therefore cannot be considered fully turbulent. By considering the ratio between the inner-viscous and diffusion layer length scales, the critical Reynolds number at which the mixing transition criterion is satisfied was able to be estimated, which translates to an initial Reynolds number around $4 \times$ larger than the current highest $Re_0$ case. This case also exhibited a narrow inertial range in the turbulent kinetic energy spectra (with a scaling close to $k^{-3/2}$), which shows that such an observation is insufficient for assessing whether the turbulence is fully developed.

As was mentioned in the introduction, if the layer width grows as $\sim t^\theta$ then the outer-scale Reynolds number grows/decays as $\sim t^{2\theta-1}$. For narrowband initial conditions this means that the Reynolds number decreases in time, however if $\theta > 0.5$ then the Reynolds number will increase in time. For broadband perturbations with an initial power spectrum $P(k) \propto k^m$ and $m < -1$, the results of Chapter 5 show that this will indeed be the case, at least while the layer is growing in the self-similar regime. These perturbations are also more representative of RMI flows encountered in reality, thus the remaining chapters will present ILES and DNS of RMI-induced turbulence evolving from broadband initial conditions. Another area for extending the current work is to evaluate the Reynolds number dependence of various quantities.
such as spectra, length scales and normalised dissipation rates at different planes in
the mixing layer. Presently these are only evaluated at the mixing layer centre plane,
however the spatial distributions of many of the quantities analysed in this paper
show that this is not necessarily the location of peak turbulent activity. Finally, it
would be useful to extend the current set of simulations to include a much larger
parameter sweep of different Schmidt, Atwood and Mach numbers. This would allow
for interaction effects between different parameters to be captured that have not been
explored in the present study.
Chapter 5

Large Eddy Simulation of the Broadband Richtmyer–Meshkov Instability

5.1 Introduction

Once the Richtmyer–Meshkov instability is initiated and has passed the initial linear growth regime, it will evolve into a nonlinear state characterised by mushroom shaped bubbles (lighter fluid penetrating into heavier fluid) and spikes (heavier fluid penetrating into lighter fluid). A key area of interest in the study of RMI is the degree to which memory of the initial conditions is retained and how this affects the statistics of the flow at late time. Thornber et al. [31] investigated RMI induced on two different, multimode initial conditions using ILES. The first of these was a narrowband perturbation, consisting of a narrow range of high wavenumber modes $k_{\text{min}}$ to $k_{\text{max}}$ where $k_{\text{min}} = k_{\text{max}}/2$, whose amplitudes are given by a constant power spectrum. This case was designed to give growth purely due to mode coupling/backscatter of the energetic scales, representing a lower bound on the expected growth rate due to pure RMI. Variations of this narrowband initial condition have appeared in subsequent studies [151, 205, 121], most notably the $\theta$-group collaboration [30], which is the same initial
condition used for the simulations presented in Chapter 4. In the turbulent regime, the width of the mixing layer grows as \( h \propto t^\theta \). For narrowband initial conditions, experiments and simulations indicate \( 0.25 < \theta < 0.33 \) [47, 193, 31, 30], while a theoretical growth rate exponent of \( \theta = 1/3 \) is possible once a sufficient number of mode coupling generations have occurred [46].

The second initial condition used in Thornber et al. [31] was a broadband perturbation, consisting of a wide range of modes \((k_{\text{max}}/k_{\text{min}} \gg 2)\) whose amplitudes satisfy a power spectrum \( P(k) \propto k^{-2} \). If the initial conditions are forgotten then the late time statistics for this case should be the same as for the narrowband case. However, as proposed by Youngs [44], it is possible that the linear growth of the largest wavelength modes is faster than that due to mode coupling, thus dictating the overall growth rate of the mixing layer. This was found to indeed be the case in the broadband simulations conducted by Thornber et al. [31], which obtained a growth rate exponent of up to \( \theta = 0.62 \) at the highest grid resolution considered, which is tending towards the theoretical prediction of \( \theta = 2/3 \) given by just-saturated mode analysis [44]. This initial condition has also been studied after reshock [83], where it was found to give a higher post-reshock growth rate than the narrowband case, as well as in two dimensions [152]. Simulations of turbulent mixing due to RMI in spherical implosions have also been performed using a \( k^{-2} \) broadband perturbation [206, 207], which is considered representative of the measured surface roughness power spectra of an ICF capsule [208].

Multiple experiments have also been performed that contain broadband initial perturbations. Weber et al. [209] performed shock tube experiments using helium (seeded with acetone) and argon. A broadband initial condition was created by first forming a stagnation plane between the two gases and then injecting streams of argon and helium above and below this stagnation plane. These two streams interact due to buoyancy and shear to generate a statistically steady and repeatable broadband initial perturbation. Due to this method of perturbing the interface, some non-linearity is already present prior to the arrival of the shock wave. The initial condition was characterised as consisting of three distinct spectral ranges that scale as \( k^{-1} \), \( k^{-3} \) and
$k^{-5}$ respectively. The ratio of largest to smallest initial wavelengths in the perturbation was approximately 100. The width of the layer, based on average mole fraction profiles, was found to have a growth rate exponent of $\theta = 0.58$. This is considerably higher than that due to high wavenumber narrowband perturbations, indicating that the overall growth of the mixing layer is being dominated by long wavelength modes that have a lower but more persistent growth rate. Subsequent experiments using the same facility gave $\theta = 0.43 \pm 0.01$ when data from two different shock Mach numbers was used [186], while a value of $\theta = 0.34 \pm 0.01$ was obtained when the mole fraction field was adjusted to remove large-scale structures from the mixing layer prior to spanwise averaging [192].

Mohaghar et al. [188] performed shock tube experiments between nitrogen (seeded with acetone) and carbon dioxide using two different initial conditions. The first of these was a predominantly single-mode interface, created by inclining the shock tube by $20^\circ$, while the second was a broadband interface that is created by injecting heavy/light gas above/below the stagnation plane between the two gases, which is inclined at $20^\circ$ as in the single-mode case. In both cases the inclination results in an amplitude to wavelength ratio of 0.088 for the large-scale single mode. As with the experiments in Weber et al. [209], it is expected that some non-linearity is present in the broadband initial perturbation due to how it is formed. Characterisation of the broadband initial condition was performed by computing the density power spectra, showing that the perturbation consisted of three distinct ranges that follow $k^{-0.1}$, $k^{-0.8}$ and $k^{-1.8}$ scalings. For this initial condition, the ratio of largest to smallest wavelengths was 67. The experimental dataset was extended in Mohaghar et al. [189] to include data at a higher shock Mach number. Comparisons between the single mode and broadband cases showed that although the layer width $h$ is very similar, the mixed-mass thickness $\delta$ is substantially larger prior to reshock, indicating greater mixing due to the presence of more fine-scale structure. Finally, Krivets et al. [6] performed shock tube experiments using air and sulphur hexafluoride, with smoke used to seed either the light or heavy gas. The initial perturbation was created by oscillating the shock tube with loudspeakers to produce Faraday waves at the interface
between the two gases. Both the bubble and spike integral widths $W_b$ and $W_s$ were obtained, with the corresponding growth rate exponents varying over a wide range from $\theta = 0.18$ to $\theta = 0.57$. This suggests the possibility that low amplitude, long wavelength modes are present in the initial perturbation, which dominate the growth rate at later times. The results were reported for a small number of experiments however ($n = 5$), hence there may be significant sample size effects in the data.

This evidence of enhanced growth rates in experiments where broadband perturbations are present, as well as the simulations and theory given in Youngs [44] and Thornber et al. [31], motivates a thorough study of RMI evolving from well-characterised broadband initial conditions. The present work generalises the $k^{-2}$ broadband perturbation used in Thornber et al. [31] to a class of perturbations with power spectra $P(k) \propto k^m$ for integer exponents $m$. Three different values of $m$ are considered, $m = -1$, $m = -2$ and $m = -3$, which represent idealised versions of the majority of initial conditions found in experiments and applications. A computational approach similar to that in Thornber et al. [31] is used to study these perturbations, where the ratio $k_{max}/k_{min}$, referred to as the bandwidth of the perturbation, increases as the grid resolution is increased. The aim of the set of simulations reported here is to validate theoretical predictions of various quantities in the self-similar regime for varying $m$ [44, 31], as well as examine how these are affected by finite bandwidth. The results represent a significant extension of these previous studies, for example the highest bandwidth $m = -2$ case is very similar to the one presented in Thornber et al. [31] but was run to $10 \times$ later dimensionless time.

This chapter is structured as follows; Section 5.2 gives specifics of the broadband initial perturbations, along with the theoretical predictions for the growth rate given by just-saturated mode analysis. Section 5.3 presents a discussion of the results for the nine simulations performed, while conclusions are given in Section 5.4.

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The work presented in this chapter has been published in Groom, M., Thornber, B. (2020). The influence of initial perturbation power spectra on the growth of a turbulent mixing layer induced by Richtmyer–Meshkov instability. *Physica D: Nonlinear Phenomena*, 407, 132463.
5.2 Problem description

5.2.1 Computational approach

The governing equations, specifically the four-equation model, presented in Chapter 3 are solved using the University of Sydney code Flamenco, which is described in Section 3.2. In this chapter, ILES is used to explore the high Reynolds number limit of key integral quantities in the regime of self-similar growth. In the ILES approach, it is assumed that the growth of the integral length scales is independent of the exact dissipation mechanism and that the species are intimately mixed within each computational cell, such that scalar dissipation rates are well represented and are insensitive to the actual values of viscosity and diffusivity. The first of these assumptions is addressed in the design of the problem such that the integral length scales are large with respect to the grid scale, while the second assumption is considered to be valid provided the Reynolds number is sufficiently high. Since the aim is to explore the high Reynolds number limit, the simulations are nominally inviscid and therefore all of the right hand side terms in Equation (3.1) are zero. However, numerical dissipation in the spatial reconstruction and Riemann solver still acts to remove kinetic energy from the flow, which is used in lieu of an explicit subgrid model. For more details on the use of ILES for shock-induced turbulent mixing see Grinstein et al. [136], as well as Thornber et al. [105] for a quantification of the numerical dissipation.

5.2.2 Initial conditions

The initial conditions used in the present simulations closely follow those used in previous fundamental studies of RMI turbulence, for example the $\theta$-group collaboration [30]. The setup consists of two quiescent gases separated by a perturbed material interface and with a shock wave initialised in the heavy gas travelling towards the interface. The interface is initially diffuse, with the profile given by an error function with characteristic initial thickness $\delta$. The volume fractions $f_1$ and $f_2 = 1 - f_1$ of the
two gases are computed as

\[ f_1(x, y, z) = \frac{1}{2} \text{erfc} \left( \frac{\sqrt{\pi} |x - S(y, z)|}{\delta} \right), \]  \hspace{1cm} (5.1)

where \( S(y, z) = x_0 + A(y, z) \) with \( A(y, z) \) the amplitude perturbation of the interface and \( x_0 \) the mean position. A Cartesian domain of dimensions \( x \times y \times z = L_x \times L \times L \) where \( L = 2\pi \) m is used for all simulations presented here. The extent of the domain in the \( x \)-direction, \( L_x \), varies depending on the cross-sectional resolution and will be detailed in Section 5.2.3. Periodic boundary conditions are used in the \( y \)- and \( z \)-directions, while in the \( x \)-direction outflow boundary conditions are imposed very far away from the test section so as to minimise spurious reflections from outgoing waves impacting the flow field. The initial mean positions of the shock wave and the interface are \( x_s = 3.0 \) m and \( x_0 = 3.5 \) m respectively and the initial pressure of both (unshocked) fluids is \( p = 1.0 \times 10^5 \) Pa. The shock Mach number is \( M = 1.8439 \), equivalent to a four-fold pressure increase, the initial densities of the heavy and light fluids are \( \rho_1 = 3.0 \text{ kg/m}^3 \) and \( \rho_2 = 1.0 \text{ kg/m}^3 \) and the post-shock densities are \( \rho_1^+ = 5.22 \text{ kg/m}^3 \) and \( \rho_2^+ = 1.80 \text{ kg/m}^3 \) respectively. This gives a post-shock Atwood number of \( A^+ = 0.487 \). The variation in \( \rho \) and \( Y_1 \) across the interface is computed using \( \rho = \rho_1 f_1 + \rho_2 (1 - f_1) \) and \( \rho Y_1 = \rho_1 f_1 \) with \( f_1 \) given by Equation (5.1). The evolution of the interface is solved in the post-shock frame of reference by applying a factor of \( \Delta u = -291.575 \text{ m/s} \) to the initial velocities of the shocked and unshocked fluids.

**Surface perturbation**

The surface perturbation of the material interface is defined in Fourier space as a power spectrum of the form

\[ P(k) = \begin{cases} Ck^m, & k_{\text{min}} < k < k_{\text{max}}, \\ 0, & \text{otherwise}, \end{cases} \]  \hspace{1cm} (5.2)
where \( k = \sqrt{k_y^2 + k_z^2} \) is the radial wavenumber of the perturbation and \( m \leq 0 \). This form is chosen as it allows for a theoretical analysis of the perturbation growth, along the lines of [44, 31]. In the majority of previous studies using initial conditions of this form, a narrowband surface perturbation was used, with \( k_{\text{min}} = k_{\text{max}}/2 \) and \( m = 0 \). In the present study, \( m = -1, -2 \) and \( -3 \) and the bandwidth \( R = k_{\text{max}}/k_{\text{min}} \) of the initial perturbation is sought to be maximised. For \( R > 2 \), the perturbation defined by \( P(k) \) is referred to as a broadband perturbation. The particular choice of \( k_{\text{min}} \) and \( k_{\text{max}} \) (and therefore \( R \)) will be detailed in Section 5.2.3 below. This ensures that the time during which the layer grows self-similarly is maximised, while also ensuring that the highest mode is sufficiently resolved by the numerics. Prior to the saturation of the lowest mode, the layer should also be free from the effects of finite domain size.

The derivation of the surface perturbation for each value of the exponent \( m \) will now be given. For a power spectrum of the form given in Equation (5.2), taking the inverse Fourier transform and simplifying using the Euler formula gives the perturbation amplitude in real space,

\[
A(y, z) = \sum_{p,q=0}^{N_k} \left[ a_{pq} \cos(p k_0 y) \cos(q k_0 z) + b_{pq} \cos(p k_0 y) \sin(q k_0 z) \\
+ c_{pq} \sin(p k_0 y) \cos(q k_0 z) + d_{pq} \sin(p k_0 y) \sin(q k_0 z) \right],
\]

(5.3)

where \( k_0 = 2\pi/L \) and \( N_k = k_{\text{max}}/k_0 \). The coefficients \( a_{pq} \ldots d_{pq} \) are chosen as (using \( a_{pq} \) as an example)

\[
a_{pq} = R S(p) S(q) \sigma_{pq},
\]

(5.4)

where \( S(p) = 1/\sqrt{2} \) if \( p = 0 \) and 1 otherwise and \( R \) is a random number taken from a Gaussian distribution. Unlike previous broadband simulations in [31, 83], the random numbers are generated using a Mersenne Twister algorithm, which is deterministic. This allows for the same random numbers to be used across multiple perturbations, which is necessary for grid convergence studies to be performed.
The standard deviation of modal amplitudes at radial wavenumber $k$, $\sigma_{pq}$, is given by

$$\sigma_{pq}^2 = \frac{1}{4} \left( a_{pq}^2 + b_{pq}^2 + c_{pq}^2 + d_{pq}^2 \right) = \frac{1}{2\pi} \frac{P(k_{pq})}{k_{pq}} \Delta k_y \Delta k_z, \quad (5.5)$$

where $\Delta k_y = \Delta k_z = 2\pi/L$, while the total standard deviation is given by

$$\sigma^2 = \int_0^\infty P(k) \, dk = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{2\pi} \frac{P(k)}{k} \, dk_y \, dk_z. \quad (5.6)$$

For each case, the total standard deviation is

$$\sigma = \begin{cases} \sqrt{C \log(R)}, & m = -1, \\ \sqrt{\frac{C k_m^{m+1}}{m + 1} \left( 1 - \frac{1}{R^{m+1}} \right)}, & m < -1. \end{cases} \quad (5.7)$$

The mean standard deviation of each mode can be related to the total standard deviation of the perturbation by

$$\sigma_{pq} = \begin{cases} \frac{2\pi \sigma}{L \sqrt{2\pi \log(R)}} \sqrt{k_{pq}^{m-1}}, & m = -1, \\ \frac{2\pi \sigma}{L} \sqrt{\frac{m + 1}{2\pi k_{pq}^{m+1} (1 - \frac{1}{R^{m+1}})}} \sqrt{k_{pq}^{m-1}}, & m < -1. \end{cases} \quad (5.8)$$

The derivation is completed by defining the constant of proportionality $C$ in Equation (5.2). Two approaches will be discussed; ensuring that all modes are initially linear and fixing the total standard deviation of the perturbation so that it is the same for all values of $m$.

**Ensuring linearity**

It is often desirable in studies of RMI that the initial amplitudes of modes in the perturbation are small, so that linear theory accurately describes their early-time evolution. Mode $k$ is assumed to be linear (i.e. growing at the rate given by linear...
theory) if \( ka_k = 1/2 \), where

\[
\left( \frac{a_k}{2} \right)^2 = \int_{k/2}^{k} P(k') \, dk'
\]  

(5.9)

is the power in a band around wavenumber \( k \) [31]. This gives the following expressions for the amplitude in the band around wavenumber \( k \):

\[
a_k = \begin{cases} 
2 \sqrt{C \log(2)}, & m = -1, \\
2 \sqrt{C k^{m+1}} \frac{(1 - 1/2^{m+1})}{m + 1}, & m < -1,
\end{cases}
\]  

(5.10)

By specifying that the highest wavenumber \( k_{\text{max}} \) must be linear, that is \( k_{\text{max}} a_{k_{\text{max}}} = 1/2 \), then the coefficient \( C \) is determined to be

\[
C = \begin{cases} 
\frac{1}{16 \log(2) k_{\text{max}}^2}, & m = -1, \\
\frac{m + 1}{16 k_{\text{max}}^{m+3} (1 - 1/2^{m+1})}, & m < -1.
\end{cases}
\]  

(5.11)

Therefore the standard deviation can be written as

\[
\sigma = \begin{cases} 
\frac{\lambda_{\text{min}}}{8\pi} \sqrt{\log(R) \log(2)}, & m = -1, \\
\frac{\lambda_{\text{min}}}{8\pi} \sqrt{\frac{1 - 1/R^{m+1}}{1 - 1/2^{m+1}}}, & m < -1,
\end{cases}
\]  

(5.12)

while the mean standard deviation of each mode that ensures linearity is determined to be

\[
\sigma_{pq} = \begin{cases} 
\frac{\lambda_{\text{min}}}{4L \sqrt{2\pi \log(2)}} \sqrt{k_{pq}^{m-1}}, & m = -1, \\
1 \frac{4L \sqrt{(2\pi)^{m+2} (1 - 1/2^{m+1})} \sqrt{k_{pq}^{m-1}}}{\sqrt{m+3} (m + 1)} & m < -1.
\end{cases}
\]  

(5.13)

The description of the perturbation is completed by a suitable choice of \( \lambda_{\text{min}} \), which is described in Section 5.2.3.
5.2 Problem description

Fixed standard deviation

An alternative approach is to keep the total standard deviation constant across all perturbations of the same bandwidth, so that changing the exponent $m$ can be thought of as changing the relative distribution of mode amplitudes. If $\sigma$ is held constant for a given bandwidth $R$, then $C$ is determined by Equation (5.7) and $\sigma_{pq}$ by Equation (5.8). Writing the total standard deviation as $\sigma = \alpha \lambda_{\text{min}}$, the only remaining choice to make is a suitable value of the constant $\alpha$ (assuming $\lambda_{\text{min}}$ has already been chosen). Here there is a trade-off that must be made between ensuring that the highest modes remain linear for the $m = -1$ perturbation while also retaining a large enough overall amplitude in the $m = -3$ perturbation such that it is computationally efficient to simulate. The standard deviation that ensures linearity of all modes for $R = 128$ (the highest bandwidth considered here) is $\sigma = 0.105 \lambda_{\text{min}}, 0.448 \lambda_{\text{min}}$ and $2.94 \lambda_{\text{min}}$ for $m = -1, -2$ and $-3$ respectively. Therefore in this study, $\alpha$ is chosen to be 0.2 for all values of $m$. This choice results in $k_{\text{max}} a_{k_{\text{max}}} = 0.950, 0.223$ and $1.32 \times 10^{-4}$, which means that the highest modes in the $m = -1$ perturbation are initially nonlinear (modes greater than $k = 135$) while for the $m = -3$ perturbation a longer physical time is required to simulate to the same non-dimensional time. A full investigation into the advantages and disadvantages of this trade-off is outside the scope of the present study and will be performed in future work.

Figure 5.1 shows a contour flood of the heavy fluid volume fraction for the three different initial conditions at a bandwidth of $R = 32$, while Figure 5.2 shows the theoretical surface power spectrum at this bandwidth as well as the initial density variance spectrum for the particular realisation used in this study. The different distribution of mode amplitudes for the same overall standard deviation can be discerned from both of these figures. Also shown in Figure 5.2 is the line separating linear and nonlinear modes so that the proportion of modes that are nonlinear in the $m = -1$ spectrum can be observed. For this particular bandwidth there is also a small fraction of modes in the $m = -2$ spectrum that are slightly nonlinear, however for higher bandwidths all modes in the $m = -2$ spectrum are linear.
5.2 Problem description

\[ (a) \ m = -1. \]

\[ (b) \ m = -2. \]

\[ (c) \ m = -3. \]

**Figure 5.1** – Initial conditions for a bandwidth of \( R = 32 \), shown using contours of heavy fluid volume fraction \( f_1 \). The major ticks on both axes correspond to a grid spacing of \( \Delta x = 0.5 \text{ m} \).

5.2.3 Numerical simulations and just-saturated mode analysis

During the early-time evolution of a broadband perturbation, shorter wavelengths will initially grow faster than longer wavelengths (except for \( m = -3 \) where they all grow at the same rate), since the initial growth rate of a single mode \( k \) is given by Richtmyer’s formula

\[ \dot{a}_k = a_k^+ A^+ \Delta u k, \quad (5.14) \]

where \( a_k^+ = (1 - \Delta u / U_s) a_k^- \) is the post-shock amplitude and \( a_k^- \) is the pre-shock amplitude, given by Equation (5.10). In Equation (5.14) \( \Delta u \) is the change in velocity induced by the shock wave and \( U_s \) is the incident velocity of the shock wave. Note that other expressions are available for \( \dot{a}_k \), such as the Vandemboomgaard formula [210], as there are certain cases where the initial linear growth rate is not well described by Equation (5.14). As the amplitude of mode \( k \) grows, its growth rate will eventually saturate due to nonlinear effects. If the linear growth rate of longer wavelength modes
Figure 5.2 – Surface perturbation power spectrum and density variance spectrum at time $t = 0$ for the $R = 32$ bandwidth cases. Also shown is the power spectrum that bisects linear and nonlinear modes for this particular bandwidth (black dashed line).

that are yet to saturate is faster than growth due to mode coupling in the range $k/2$ to $k$, then these modes will begin to dominate the overall growth rate of the layer and the growth rate exponent $\theta$ will be dependent on the initial conditions [31]. If the bandwidth of the initial perturbation is large (i.e. $R \gg 2$) then this regime of self-similar growth can extend for a significant amount of time, until the longest wavelength saturates.

In just-saturated mode analysis, the growth rate of the mixing layer at time $t$ is assumed to be dominated by the growth rate of the mode that is saturating at time $t$. The model was first proposed by Dimonte et al. [211] and was extended to include the effects of initial conditions by Youngs [44]. For a broadband perturbation of the form given in Equation (4.1), the linear growth rate in a band around mode $k$ is given by

$$\dot{\alpha}_k = B \sqrt{CA} \Delta u k^{\frac{m+3}{2}},$$

\(5.15\)
where $C$ is determined as described in Section 5.2.2 and $B$ is given by

$$B = \begin{cases} 
(1 - \Delta u/U_s)2\sqrt{\log(2)}, & m = -1, \\
(1 - \Delta u/U_s)2, & m = -2, \\
(1 - \Delta u/U_s)2\sqrt{3/2}, & m = -3.
\end{cases}$$

(5.16)

Following Thornber et al. [31], a structure of size $1/k$ becomes nonlinear at time $t = 1/(k\lambda_k)$. Assuming that the growth of $W$ is dominated by the growth of mode $k$ at time $t$ gives

$$W \propto \frac{1}{k} = \left(B\sqrt{CA^+}\Delta u t\right)^{\frac{2}{m+5}},$$

(5.17)

and therefore $W \propto t^\theta$ where $\theta = 2/(m + 5)$.

The duration of time for which Equation (5.17) is valid can be estimated by estimating the time at which the smallest and largest modes saturate. Assuming that mode $k$ saturates when $a_k = 0.1\lambda_k$, the saturation time can be estimated as

$$t_{sat} = \frac{0.1\lambda_k - a_k^+}{\dot{a}_k},$$

(5.18)

where the linear growth rate $\dot{a}_k$ is given by Equation (5.14). An additional consideration must be made for the initial inversion that occurs due to the heavy–light configuration. The time for this inversion to occur may be estimated as

$$t_{inv} = \frac{2a_k^+}{\dot{a}_k} = \frac{2}{A^+\Delta u k}.$$  

(5.19)

Therefore the time to saturation of the longest wavelength in the initial perturbation may be estimated as $t_{sat}(k_{min}) + t_{inv}(k_{min})$.

For each value of $m$, three different bandwidths are simulated for a total of nine cases. The choice of $k_{min}$ and $k_{max}$ is made so as to maximise the time during which the layer is growing self-similarly, while also keeping numerical errors below an acceptable level. It is important to clarify how convergence is defined in the present set of implicit large eddy simulations, as this determines the particular choice of $k_{min}$ and $k_{max}$. In fact,
Table 5.1 – Saturation time (s) of the longest wavelength for each simulation, estimated using Equation (5.18).

<table>
<thead>
<tr>
<th></th>
<th>$m = -1$</th>
<th>$m = -2$</th>
<th>$m = -3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R = 16$</td>
<td>0.036</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$R = 32$</td>
<td>0.083</td>
<td>0.044</td>
<td>0.031</td>
</tr>
<tr>
<td>$R = 64$</td>
<td>0.184</td>
<td>0.090</td>
<td>0.064</td>
</tr>
<tr>
<td>$R = 128$</td>
<td>-</td>
<td>0.183</td>
<td>0.129</td>
</tr>
</tbody>
</table>

there are two different notions of convergence that are relevant here; convergence with respect to the initial impulse and convergence with respect to the infinite bandwidth limit. The first of these is straightforward to assess and has been performed in the previous study of broadband RMI by Thornber et al. [31]. In that study, a grid convergence analysis was performed using the CNS3D code, which uses very similar numerics to Flamenco, by varying the grid resolution for a fixed initial condition so that $\lambda_{\text{min}} = 4\Delta x$, $8\Delta x$ and $16\Delta x$. By the end of the simulations, the difference in integral width when $\lambda_{\text{min}} = 8\Delta x$ vs. $\lambda_{\text{min}} = 16\Delta x$ was less than 1.5%. A comparison of the kinetic energy spectra between these two grid resolutions also showed that the first 48 modes were well resolved (i.e. 75% of the possible modes supported by the grid), which was deemed to be a sufficient level of convergence. Given that the present study uses a very similar computational setup, the restriction of the shortest wavelength to $\lambda_{\text{min}} = 8\Delta x$ is also adopted here.

The second notion, that of convergence with respect to the infinite bandwidth limit, may be analysed by considering the results of simulations with successively increased bandwidths that have the same number of grid points per minimum wavelength. If the results for a given quantity at two different bandwidths are the same (when appropriately non-dimensionalised) then these results are considered to be representative of those that would be obtained in the limit of infinite bandwidth. This is expected to be true for as long as the mixing layer evolving from a given bandwidth is growing self-similarly, which according to just-saturated mode theory should be between the saturation times of the shortest and longest wavelengths in the perturbation. This therefore motivates choosing $\lambda_{\text{max}}$ to be as large as possible. In actual simulations there are other sources of error that may cause the results at a given bandwidth to
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Table 5.2 – Total physical time (s) of each simulation.

<table>
<thead>
<tr>
<th></th>
<th>$m = -1$</th>
<th>$m = -2$</th>
<th>$m = -3$</th>
</tr>
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<tbody>
<tr>
<td>$R = 16$</td>
<td>0.5</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$R = 32$</td>
<td>0.25</td>
<td>0.15</td>
<td>0.1</td>
</tr>
<tr>
<td>$R = 64$</td>
<td>0.4</td>
<td>0.2</td>
<td>0.15</td>
</tr>
<tr>
<td>$R = 128$</td>
<td>-</td>
<td>0.185</td>
<td>0.13</td>
</tr>
</tbody>
</table>

depart from the infinite bandwidth limit earlier than this. Aside from errors due
to insufficient resolution of the smallest scales, there will also be errors due to in-
sufficient statistical sampling of the largest scales. In other words, the results may
become sensitive to the particular choice of random numbers used to initialise these
scales once they begin to dominate the growth of the layer. In Thornber et al. [31] it
was concluded that simulations with $\lambda_{max} = L/2$ did not show any influence of the
domain size over the time scales being considered and for that reason the same choice
of maximum wavelength is also made here.

Therefore the choice of $k_{min} = 2$ and $k_{max} = N/8$ determines the bandwidth $R$, which
in turn is determined by the number of cells in the $y$- and $z$-directions $N = L/\Delta x$.
The three different bandwidths simulated are $R = 16$, $R = 32$ and $R = 64$ for the
$m = -1$ case, and $R = 32$, $R = 64$ and $R = 128$ for the $m = -2$ and $m = -3$ cases.
The corresponding grid resolutions used are $384 \times 256^2$, $768 \times 512^2$, $768 \times 1024^2$ and
$768 \times 2048^2$ in order of increasing bandwidth. To minimise computational expense,
the domain length of uniformly refined mesh in the $x$-direction $L_x$ is set to be $1.5L$
for the $256^2$ and $512^2$ grids, $0.75L$ for the $1024^2$ grid and $0.375L$ for the $2048^2$ grid,
such that the grid spacing $\Delta x$ is the same as $\Delta y = \Delta z$. Each simulation is run
until the at least the saturation time of the longest wavelength, which is estimated
using Equation (5.18), although some simulations were extended beyond this time to
explore the behaviour of the layer once it had fully saturated. The estimated time
to saturation of the longest wavelength in each initial perturbation is given in Table
5.1, while the total physical time of each simulation is given in Table 5.2.
5.3 Effects of bandwidth and initial power spectrum

Figure 5.3 – Contours of heavy fluid volume fraction $f_1$ between the isosurfaces $f_1 = 0.01$ (blue) and $f_1 = 0.99$ (red), for the $m = -2$ case with an initial bandwidth $R = 128$ at time $t = 0.185$ s.

5.3 Effects of bandwidth and initial power spectrum

Figure 5.3 gives a visualisation of the highest bandwidth $m = -2$ case, showing red bubbles rising into the heavy fluid and blue spikes penetrating into the light fluid. The data are plotted at the latest time in the simulation, just after the saturation of the longest wavelength in the initial perturbation. The long wavelength modes are still clearly visible at this time, with fine-scale turbulent structures due to the breakdown of shorter wavelength modes superimposed on top of them. At this point in the simulation, the width of the layer is still relatively narrow compared to the longest wavelength.

The width of the mixing layer may be defined in a number of ways, for example the visual width $H$ based on the mean volume fraction profile $\langle f_1 \rangle$ [3]. An alternative definition is the peak-to-peak width $h$, taken as the distance between the minimum and maximum $x$-positions where the volume fraction of fluid 1 $f_1 = 0.5$. Note that both definitions are susceptible to fluctuations caused by turbulent breakup of the interface and acoustic waves, hence they are not well suited for estimating the growth
rate exponent $\theta$. It is still useful to examine $h$ (or $H$) however as a way of comparing the growth of the layer for different bandwidths and values of $m$. It might be expected that the different cases will all have the same value of $h$ at the saturation time of the longest wavelength, since $\lambda_{\text{max}}$ is the same for all cases. This comes from observation of Figure 5.3, where it is plausible that the fine scale turbulence superimposed on top of large scale coherent structures has a negligible impact on the overall width of the layer. However, as shown in Figure 5.4, this expectation of the same value of $h$ at saturation time is only realised between cases with the same value of $m$; as $m$ decreases the peak-to-peak width at saturation time also decreases.

The differences in $h$ between cases with the same value of $m$, which are small compared to the differences between cases with different $m$, are most likely due to inaccuracies in estimating the true saturation time of the layer. To investigate the cause of the larger differences between cases with different $m$, 2D slices of the $f_1$ volume fraction field are plotted in Figure 5.5, as well as lines along the $f_1 = 0.5$ contour that is used to calculate the peak-to-peak width $h$. One immediate observation is that there is more fine-scale structure in the $m = -1$ simulation than in the $m = -2$ simulation and similarly in the $m = -2$ simulation compared to the $m = -3$ simulation. This is because the smallest wavelengths have had more time to become nonlinear and transition to turbulence in the $m = -1$ simulation due to the longer time to saturation of the longest wavelength. It is also because of this additional time to develop more fine-scale structure that the values of $h$ at saturation time differ between the different simulations. In the $m = -1$ simulation (and less so in the $m = -2$ simulation), the interface is less coherent and there are multiple regions in the flow where blobs of fluid with $f_1 \geq 0.5$ have separated from the main interface. In contrast to this, the interface at the end of the $m = -3$ simulation is for the most part still simply connected as the smallest wavelengths are still in a relatively early stage of nonlinear development.

These observations can be quantified more precisely by considering a measure of the spectral bandwidth, which is expected to rapidly increase during transition to turbulence. Following Gowardhan et al. [7], the integral thickness $\delta$ and mean zero-
5.3 Effects of bandwidth and initial power spectrum

![Figure 5.4](image)

**Figure 5.4** – Peak-to-peak width (m) of the mixing layer vs. physical time (s). Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth. The data are plotted between $t = 0$ and the saturation time of the longest wavelength.

The crossing frequency $\kappa$ are defined as

$$\delta = \int_{-\infty}^{\infty} 4\langle Y_1 \rangle \langle Y_2 \rangle \, dx,$$  \hspace{1cm} (5.20a)

$$\kappa^2 = \frac{\int_{0}^{\infty} k^2 E_\rho(k) \, dk}{\int_{0}^{\infty} E_\rho(k) \, dk},$$  \hspace{1cm} (5.20b)

where $\langle \ldots \rangle$ indicates a plane average taken over the statistically homogeneous directions and $E_\rho(k)$ is the density variance spectrum, calculated using the method.
5.3 Effects of bandwidth and initial power spectrum

Figure 5.5 – Contour flood of volume faction $f_1$ and contour line of $f_1 = 0.5$ at saturation time for the medium bandwidth cases. The major ticks on both axes correspond to a grid spacing of $\Delta x = 0.5$ m.

given in Equation (4.27). A measure of the spectral bandwidth is then given by $\eta(t) = \delta(t)\kappa(t)$. Figure 5.6 gives the evolution of $\eta$ in time for each case, showing easily discernible differences between cases with different values of $m$. For a given initial bandwidth $R$, the increase in spectral bandwidth is most rapid for $m = -1$ and most slow for $m = -3$. This indicates that the $m = -1$ cases transitions to turbulence first and has the most fine-scale structure present at saturation time, in
5.3 Effects of bandwidth and initial power spectrum

Figure 5.6 – Spectral bandwidth measure vs. physical time. Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth. The data are plotted between \( t = 0 \) and the saturation time of the longest wavelength.

accordance with the observations made in Figure 5.5.

The contour plots in Figure 5.5 also resemble quite closely the experimental images reported in Krivets et al. [6]. Those image sequences, particularly for Experiment 4, show a transitional mixing layer containing a broad range of modes, the smallest of which have become turbulent by the end of the experiment, while the largest modes are still mostly linear. Figure 5.7 gives a comparison of the final images from Experiment 4 with an image taken from a section of the \( m = -2 \) simulation at a bandwidth of \( R = 64 \), highlighting the very similar phenomenology. The majority
5.3 Effects of bandwidth and initial power spectrum

Figure 5.7 – Comparison of (a) experimental images from Experiment 4 and (b) volume fraction contour flood from a section of the $m = -2$, $R = 64$ simulation at time $t = 0.1$ s. Source: From Figure 1 of Krivets et al. [6].

of values reported for $\theta$ in [6] are also higher than the range of values typically reported for narrowband, short wavelength perturbations, suggesting that the growth rate of the layer is being influenced by linear growth of longer wavelengths. For example, in Experiment 4 the bubble and spike growth rates were $\theta_b = 0.42$ and $\theta_s = 0.51$ respectively, which suggests the perturbations used were broadband in nature. Relating those experiments to the present work, a perturbation with spectral exponent $-1 \leq m \leq -2$ and relatively narrow bandwidth (i.e. $R = 32$) would produce a similar growth rate, as will be shown in Section 5.3.1. A more realistic representation would be a power spectrum consisting of multiple distinct ranges, each with a different exponent, such as in the initial conditions used in Weber et al. [209]. This will be explored further in future work.

5.3.1 Mixing measures

In this section, various integral mixing measures based on plane-averaged volume fraction profiles are presented for each of the nine simulations. The most fundamental
of these is the integral width, given by Equation (4.5). As with \( h \), the integral width evolves as \( W \propto t^\theta \) and is the more useful quantity for estimating \( \theta \) as it is more robust to fluctuations. Bubble and spike integral widths may also be defined and are given by Equation (4.18). Another useful quantity, based on second-order moments, is the (global) molecular mixing fraction [41], given by Equation (4.6). \( \Theta \) can take values anywhere between 0 and 1, with \( \Theta = 0 \) corresponding to complete heterogeneity and \( \Theta = 1 \) corresponding to complete homogeneity of mixing. A steady-state value of \( \Theta \) is also an indication that the mixing layer is evolving in a self-similar fashion.

### Non-dimensionalisation

In order to compare the evolution of \( W \) across different bandwidths and values of \( m \), a suitable non-dimensionalisation is sought, along the same lines of the analysis presented in Thornber et al. [30] for narrowband perturbations. For a multimode perturbation of the form given in Equation (5.3) with normally distributed coefficients, the initial growth rate of the integral width is

\[
\dot{W}_0 = 0.564 \sigma^+ A^+ \Delta u \bar{k},
\]

where \( \sigma^+ = (1 - \Delta u/U_s)\sigma \) and \( \bar{k} \) is a weighted average wavenumber of the perturbation, given by

\[
\bar{k} = \frac{\int_{k_{\min}}^{k_{\max}} k^2 P(k) \, dk}{\sqrt{\int_{k_{\min}}^{k_{\max}} P(k) \, dk}}.
\]

For each of the simulations \( \sigma = 0.2 \lambda_{\min} \) and \( \bar{k} \) is

\[
\bar{k} = \begin{cases} 
  k_{\max} \sqrt{\frac{1 - 1/R^2}{2 \log(R)}}, & m = -1, \\
  k_{\max} \sqrt{\frac{1}{R}}, & m = -2, \\
  k_{\max} \sqrt{\frac{2 \log(R)}{R^2 - 1}}, & m = -3.
\end{cases}
\]
5.3 Effects of bandwidth and initial power spectrum

Table 5.3 – Initial growth rate $\dot{W}_0$ (m/s) for each simulation.

<table>
<thead>
<tr>
<th>$m$</th>
<th>$R = 16$</th>
<th>$R = 32$</th>
<th>$R = 64$</th>
<th>$R = 128$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m = -1$</td>
<td>11.99</td>
<td>10.91</td>
<td>10.08</td>
<td>-</td>
</tr>
<tr>
<td>$m = -2$</td>
<td>-</td>
<td>5.466</td>
<td>3.942</td>
<td>2.827</td>
</tr>
<tr>
<td>$m = -3$</td>
<td>-</td>
<td>2.639</td>
<td>1.467</td>
<td>0.7983</td>
</tr>
</tbody>
</table>

An additional correction factor may be included to account for the initial diffuse width of the interface. Following Duff et al. [37] and Youngs & Thornber [48], the initial impulse is written as $\dot{W}_0 = 0.564\sigma^+ A^+ \Delta u \bar{k}/\psi$, where $\psi$ is given by

$$\psi = 1 + \sqrt{\frac{2}{\pi}} \bar{k} \epsilon. \quad (5.24)$$

In Equation (5.24), $\epsilon = \delta^+ / \sqrt{\pi}$ where $\delta^+ = \overline{C} \delta^-$ is the post-shock characteristic thickness of the interface, $\delta^- = \lambda_{\text{min}}/4$ is the pre-shock characteristic thickness and $\overline{C}$ is the mean compression rate, given by

$$\overline{C} = \frac{\rho_1 \bar{\rho}_2 + \rho_2 \bar{\rho}_1}{\rho_1 \bar{\rho}_2 + \rho_2 \bar{\rho}_1}. \quad (5.25)$$

The initial growth rates of $W$ are tabulated in Table 5.3. In the following sections, all quantities are non-dimensionalised by $\dot{W}_0$ and $\lambda_{\text{min}}$, for example dimensionless time $\tau = t \dot{W}_0 / \lambda_{\text{min}}$.

The evolution of integral width in time is shown in Figure 5.8. The data are plotted from the shock arrival time ($t_0 = 0.0011$ s) up to the saturation time of the largest wavelength. A good collapse of the data is observed at early time across all cases, as well as at late time between cases with the same value of $m$. This indicates that with this non-dimensionalisation, cases that are growing with a larger value of $\theta$ also have a larger value of $W/\lambda_{\text{min}}$ for a given dimensionless time. Figure 5.8 also shows how it becomes increasingly difficult to simulate to late dimensionless times with decreasing values of $m$ (prior to the largest wavelength saturating), which is in line with the qualitative observations made for Figure 5.5. In other words, to obtain the same dimensionless time at the point of saturation of the largest wavelength for the
m = −3 case compared to the m = −1 case, a much larger bandwidth is required (or alternatively a larger impulse must be used). This is the reason why smaller bandwidths were used in the m = −1 cases compared to the other cases.

As a comparison, the non-dimensionalisation presented in Gowardhan et al. [7] is also performed here. The integral width is scaled by κ₀ = κ(0) and time is scaled by κ₀W₀, with the results shown in Figure 5.9. Compared with the present non-dimensionalisation, the data are collapsed to approximately a single curve, although the collapse between cases with the same value of m is not as good. The difference
5.3 Effects of bandwidth and initial power spectrum

Figure 5.9 – Integral width vs. time using the non-dimensionalisation of Gowardhan et al. [7] (left) and an equivalent non-dimensionalisation based on \( \bar{k} \) (right). Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth.

in dimensionless time between cases with different \( m \) has also been substantially enhanced. It is interesting to note that \( \kappa_0 \) is very similar to the weighted average wavenumber \( \bar{k} \) introduced in Equation (4.13). For example, for the \( m = -2 \) case at a bandwidth of \( R = 128 \), \( \kappa_0 = 23.46 \text{ m}^{-1} \) and \( \bar{k} = 22.62 \text{ m}^{-1} \). This suggests that a very similar collapse should occur if \( \bar{k} \) is used instead to non-dimensionalise \( W \) and \( t \), with Figure 5.9 confirming that this is indeed the case. Since this scaling was introduced by Gowardhan et al. [7] to distinguish between cases with linear vs. nonlinear initial perturbations, it is not surprising that all of the present cases collapse to a single group. This can also be explained in terms of the initial impulse \( W_0 \), which varies between cases with different \( m \) due to varying \( \bar{k} \). Given that the purpose here is to distinguish between cases with different \( m \), the original non-dimensionalisation is used for the remainder of this study.

Growth rates

To estimate the growth rate exponent \( \theta \) for each simulation, nonlinear regression was used to fit a model of the form \( W = \beta (\tau - \tau_0)^\theta \). The interval over which this regression was performed was taken to be the period of time between the inversion.
5.3 Effects of bandwidth and initial power spectrum

Table 5.4 – Growth rate exponent $\theta$ for each simulation.

<table>
<thead>
<tr>
<th></th>
<th>$m = -1$</th>
<th>$m = -2$</th>
<th>$m = -3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R = 16$</td>
<td>0.426</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>$R = 32$</td>
<td>0.432</td>
<td>0.571</td>
<td>0.872</td>
</tr>
<tr>
<td>$R = 64$</td>
<td>0.488</td>
<td>0.574</td>
<td>0.805</td>
</tr>
<tr>
<td>$R = 128$</td>
<td>-</td>
<td>0.622</td>
<td>0.790</td>
</tr>
</tbody>
</table>

time to the saturation time of the largest wavelength, as during this period the results are expected to be representative of the infinite bandwidth limit. The estimate of $\theta$ taken from the nonlinear regression for each simulation is given in Table 5.4. It can be seen that for the $m = -1$ and $m = -2$ cases $\theta$ is increasing with the increasing bandwidth of the perturbation and is approaching the theoretical value of $2/(m + 5)$, particularly in the $m = -1$ simulations. In the $m = -3$ cases, $\theta$ is actually decreasing with increasing bandwidth. One possible explanation for this is that as the bandwidth increases, the shortest wavelengths are more nonlinear by the time the largest wavelength saturates and hence there is more dissipation of kinetic energy in the layer (for this specific value of $m$). In all cases the error in the regression is very low; the coefficient of determination $R^2$ is at least 0.999 and the standard error is at most 0.096%. This is not equivalent to the uncertainty in the value of $\theta$ but is merely a measure of how well the functional form $W = \beta(\tau - \tau_0)^\theta$ can explain the variation in the integral width data; the uncertainty in the data itself has not been taken into account. In order to obtain meaningful error bounds on $\theta$ multiple realisations would need to be run, or the same realisation simulated using multiple codes as in Thornber et al. [30]. However, by carefully designing the problem it is assumed these error bounds are small [121].

The evolution of the bubble and spike integral widths in time is shown in Figure 5.10. Qualitatively, both $W_b$ and $W_s$ evolve quite similarly, however $W_s$ is greater than $W_b$ for the entire duration of the simulation in all cases. To explore the relationship between $W_b$ and $W_s$ further, the evolution of the ratio $W_s/W_b$ in time is plotted in Figure 5.11. In all cases this ratio is initially around 3 just after shock passage, but quickly reduces and asymptotes to a constant value. The early-time variation in $W_s/W_b$ indicates that the initial impulsive growth rate of $W_s$ is greater than that of
5.3 Effects of bandwidth and initial power spectrum

Figure 5.10 – Bubble and spike integral widths vs. dimensionless time. Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth.

However, the fact that $W_s/W_b$ approaches a constant value at late time indicates that the bubbles and spikes eventually scale with the same exponent $\theta_b = \theta_s = \theta$. This is confirmed using nonlinear regression; for the highest bandwidth cases the difference between $\theta_b$ and $\theta_s$ when fit between the inversion and saturation times is 3.9%, 4.3% and 0.63% for $m = -1, -2$ and $-3$ respectively. This implies that at late time the self-similar evolution of the mixing layer can be described by a single length scale $W$. The constant value is also not the same for different values of $m$; at the latest dimensionless time in each simulation the ratio $W_s/W_b$ is 1.16, 1.12 and 1.08 for decreasing $m$.

The instantaneous value of $\theta$ can be computed by using a simple buoyancy-drag model (which also follows from self-similarity arguments), written as

$$\ddot{W} = -C_d \frac{\dot{W}^2}{W},$$

which has the solution $W = W_0(t - t_0)^\theta$ with $\theta = 1/(1 + C_d)$. This can be used to estimate $\theta$ by calculating the derivatives of $W$ with finite differences, the results of which are shown in Figure 5.12. There is some noise in the data, mainly due to division by the numerical second derivative, however clear trends are still able
to be determined. In the $m = -1$ case, the $R = 64$ bandwidth is sufficient for the theoretical growth rate of $\theta = 1/2$ to be obtained for a significant period of time; taking the average of instantaneous $\theta$ from $\tau = 10$ to $\tau = 30$ gives $\theta = 0.50$. Performing the nonlinear regression over this same interval also yields $\theta = 0.50$. For the $m = -2$ case, the largest bandwidth simulation comes close to obtaining the theoretical growth rate of $\theta = 2/3$. If the average of instantaneous $\theta$ is taken over the interval from $\tau = 5$ to $\tau = 10$ this gives $\theta = 0.63$, which is also the same value obtained from nonlinear regression performed over this interval. For all bandwidths in the $m = -3$ case, the instantaneous $\theta$ obtained from the buoyancy-drag model is substantially less than the theoretical value of $\theta = 1$. For the largest bandwidth, taking the average of instantaneous $\theta$ from $\tau = 2$ to $\tau = 4$ gives $\theta = 0.75$, which again matches the value obtained from nonlinear regression on this interval.

**Molecular mixing**

Finally, the evolution of the molecular mixing fraction $\Theta$ in time is plotted in Figure 5.13. Shown are data for all simulations plotted until the saturation time of the
longest wavelength, as well as data for some simulations that were extended beyond this saturation time to explore the late time behaviour. When the data are only plotted up to the saturation time, a good collapse is observed between cases with the same value of $m$. Beyond this point, the results for the smaller bandwidth cases begin to depart from those of the largest bandwidth, indicating that they are no longer representative of the infinite bandwidth layer. As stated earlier, a constant value of $\Theta$ is one measure of self-similarity of the mixing layer. However, over the interval where the instantaneous growth rate $\theta$ is approximately constant in each of the largest bandwidth simulations, $\Theta$ is either slowly decreasing in the $m = -1$ case or slowly increasing in the $m = -2$ and $m = -3$ cases. For the $m = -1$ case, a local maximum in $\Theta$ occurs after the initial (global) minimum, beyond which $\Theta$ gradually decays to an asymptotic value. Similar behaviour was also observed for the narrowband mixing layer in Thornber et al. [30]. Given that the largest bandwidth $m = -1$ case was shown previously to be growing self-similarly at the theoretically predicted rate over this interval, it is reasonable to assume that the late time value of $\Theta = 0.560$ is close to that which would be obtained in the limit of infinite bandwidth. For the $m = -2$ and $m = -3$ cases, $\Theta = 0.388$ and 0.197 respectively, although this is

**Figure 5.12** – Instantaneous growth rate exponent $\theta$ estimated from derivatives of $W$. Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth.
not necessarily indicative of the infinite bandwidth asymptotic value (particularly in the \( m = -3 \) case). Simulations at higher bandwidths are likely required to determine whether \( \Theta \) in the \( m = -2 \) and \( m = -3 \) cases behaves similarly to the \( m = -1 \) case.

### 5.3.2 Self-similarity

Another method for assessing the degree to which the layer is evolving self-similarly is to plot plane-averaged volume fraction profiles at different points in time, scaled by the integral width. If a perfect collapse is obtained then this shows that the evolution of the mixing layer can be completely described by a single length scale, in this case \( W \), and is therefore self-similar. Figure 5.14 gives both the plane-averaged volume fraction \( \langle f_1 \rangle \) (denoted by \( \bar{f}_1 \) in the figures) as well as the product \( \langle f_1 \rangle \langle 1 - f_1 \rangle \) to highlight the variation at the extremes of the mixing layer for the \( m = -1 \) case. A good collapse is observed across all of the later times considered (solid lines), particularly for the largest bandwidth, showing that the layer is evolving self-similarly and can be appropriately scaled by \( W \). There is a narrowing of the \( \langle f_1 \rangle \langle 1 - f_1 \rangle \) profile in time at the fringes of the spike side in the larger bandwidth cases, which suggests that the
5.3 Effects of bandwidth and initial power spectrum

integral width is becoming increasingly dominated by mixing in the core of the layer. To give some more context to the figures, the 1% bubble and spike heights $H_b$ and $H_s$ can be calculated, in a similar manner to the visual width, as

$$H_b = x_c - x(f_1 = 0.99), \quad (5.27a)$$

$$H_s = x(f_1 = 0.01) - x_c. \quad (5.27b)$$

Based on these definitions, the ratios $H_b/W$ and $H_s/W$ are found to be 3.0 and 4.3 on average for the largest bandwidth simulation. Therefore the departure from self-similarity observed on the spike side is occurring at the absolute fringes of the layer ($x/W \approx 6$), at a much greater distance from the layer centre than the 1% spike height. The same profiles are shown for the $m = -2$ case in Figure 5.15 and for the $m = -3$ case in Figure 5.16. For the medium and large bandwidths in the $m = -2$ case, the collapse of the data when scaled by $W$ is the best of all the cases, even at the fringes of the layer. For the largest bandwidth the ratios $H_b/W$ and $H_s/W$ are 3.3 and 4.2 respectively. For the $m = -3$ case the overall collapse in the data is less good, most notably on the bubble side, although still acceptable when considering that the scaled bubble and spike heights are $H_b/W = 3.7$ and $H_s/W = 4.1$ based on the largest bandwidth case. Again, the fact that the $\langle f_1 \rangle \langle 1 - f_1 \rangle$ profiles are narrowing in time suggests that the degree to which mix at the boundaries of the layer influences the integral width is decreasing. Another notable trend is that the scaled bubble heights increase with decreasing $m$ while the scaled spike heights decrease. This trend is also observed in the width of the $\langle f_1 \rangle \langle 1 - f_1 \rangle$ profiles.

Based on the just-saturated mode analysis given in Section 5.2.3, as well as the observations of self-similarity made in this section, another non-dimensionalisation is proposed with the aim of collapsing the data at late time across different values of $m$. Under the assumption that the layer is growing self-similarly and is dominated by linear growth, just-saturated mode analysis yields the relation in Equation (5.17).
Figure 5.14 – Plane averaged volume fraction profiles for $m = -1$. Dimensionless times are given in the legend.
5.3 Effects of bandwidth and initial power spectrum

Figure 5.15 – Plane averaged volume fraction profiles for $m = -2$. Dimensionless times are given in the legend.
5.3 Effects of bandwidth and initial power spectrum

Figure 5.16 – Plane averaged volume fraction profiles for $m = -3$. Dimensionless times are given in the legend.
Non-dimensionalising $W$ by $\lambda_{\text{min}}$ gives

$$\frac{W}{\lambda_{\text{min}}} \propto \left( \frac{B\sqrt{CA^+\Delta t}}{\lambda_{\text{min}}^{\frac{m+5}{2}}} \right)^{\frac{2}{m+5}} \approx \hat{\tau}^{\frac{2}{m+5}}.$$ (5.28)

Therefore plotting $(W/\lambda_{\text{min}})^{(m+5)/2}$ vs. $\hat{\tau}$ should yield a linear relationship, provided $W$ is growing at the theoretical rate of $\theta = 2/(m + 5)$. This is shown in Figure 5.17, with the data plotted up until saturation time, as well as until the very end of all simulations to explore the late time behaviour. As expected, since the $R = 64$, $m = -1$ case obtains the theoretical growth rate, a linear relationship is obtained for this case over the majority of the simulation time. In all other cases, departure from the theoretical growth rate is reflected in Figure 5.17 as departure from a linear relationship. The $R = 64$, $m = -1$ case can also be used to estimate the constant of proportionality for Equation (5.28). Performing linear regression over the interval for which $\theta = 0.5$, i.e. from $\tau = 10$ to $\tau = 30$ (or equivalently $\hat{\tau} = 7.58$ to $\hat{\tau} = 22.7$), gives the following line of best fit

$$\left( \frac{W}{\lambda_{\text{min}}} \right)^{\frac{m+5}{2}} = 0.25(\hat{\tau} - \hat{\tau}_0) + 0.01.$$ (5.29)

If the intercept, which is only important at very early time, is ignored then this gives the constant of proportionality for Equation (5.28) to be $0.25^{2/(m+5)}$.

### 5.3.3 Turbulent kinetic energy

The total fluctuating kinetic energy, presented here in terms of Favre averages, is defined in Equation (4.8). As before, the $x$-, $y$- and $z$-components of TKE are denoted by TKX, TKY and TKZ respectively. Since TKE is a large scale quantity, it is expected to converge in ILES provided there is a reasonable separation of the energetic scales from the dissipative scales. Figure 5.18 shows the evolution of TKE and its components in time. Since isotropy is expected in the transverse directions, the TKY and TKZ components are averaged and a single quantity, referred to as TKYZ, is presented for the transverse total fluctuating kinetic energy. The data are presented
in dimensionless form and are non-dimensionalised by the initial growth rate i.e. by $\widetilde{\rho} \widetilde{W}_0^2 \lambda_{\text{min}} L^2$, where $\widetilde{\rho} = 3.51 \text{ kg/m}^3$ is the mean post-shock density and $L$ and $\lambda_{\text{min}}$ are the characteristic length scales in the homogeneous and inhomogeneous directions respectively. This non-dimensionalisation is useful for determining the degree to which the results are converged with respect to the infinite bandwidth limit. A reasonable collapse is observed for the $m = -1$ cases, indicating that the results for largest bandwidth are representative of the infinite bandwidth limit, at least up until the saturation time of the longest wavelength. The collapse is not as good for the $m = -2$ cases, while for the $m = -3$ cases the data are not converged at all with respect to the infinite bandwidth limit (note that as outlined in Section 5.2.3 they are still considered converged for a given bandwidth). This suggests that even larger bandwidths are needed in order to obtain results that are representative of this limit. Figure 5.18 also shows that in dimensionless terms, the $m = -3$ perturbations have the most kinetic energy deposited by the shock wave for a given bandwidth since all modes in the perturbation have the same growth rate, whereas for the $m = -2$ and $m = -1$ perturbations the growth rates are smaller for larger wavelengths. In the $m = -1$ cases, the TKE is decaying throughout the entirety of the simulation,
Figure 5.18 – Total fluctuating kinetic energy vs. dimensionless time. Dotted lines represent the smallest bandwidth, dashed lines the medium bandwidth and solid lines the largest bandwidth.
and at early time there is a transfer of energy to the transverse directions due to the shorter wavelengths becoming nonlinear. The TKE in the $m = -2$ cases also decays throughout the simulation, however there is a less noticeable transfer of energy to the transverse directions; more energy is contained in the longer wavelengths which take a longer time to saturate and become nonlinear. An interesting phenomenon is observed in the $m = -3$ cases where at early time, starting from about the inversion time of the longest wavelength, the TKE is approximately constant, indicating zero dissipation. However, during this period there is a transfer of energy from the transverse directions to the $x$-direction. At 'late' time the TKE beings to decay, mainly driven by a decay in TKX.

The scaling of TKE over the period of dimensionless time corresponding to constant instantaneous $\theta$ is also given in Figure 5.18. In the self-similar regime TKE is expected to scale as $t^{-n}$ for some constant $n$, the value of which can be determined from the slope of these scalings. For $m = -1$, $m = -2$ and $m = -3$ the decay rates of TKE during this period are $n = 0.66$, $n = 0.26$ and $n = 0.11$ respectively. An argument based on dimensional analysis was given in Thornber et al. [31] for the value of $n$ in terms of $\theta$. Using either the empirical relation $\epsilon \propto u^3/l$ (and equating $l$ with the integral width) or by assuming that the mean velocity in the mixing layer is proportional to the growth rate of the mixing layer itself gives $q_k \propto t^{2\theta-2}$, where $q_k$ is the mean fluctuating kinetic energy. Since the TKE is proportional to the width of the mixing layer multiplied by the mean fluctuating kinetic energy, this gives $\text{TKE} \propto Wq_k \propto t^{3\theta-2}$. This predicted value of $n = 2 - 3\theta$ has been found to be in good agreement with the measured decay rate of TKE in multiple studies of narrowband RMI [31, 30], however for the present set of broadband cases the measured decay rates do not agree with this theoretical prediction. This is true even for the $m = -1$ case, which is converged with respect to the infinite bandwidth limit. Furthermore, for $\theta > 2/3$ this analysis predicts that TKE will increase in time, which is also not observed in Figure 5.18.

An explanation for why the TKE in the broadband case does not scale as $t^{3\theta-2}$ can be found by considering the assumptions behind the original derivation given in [31].
Starting with the relationship $\epsilon \propto u^3/l$ but retaining the constant of proportionality and equating $l$ with the integral width $W$ gives

$$\epsilon = \frac{dq_k}{dt} = C_\epsilon \frac{u^3}{l} \propto C_\epsilon \frac{q_k^{3/2}}{W}. \tag{5.30}$$

Since TKE $\propto Wq_k$, then it follows that

$$\frac{dTKE}{dt} \propto \frac{dW}{dt} \frac{TKE}{W} + C_\epsilon \left(\frac{TKE}{W}\right)^{3/2},$$

and therefore

$$C_\epsilon \propto \left(\frac{dTKE}{dt} - \frac{dW}{dt} \frac{TKE}{W}\right) \left(\frac{TKE}{W}\right)^{-3/2} = D. \tag{5.30}$$

A dimensional analysis can be performed on Equation (5.30), assuming TKE $\sim t^{-n}$ and $W \sim t^\theta$, which gives $C_\epsilon \sim t^{n/2-3\theta/2-1}$ and hence if $C_\epsilon$ is constant this implies $n = 2 - 3\theta$ as before. More importantly however, all of the terms on the RHS of Equation (5.30) are available, allowing for an assessment of the assumption that $C_\epsilon$ is constant. These terms are plotted in Figure 5.19 for each of the largest bandwidth cases, along with data for the narrowband case at late time taken from the $\theta$-group collaboration [30]. Note that the $y$-axis is not meaningful (since the data plotted is merely proportional to $C_\epsilon$) and has been scaled so that the minimum of the data is zero. The $\theta$-group data $x$-axis has also been shifted to make the figure more compact. It is clear that in the narrowband case, for which TKE scales as $t^{3\theta-2}$ at late time, the assumption that $C_\epsilon$ is constant is justified. However, for the broadband cases $C_\epsilon$ is not constant and therefore the result TKE $\propto t^{3\theta-2}$ does not hold. The decay rate in the $m = -1$ case is closest to the predicted value ($n = 0.5$), which agrees with the observation that $C_\epsilon$ is plateauing over the period which this decay rate was measured. In theory, if the functional form of $C_\epsilon$ was known, then a new estimate for the decay rate $n$ in the broadband case could be derived. This is analogous to the recently proposed modification of a buoyancy-drag model [48], and points to a means of adapting the dissipation terms commonly employed in Reynolds-averaged Navier–Stokes models.
5.3 Effects of bandwidth and initial power spectrum

Figure 5.19 – Plot of the RHS of Equation (5.30) vs. dimensionless time for each of the largest bandwidth cases, as well as a portion of the quarter-scale \( \theta \)-group data.

Spectra

The distribution of turbulent kinetic energy in wavenumber space may be analysed by computing the radial power spectrum over the \( y-z \) plane located at the mixing layer centre \( x_c \). Variable-density spectra of both the normal and transverse velocity components are calculated according to Equation (4.27). Since isotropy is expected in the transverse directions, a single transverse energy spectrum is defined as \( E_{v_{yz}} = (E_{v_y} + E_{v_z})/2 \). The energy spectra of the transverse and normal velocity components are shown in Figure 5.20 for each of the largest bandwidth cases at four different dimensionless times, with the data non-dimensionalised by \( \rho \bar{W}_0^2 \). Each
dimensionless time plotted corresponds to; same physical time (t=0.005 s), same dimensionless time (τ = 2.87), dimensionless time at which W/λ_{min} = 2 and dimensionless time at saturation of the longest wavelength respectively. At the earliest time plotted, there is a visible discontinuity located at the highest wavenumber in the initial perturbation, particularly for the E_{vz} spectra, due to there being insufficient time for a significant amount of energy to cascade to scales smaller than 8Δx. The theoretical scalings in wavenumber space are also shown in Figure 5.20. Following Youngs [44], a scaling of E_v ∼ k^{(m+2)/2} is expected at early time. This scaling is most easily visible for wavenumbers 10 ≲ k ≲ 50 at the earliest time shown in Figure 5.20, as the highest wavenumbers in the initial perturbation break down rapidly, while the statistics of the lowest wavenumbers are not sufficient to produce a smooth line. In general, the spectra of the transverse velocity components follow this early time scaling more closely than those of the normal velocity component. The k^{(m+2)/2} scaling at early time also shows that, right after shock passage, the peak kinetic energy is located at k_{max} for the m = −1 cases, at k_{min} in the m = −3 cases while the m = −2 cases have a uniform distribution of kinetic energy across all wavenumbers.

At late time, the analysis of Zhou [191] was modified by Thornber et al. [31] to take into account the effects of the initial perturbation spectrum. This gave an expected scaling of E_v ∼ k^{(m-6)/4} provided τ_{RM} < τ_{HDT}, where τ_{RM} and τ_{HDT} are the characteristic eddy turnover times of Richtmyer–Meshkov and homogeneous decaying turbulence respectively, otherwise the spectra should revert to a k^{-5/3} scaling [31]. The k^{(m-6)/4} scaling is shown in Figure 5.20 at high wavenumbers and in general the agreement with the data is mixed. In the m = −1 case, the transverse spectra scale as k^{-1.47} at late time, which is close to the scaling observed in the narrowband case [121]. The early and intermediate time transverse spectra do suggest however that a k^{-7/4} scaling is briefly obtained at higher wavenumbers. This is also observed in the normal spectra, which also retain this scaling (k^{-1.73}) at later times. A similar trend is observed in the m = −2 case, where again the transverse spectra scale as k^{-1.47} at late time while at earlier times a scaling close to k^{-2} is observed at high wavenumbers. The k^{-2} scaling is also seen briefly in the normal spectra, which at late
5.3 Effects of bandwidth and initial power spectrum

Figure 5.20 – Variable-density turbulent kinetic energy spectra for each of the largest bandwidth cases. Dimensionless times are given in the legend.
time are tending towards a $k^{-5/3}$ scaling. Finally in the $m = -3$ case, the transverse spectra follow a scaling of $k^{-1.53}$ at intermediate wavenumbers and a scaling close to $k^{-9/4}$ at higher wavenumbers (above the smallest initial wavelength). Meanwhile the normal spectra scale as $k^{-5/3}$ at intermediate wavenumbers and as $k^{-9/4}$ at higher wavenumbers. The fact that very little TKE is dissipated in the $m = -3$ simulation can also be seen here, with the spectra at later times collapsing almost perfectly on top of each other.

5.4 Conclusions

This chapter has investigated the influence of different broadband perturbations on the evolution of a turbulent mixing layer induced by RMI through a series of carefully designed numerical simulations. In particular, the effects of varying the bandwidth $R$ and spectral exponent $m$ of the initial perturbation have been analysed for three different values of both $m$ and $R$. For a given bandwidth, the total standard deviation of the perturbation was held constant for all values of $m$, and the initial amplitudes of all modes were linear (or weakly nonlinear in the $m = -1$ case). Upon non-dimensionalisation, a good collapse of the data was obtained for various integral measures such as the integral width $W$ and molecular mixing fraction $\Theta$. Both non-linear regression and direct calculation through derivatives of $W$ were used to extract the growth rate exponent $\theta$. For the largest bandwidth cases, $\theta$ was found to be 0.5, 0.63 and 0.75 for $m = -1$, $m = -2$ and $m = -3$ respectively, while the values of $\Theta$ at the latest times considered were 0.56, 0.39 and 0.20. The degree to which the layer is evolving self-similarly was assessed using plane-averaged volume fraction profiles, with all cases showing a good collapse when scaled by a single length scale $W$. The temporal evolution of total fluctuating kinetic energy was also presented, along with the observed decay rates for each case and an argument for why they do not match the predicted value of $n = 2 - 3\theta$. Finally, the scaling of turbulent kinetic energy was analysed in spectral space and was shown to follow the theoretical scaling of $k^{(m+2)/2}$ at low wavenumbers. At high wavenumbers the spectra of the transverse velocity
5.4 Conclusions

Components tend towards a $k^{-3/2}$ scaling at late time, while the normal velocity spectra approach a $k^{-5/3}$ scaling. In general, the results provide a good validation for analysing the mixing layer in terms of linear growth rates of individual modes in the perturbation, as well as highlighting where this analysis fails to accurately capture the behaviour of the mixing layer.

This work highlights multiple avenues for further investigation. Given the promising comparisons that were drawn between the present simulations and experiments with broadband perturbations, a full study that aims to more closely match experimental conditions would likely provide a lot of useful insight. A first step in this direction is given in Chapter 6. Another option is to perform a complete analysis of the budgets of transport equations for quantities such as turbulent kinetic energy to inform RANS modelling, as was recently done for narrowband RMI [105]. Finally, it would be useful to extend the just-saturated mode theory presented here to include the effects of viscosity and diffusivity on the growth rates of each mode, as well as to extend the recently proposed modifications for a buoyancy-drag model given in Youngs and Thornber [48, 49] to broadband perturbations.
Chapter 6

Direct Numerical Simulation of an Idealised Air–SF6 Shock Tube Experiment

6.1 Introduction

In this chapter, DNS and ILES are performed of 3D RMI with both narrowband and broadband perturbations, using a setup that represents an idealised version of the RMI shock tube experiments performed by the research group of J. Jacobs at the University of Arizona [212, 213, 180, 34]. There are several reasons for doing this, each of which will be listed in turn. Firstly, the standard by which simulations are ultimately judged by more often than not is whether they agree with experimental results. While there are sometimes good reasons for not doing so, it is typically much easier to design a simulation that aims to match an experiment rather than the other way around. Therefore using experimentally motivated gas combinations, shock Mach numbers, pressures and temperatures in fundamental RMI studies helps to address a potential criticism of the work presented in Chapter 4 and Chapter 5, which is that those simulations cannot be replicated in an experiment.

There are also other good reasons for using a real gas combination, one of which is
that it provides data at a different Atwood number to what has already been presented here. Using a light-heavy configuration, common to almost all shock tube experiments, adds another element of variation from the simulations of Chapters 4 and 5. Somewhat coincidentally, this configuration is more challenging for numerical simulations, mainly due to post-shock oscillations that are induced behind the transmitted shock as it travels through the heavy fluid. Such oscillations are common to all shock capturing methods for shock waves that move slowly with respect to the computational mesh and must be carefully managed so that they do not influence the solution. The simulations presented in this chapter therefore represent close to the limit of what the current numerical method is capable of.

Perhaps the biggest motivation for using an experimentally matched setup however, is the need to explain results from shock tube experiments with 3D multimodal perturbations. For example, Jacobs et al. [8] found that their measurements of mixing layer width prior to reshock could be partitioned into two groups with different power law exponents. The particular diagnostic used was the mixing layer half width \( h \), found by taking the distance between the 10% and 90% average concentration locations and halving this. As with the integral width, \( h \) obeys a power law \( h = C t^\theta \). Prior to reshock, both groups initially have exponents approximately equal to 0.5 (\( \theta = 0.51 \) and \( \theta = 0.54 \)), while at later times the exponents are less but also notably different (\( \theta = 0.38 \) and \( \theta = 0.29 \) respectively). Similarly, Krivets et al. [6] found a wide range of growth exponents \( \theta \) for the integral width prior to reshock, ranging from \( \theta = 0.18 \) to \( \theta = 0.57 \), using a similar experimental setup.

A plausible explanation for this behaviour is that in addition to the high wavenumber, high amplitude (relative to wavelength) modes that are initialised on the membrane-less interface by vertical oscillations produced using loudspeakers, there are also some low wavenumber, low amplitude modes present in the initial perturbation. Based on the theory given in Chapter 5, these modes would dominate the growth of the layer while they are growing linearly and have not yet saturated. Long after saturation has occurred, the growth rate of the layer would be expected to tend towards that of a narrowband perturbation that grows purely due to mode coupling with \( \theta = 1/3 \) [46].
6.2 Setup

However, in the intermediate time prior to this, but after saturation of the longest initial wavelength, there are likely to be some lingering effects on the growth rate due to the presence of additional low wavenumber modes that could account for the observed values of $\theta$ in Jacobs et al. [8], Krivets et al. [6]. Given that behaviour of the two groups in Jacobs et al. [8] was identical after reshock, this would suggest that saturation of the longest initial wavelength has occurred prior to reshock time, as otherwise it would continue to dominate the growth rate after reshock as well [83]. This implies that the bandwidth of the initial perturbation is not extremely large, in other words the wavelengths of the lowest modes initialised are likely only about an order of magnitude larger than those of the highest wavenumbers. These estimates are used to design a series of numerical simulations that incorporate a lot of the features of these experiments but with idealised initial surface perturbations, so as to explore the effects that additional low wavenumber modes may have on the results.

6.2 Setup

The computational setup is essentially the same as in Chapter 4 and Chapter 5 but with a few key differences that will be described here. The governing equations are given by the new five-equation model presented in Chapter 3, which are solved using Flamenco. A Cartesian domain of dimensions $x \times y \times z = L_x \times L \times L$ where $L = 2\pi$ m is used for all simulations. As in Chapter 5, the extent of the domain in the $x$-direction, $L_x$, is varied and will be detailed below in Section 6.3. Periodic boundary conditions are used in the $y$- and $z$-directions, while in the $x$-direction outflow boundary conditions are imposed very far away from the test section so as to minimise spurious reflections from outgoing waves impacting the flow field. The initial mean positions of the shock wave and the interface are $x_s = 2.5$ m and $x_0 = 3.0$ m respectively and the initial pressure and temperature of both (unshocked) fluids is $p = 0.915$ atm and $T = 298$ K, equal to that in the experiments of Jacobs et al. [8]. All computations employ the ideal gas equation of state with a fixed value of $\gamma$ for each species.
Table 6.1 – The molecular weight \( W_l \) (g/mol), ratio of specific heats \( \gamma \), dynamic viscosities \( \times 10^5 \) Pa-s) and Prandtl and Schmidt numbers of air and SF\(_6\).

<table>
<thead>
<tr>
<th>Property</th>
<th>Air</th>
<th>SF(_6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( W_l )</td>
<td>28.964</td>
<td>146.057</td>
</tr>
<tr>
<td>( \gamma_l )</td>
<td>1.4</td>
<td>1.1</td>
</tr>
<tr>
<td>( \mu_l )</td>
<td>1.836</td>
<td>1.535</td>
</tr>
<tr>
<td>( Pr_l )</td>
<td>0.71</td>
<td>0.90</td>
</tr>
<tr>
<td>( Sc_l )</td>
<td>0.71</td>
<td>0.90</td>
</tr>
</tbody>
</table>

The shock Mach number is \( M = 1.5 \), which is higher than the \( M = 1.2 \) shock used in Jacobs et al. [8], Krivets et al. [6]. This is so that the initial impulse is larger, which makes more efficient use of the explicit time stepping algorithm, but not so large that it introduces significant post-shock compressibility effects. Therefore the post-shock evolution of the mixing layer is still approximately incompressible in both the present simulations and the experiments in [8, 6]. The initial densities of air and SF\(_6\) are \( \rho_1 = 1.083 \) kg/m\(^3\) and \( \rho_2 = 5.465 \) kg/m\(^3\) and the post-shock densities are \( \rho_1^+ = 2.469 \) kg/m\(^3\) and \( \rho_2^+ = 15.66 \) kg/m\(^3\) respectively. This gives a post-shock Atwood number of \( A^+ = 0.72 \), which is essentially the same as the value of 0.71 given in Jacobs et al. [8], indicating that the effects of compressibility are minimal. The variation in \( \rho \) and \( Y_1 \) across the interface are computed as in Section 4.2.2. The evolution of the interface is solved in the post-shock frame of reference by applying a shift of \( \Delta u = -158.08 \) m/s to the initial velocities of the shocked and unshocked fluids. The initial velocity field is also modified to include an initial diffusion velocity at the interface, which is calculated according to Equation (4.4). To improve the quality of the initial condition, three-point Gaussian quadrature is used in each direction to accurately compute the cell averages required by the finite-volume algorithm.

Table 6.1 gives the thermodynamic properties of each fluid. The dynamic viscosities of both fluids are calculated using the Chapman–Enskog viscosity model at a temperature of \( T = 298 \) K, while the diffusivities are calculated under the assumption of Lewis number equal to unity (hence \( Pr_l = Sc_l \)). In the DNS calculations, the actual values of viscosity used are much higher, so as to give a Reynolds number that is able
to be fully resolved, but are kept in the same proportion to each other. The initial Reynolds number is given by

$$Re_0 = \frac{\bar{\lambda}\bar{W}_0\rho^+}{\mu},$$

(6.1)

where $\bar{\lambda}$ and $\bar{W}_0$ are the weighted-averaged wavelength and initial growth rate of integral width and are hence different for the different perturbations considered. Meanwhile $\rho^+ = 9.065 \text{ kg/m}^3$ is the mean post-shock density and $\mu = 0.3228 \text{ kg/m/s}$ is the mean dynamic viscosity used for all cases unless otherwise stated.

Three different initial perturbations are considered; a narrowband perturbation and two broadband perturbations, all of the form given by Equation (5.2). For the narrowband perturbation, $k_{\text{min}} = 16$, $k_{\text{max}} = 32$ and $m = 0$. This is essentially the same perturbation as the quarter-scale scale of Thornber et al. [30], however the initial amplitudes are larger and are defined such that $a_{k_{\text{max}}} k_{\text{max}} = 1$, which is at the limit of the linear regime. Note that in the experiments of Jacobs et al. [8], $a_{k_{\text{max}}} k_{\text{max}}$ ranged between 2.82 and 3.14, which is much more nonlinear. The choice of restricting the mode amplitudes such that all modes are initially linear is made so that the results may be easily scaled by the initial growth rate and compared with the results of the previous chapters. Future work should investigate if any significant differences are observed when nonlinear initial amplitudes are used. For the two broadband perturbations, $k_{\text{min}}$ is taken to be 2, while $k_{\text{max}}$ is kept at 32 and $m$ is either $-1$ or $-2$. The amplitudes are defined by setting $a_{k_{\text{max}}} k_{\text{max}} = 1$, in other words the amplitudes of shortest wavelength mode are the same as for the narrowband perturbation. These broadband perturbations therefore incorporate additional longer wavelength, low amplitude modes relative to the narrowband perturbation and are used to study the effects these may have on the growth of the mixing layer in an idealised setting. Unlike the broadband perturbations analysed in Chapter 5, the perturbations considered here have different total standard deviations for the same bandwidth.

Based on the bandwidths and mode amplitudes defined above, the weighted-average wavelength, given by Equation (5.22), of each perturbation is $\bar{\lambda} = 0.278$ m, 0.463 m and 0.785 m for $m = 0$ (narrowband), $m = -1$ and $m = -2$ (broadband) respectively.
Table 6.2 – The weighted-average wavelength (m), initial growth rate of integral width (m/s) and average dynamic viscosity (Pa-s) for each case.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>( Re_0 = 122 )</th>
<th>( Re_0 = 261 )</th>
<th>( Re_0 = 526 )</th>
<th>( Re_0 = 1051 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>0</td>
<td>-1</td>
<td>-2</td>
<td>-2</td>
</tr>
<tr>
<td>( \bar{\lambda} )</td>
<td>0.278</td>
<td>0.463</td>
<td>0.785</td>
<td>0.785</td>
</tr>
<tr>
<td>( \bar{W}_0 )</td>
<td>15.67</td>
<td>20.03</td>
<td>23.84</td>
<td>23.84</td>
</tr>
<tr>
<td>( \bar{\mu} )</td>
<td>0.3228</td>
<td>0.3228</td>
<td>0.3228</td>
<td>0.1614</td>
</tr>
</tbody>
</table>

Similarly, the initial growth rate of integral width is given by

\[
\bar{W}_0 = 0.564 \sigma_0^+ A^+ \Delta u \bar{k}/\psi, \tag{6.2}
\]

where \(\sigma_0^+ = C_V (1 - \Delta u/U_s) \sigma_0\), \(\sigma_0\) is given by Equation (5.12) and \(\psi\) is given by Equation (5.24). Here \(C_V = (A^- + C_RA^+) / (2C_RA^+)\) is an additional correction factor that is applied to the Richtmyer compression factor \(C_R = (1 - \Delta u/U_s)\) to give the impulsive model of Vandenboomgaerde et al. [210]. For the present gas combination and configuration, \(C_V = 1.16\) and is used to account for deficiencies in the original impulsive model of Richtmyer [16] for certain cases. Therefore the initial growth rates are \(\bar{W}_0 = 15.67\) m/s, \(\bar{W}_0 = 20.03\) m/s and \(\bar{W}_0 = 23.84\) m/s for \(m = 0\), \(m = -1\) and \(m = -2\) respectively. This gives an initial Reynolds number of \(Re_0 = 122\), \(Re_0 = 261\) and \(Re_0 = 526\). An additional case is run for the \(m = -2\) broadband perturbation with an initial Reynolds number of \(Re_0 = 1051\) (obtained by halving the viscosity), to explore the Reynolds number effects on the growth rate and other quantities. The initial Reynolds number, and associated quantities, for each case is given in Table 6.2

### 6.3 Preliminary results

Both ILES and DNS are performed using the computational setup described in Section 6.2, the preliminary results of which are reported here. Attention will be restricted to integral quantities given in Section 4.3.1, namely the integral width, molecular mixing fraction, total fluctuating kinetic energy and domain-integrated enstrophy.
and scalar dissipation rate. This allows for both an assessment of grid convergence in
the DNS, along with a meaningful comparison between DNS and ILES results. For
the ILES cases, a domain length of $L_x = 1.5\pi$ m was used with a grid resolution
of $384 \times 512 \times 512$. These simulations were run up to time $t = 0.3$ s, at which
point some of the spikes were observed to have reached the domain boundaries. For
comparison, the saturation times of the longest initial wavelengths in the $m = -1$ and
$m = -2$ perturbations are $t_{sat} = 0.084$ s and $t_{sat} = 0.018$ s respectively. Similarly,
a domain length of $L_x = 1.5\pi$ m was used for the $Re_0 = 122$, $Re_0 = 261$ and
$Re_0 = 526$ DNS cases, which were all found to be suitably converged on a grid
resolution of $768 \times 1024 \times 1024$. These simulations were run up to a time of $t = 0.1$
s due to limitations on computational resources. For the $Re_0 = 1051$ DNS case, a
reduced domain size of $L_x = 0.75\pi$ m was used, with a maximum grid resolution of
$768 \times 2048 \times 2048$. The simulations were run up to time $t = 0.08$ s, at which point
some of the spikes were observed to have reached the domain boundaries.

Figure 6.1 shows a contour flood of the volume fraction $f_1$ (i.e. the volume fraction of
air) for the three initial conditions. Whilst there is a noticeable difference between the
narrowband ($m = 0$) and broadband ($m = -1, m = -2$) surface perturbations, the
differences between the $m = -1$ and $m = -2$ perturbations are quite subtle. Never-
theless these subtle differences in the amplitudes of the additional, longer wavelengths
are responsible for quite noticeable differences in the subsequent evolution of the mix-
ing layer, as will be shown below. This highlights the importance of understanding
the sensitivity to initial conditions in RMI-induced flows.

The results in the following sections are appropriately non-dimensionalised to allow for
direct comparisons with the experiments in Jacobs et al. [8] (although only qualitative
comparisons are performed here). All length scales are normalised by $\lambda_{min}$, which is
equal to 0.196 m in the simulations and is estimated to lie between 2.9 mm and
3.2 mm in the experiments. As the effects of different initial impulses are of primary
interest, it does not makes sense to use $\dot{W}_0$ as the normalising velocity scale, therefore
all velocities are normalised by $A^+\Delta u$ instead. In the simulations $A^+ = 0.72$ and
$\Delta u = 158.08$ m/s, while in the experiments $A^+ = 0.71$ and $\Delta u = 74$ m/s. Therefore
6.3 Preliminary results

The non-dimensional time is given by

$$\tau = \frac{(t - t_0)A^+\Delta u}{\lambda_{\text{min}}},$$

where \( t_0 = 0.0011 \) s is the shock arrival time. This equates to a dimensionless time of \( \tau = 175 \) at the latest time considered in the simulations (\( t = 0.3 \) s) and \( 107 \leq \tau \leq 118 \) at the latest time prior to reshock in the experiments (\( t - t_0 = 6.5 \) ms).

Figure 6.1 – Initial conditions for the narrowband \((m = 0)\) and broadband \((m = -1, m = -2)\) cases, shown using contours of heavy fluid volume fraction \( f_1 \). The major ticks on both axes correspond to a grid spacing of \( \Delta x = 1 \) m.
6.3 Preliminary results

6.3.1 ILES

Figures 6.2–6.4 show the development of the mixing layer and transition to turbulence for the $m = 0$ (narrowband), $m = -1$ and $m = -2$ (broadband) ILES cases respectively in the $x$-$y$ plane located at $z = 0$. Note that these cases were run using the low Mach correction of Xie et al. [10], due to the results of the isentropic vortex test case presented in Appendix C. All other aspects of the algorithm are the same as for the DNS cases. Comparing between cases, even at early time ($\tau = 11.1$) the effects of the additional low wavenumber modes in the broadband cases can be seen quite clearly, where similar fine-scale structures as in the narrowband case are superimposed on top of increasingly large long wavelength variations. This particular dimensionless time also corresponds to slightly after the estimated saturation time of the longest initial wavelength in the $m = -2$ perturbation, which seems to agree qualitatively with observations of Figure 6.4. Comparing to the experiments in Jacobs et al. [8], the dimensionless time of $\tau = 11.1$ corresponds to a physical (post-shock) time of $0.61 \leq t \leq 0.67$ ms. Observing the experimental image sequence reproduced in Figure 6.5, there appears to be reasonable qualitative agreement with the simulations at this time in terms of fine-scale structure and the amplitudes of longer wavelengths.

At the next time shown ($\tau = 57.9$), the differences between cases are now more substantial. In the narrowband case the mixing layer has remained relatively uniform over the span of the domain, whereas in the broadband cases, particularly the $m = -2$ case, large-scale entrainment is starting to occur at scales on the order of the domain width. This time is also soon after the estimated saturation time of the longest initial wavelength in the $m = -1$ perturbation, and comparing this image with the image at earlier time for the $m = -2$ perturbation shows good qualitative agreement for the amplitude of this mode. Another noticeable phenomenon at this time is that in the narrowband case, and to a lesser degree in the $m = -1$ case, some spikes have escaped the main mixing layer, which does not appear to occur in the $m = -2$ case. These are only visible in the contour plots due to the particular contour levels used, which range between $f_1 = 0.001$ and $f_1 = 0.999$, indicating that the escaping spikes only contain very small amounts of SF$_{6}$ (i.e. $\leq 1\%$ by volume). Such small amounts of material
6.3 Preliminary results

may also not show up in an experimental diagnostic such as PLIF or Mie scattering, although there appears to be some visible material ejected from the main layer in the experiments of Jacobs et al. [8] at the relevant time \(3.2 \leq t \leq 3.5\) ms. Comparisons between the simulations and the experiments at this time also show greater differences than at earlier times, although some useful comments can still be made. The biggest reason for the differences is likely due to the different initial perturbations, where the mode amplitudes in the experiment where much more nonlinear (which is not taken into account in the present non-dimensionalisation). Even so, there is clear visual evidence of long wavelength perturbations in the experimental images at this time, which most closely resemble the images in the \(m = -2\) broadband case.

Finally, Figures 6.2–6.4 also show results for a dimensionless time that is much later than the reshock time in the experiments. There are now major differences in the degree of large-scale entrainment, which is significantly greater in the \(m = -2\) broadband case. The other major difference is in the small amounts of material ejected far away from the layer, which appears to occur most frequently in the narrowband case. A caveat should be made with regards to this, in that although the highest wavenumbers in the narrowband and broadband perturbations have the same amplitudes, different random numbers are used hence the phases of these modes will be different. Therefore more simulations with different random numbers are likely required to reduce the uncertainty when making conclusions about statistically rare events such as these. Nevertheless, it seems at least plausible that the slower but more persistent growth of the low wavenumber modes in the broadband cases may cause the main mixing layer to eventually disrupt the trajectory of any spikes that were initially ejected. The plane-averaged volume fraction profiles in Figure 6.6 also support this claim, showing a distinct secondary peak in \(\bar{f}_1\bar{f}_2\) on the spike side of the layer in the \(m = 0\) and \(m = -1\) cases but not the \(m = -2\) case. This also indicates that the ejected spikes are present throughout the entire cross-section of the flow field in these cases and do not just happen to be unique to the particular 2D slice shown in Figures 6.2–6.4.

Figure 6.6 also shows the temporal evolution of integral width, while the mixing
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Figure 6.2 – Contours of volume fraction $f_1$ for the narrowband ($m = 0$) ILES case. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1 \text{ m.}$
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(a) $\tau = 11.1$.

(b) $\tau = 57.9$.

(c) $\tau = 175$.

Figure 6.3 – Contours of volume fraction $f_1$ for the $m = -1$ broadband ILES case. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
Figure 6.4 – Contours of volume fraction $f_1$ for the $m = -2$ broadband ILES case. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
Figure 6.5 – Image sequence taken from a typical experiment using the Mie diagnostic. Times relative to shock impact are shown in each image. Reshock occurs at $t = 6.50$ ms. Source: From Figure 3 of Jacobs et al. [8].
measures $\Theta$ and $\Xi$ are shown in Figure 6.7. Substantial differences are observed in all of these measures between cases, with the integral width in the $m = -2$ case being over twice as large as that in the narrowband case at the latest time. This is due to the additional low wavenumber modes providing greater overall width to the layer. The mixing layer in the $m = -2$ case is also the most heterogeneous throughout the entire simulation, although there is a greater degree of large-scale entrainment which should lead to more material being mixed overall. The minimum in $\Theta$ and $\Xi$ is also lowest for the $m = -2$ case due to the greater initial impulse causing greater stretching of the layer at early time, similarly the minimum in $\Theta$ and $\Xi$ for the $m = -1$ case is lower than in the $m = 0$ case. None of the cases have reached self-similar decay, however based on gradients of $\Theta$ at the latest time considered it appears that $\Theta$ is most quickly approaching a constant value in the $m = -1$ case. The late-time values of $\Xi$ and $\Theta$ are approximately the same for the narrowband case, while $\Xi < \Theta$ in the broadband cases. Again this is due to the greater overall heterogeneity of the mixing layer in these cases, which affects $\Xi$ more than $\Theta$.

Using nonlinear regression to fit a model of the form $W = \beta(\tau - \tau_0)^\theta$, the growth exponent $\theta$ can be estimated for each simulation. The interval over which this re-

Figure 6.6 – Integral width vs. dimensionless time and product of plane-averaged volume fraction profiles at time $t = 0.3$ s for the narrowband ($m = 0$) and broadband ($m = -1$, $m = -2$) ILES cases.
gression is performed is different for each simulation and reflects the different growth regimes that are expected. For the narrowband case, the fit is performed from the time of peak mix velocity $V = dW/dt$, evaluated to occur at $\tau = 0.82$, to the end of the simulation at $\tau = 175$. This gives the value of $\theta$ to be 0.34, which is very close to the theoretical value of $1/3$ for narrowband initial conditions Elbaz and Shvarts [46]. For the broadband cases, two different fits are performed; the first between the saturation time of the smallest and largest initial wavelengths, with the second performed between the saturation time of the largest initial wavelength and the end of the simulation. For the $m = -1$ case, the first fit gives a value of $\theta = 0.47$, which is close to the theoretical value of $1/2$ given in Chapter 5, while the second fit gives a value of $\theta = 0.41$. Therefore the additional long wavelengths in the initial perturbation influence the growth rate well after they have saturated. Similar behaviour is seen for the $m = -2$ case, where the first fit gives a value of $\theta = 0.69$, which is also close to the theoretical value of $2/3$ given in Chapter 5, while the second fit gives a value of $\theta = 0.44$.

Figure 6.8 shows the instantaneous value of $\theta$ obtained from the simple buoyancy-drag model, given in Equation (5.26), for the three cases. Some interesting behaviour is observed here. For each case, $\theta$ initially decreases then increases briefly before
continuing to decrease for the rest of the simulation. This is most prominent for the narrowband case, which increases to a value greater than 0.5 before decaying to almost 0.2 by the end of the simulation. In contrast to this, both of the broadband cases increase to a similar value at early time however the subsequent decay is much more gradual, with both cases maintaining a constant value close to 0.4 for the latter half of the simulation. In both cases this is in good agreement with the value of $\theta$ obtained from the second nonlinear regression. For the narrowband case however, the instantaneous value of $\theta$ is almost never equal to the value of 0.34 obtained from the nonlinear regression, although the average of this instantaneous value is equal to 0.28. The reason for the peak in $\theta$ that occurs at around $\tau = 20$ is unclear at this stage and requires further investigation. The results are still at a relatively early dimensionless time compared to the quarter-scale $\theta$-group case in Thornber et al. [30] (here $t = 0.3$ s corresponds to $\tau = 16.9$ with that non-dimensionalisation), for which $0.2 \leq \theta \leq 0.25$ during this same period. Therefore $\theta$ may very likely start to increase again if the simulation is run to later times.

Comparing the results for $\theta$ to those presented in Jacobs et al. [8] provides some possible explanations for the differences between the two groups. Firstly, at early time the higher than expected values of $\theta$ (which are 0.51 and 0.54 respectively for the two groups) may be due to either the presence of unsaturated long wavelengths, or due to the interesting dynamics of the narrowband perturbation shown in Figure 6.8. However at later times it is clear that values of $\theta > 1/3$ are likely due to additional long wavelength modes that were present in the initial perturbation, which have saturated but are still dominating the overall growth rate of the layer. For example, in the experiments the two values of $\theta$ obtained at later times up until reshock were 0.38 and 0.29 respectively, which are close to the late-time values obtained for $\theta$ in the broadband and narrowband cases respectively. In reality, there was likely to have been additional long wavelength modes present in the initial perturbations for both groups, just that the amplitudes/wavelengths were larger in one group than the other such that these had a more significant effect on the growth of the layer.

Figure 6.9 shows the total fluctuating kinetic energy for each case along with a simple
anisotropy measure defined as

$$TKR = \frac{2 \times TKX}{TKY + TKZ}.$$  

where TKX, TKY and TKZ are the components of TKE in the x-, y- and z-directions respectively. The data are normalised by $\rho \tau (A_p \Delta u)^2 \lambda_{min} L^2$. Throughout the simulation, there is more TKE in the $m = -2$ than the $m = -1$ case, and similarly for the $m = -1$ case and the $m = 0$ case. This is due to the different initial impulses for the three cases, where a larger initial impulse deposits more kinetic energy. The discontinuous change in TKE that occurs shortly after $\tau = 10$ is due to the shock exiting the domain and thus the disappearance of the high frequency post-shock oscillations that are present when the shock propagates through SF$_6$.

**Figure 6.8** – Instantaneous growth rate exponent $\theta$ vs. dimensionless time for the narrowband ($m = 0$) and broadband ($m = -1, m = -2$) ILES cases. The data are plotted from the time of peak mix velocity (denoted by $\tau_p$) to the end of each simulation.
Beyond this time, the TKE that is contained in the mixing layer begins to decay and at late time each case decays at a noticeably different rate. Using linear regression from times $\tau = 100$ to $\tau = 175$, these decay rates are estimated to be $n = -1.2$, $n = -0.85$ and $n = -0.65$ for the $m = 0$ (narrowband), $m = -1$ and $m = -2$ (broadband) cases respectively. Based on the analysis presented in Section 5.3.3, these decay rates can also be used to estimate the value of theta over this period using the relation $n = 3\theta - 2$. In Chapter 5 it was shown that this relation does not hold for broadband initial perturbations, at least during the period of self-similar growth. However for the current cases, inverting the relation gives values of $\theta = 0.27$, $\theta = 0.38$ and $\theta = 0.45$ respectively, indicating that once the longest initial wavelength has saturated the decay rates $n$ tend towards values that are close to satisfying $n = 3\theta - 2$ (for the measured values of $\theta$ at late time). This indicates that care must be taken when using this relation to infer the value of $\theta$, as its accuracy will largely depend on whether the measurement of $n$ is made well after the saturation time of any long wavelength modes that may be present in the initial perturbation. Nevertheless it should also offer some reassurance to experimentalists that it is still possible to use
the measured decay rate of TKE to estimate $\theta$, just with a few caveats.

Briefly examining the simple anisotropy measure TKR, it is clear that each case is persistently anisotropic, in line with similar observations for purely narrowband perturbations made in Chapter 4 and Appendix D. There is a sharp initial drop in anisotropy that occurs when the shock exits the domain, after which TKR plateaus to a constant value in the broadband cases and a slow decay in the narrowband case. At the latest time TKR is equal to 1.54, 1.77 and 2.09 for the $m = 0$, $m = -1$ and $m = -2$ cases respectively. There is potentially an Atwood number dependence for this measure, for example see the results for TKR in Appendix D for the standard and quarter-scale $\theta$-group cases where $A = 0.5$, as well as what appears to be a dependence on the initial conditions, although this could just be due to the different initial impulses. For example, in Chapter 5 the $m = -1$ cases were seen to be the most anisotropic (as measured by the ratio $W_s/W_b$) but they also had the largest initial impulse.

6.3.2 DNS

The same preliminary analysis that was performed above for the ILES cases is now also performed for the DNS cases. Prior to this however, it is important to restate the motivation for performing DNS of this setup, since the ILES results appear to be much more representative of the experiments of Jacobs et al. [8] and Krivets et al. [6] and are perhaps sufficient for demonstrating the effects of additional long wavelength perturbations. There are limitations to what can be appropriately analysed using ILES however, such as the transitional phase of mixing layer development as well as small-scale quantities in fully-developed flow, and in the absence of accurate subgrid models for these types of flows one must resort to DNS. Indeed, in order to develop accurate subgrid models for these types of flows, DNS, along with experiments, should be what is used to guide this development. Therefore the motivation remains the same as that which was stated in Chapter 4; to improve the understanding of turbulent mixing due to RMI and guide the development of reduced-order modelling techniques.
and sub-grid models for these flows. Using a computational setup that is possible to replicate experimentally is therefore a useful step in that direction. It is also highly desirable to perform DNS of broadband initial conditions specifically, both to extend the analysis of Chapter 4 and also to verify the results of Chapter 5 (for example the variation in $C_\epsilon$).

Figures 6.10 and 6.11 show the development of the mixing layer for the $Re_0 = 122$ (narrowband), $Re_0 = 261$, $Re_0 = 526$ and $Re_0 = 1051$ (broadband) DNS cases at times $\tau = 11.1$ and $\tau = 46.2$ respectively, in the $x$-$y$ plane located at $z = 0$. The effects of viscosity (and diffusivity) are quite noticeable at these Reynolds numbers, with the significant damping of the small-scale structures that were present in the ILES cases occurring, particularly at later times. There is still a wide range of scales and more heterogeneity present in the broadband cases, due to the bandwidth of the initial perturbation, however the narrowband case is quite homogeneous and diffuse. Higher Reynolds numbers could be achieved for this case by increasing $\lambda_{\text{min}}$ relative to the grid size, in other words by using a perturbation similar to the one used in Chapter 4, however the aim here is to demonstrate the effects of additional long wavelength modes for the same value of $\bar{\mu}$.

It is interesting to observe that even for the $Re_0 = 1051$ case, there are virtually no secondary instabilities present, whereas equivalent values of $Re_0$ in the narrowband DNS cases of Chapter 4 have much greater amounts of small-scale fluctuations due to secondary instabilities. This is most likely due to much smaller ratios of the amplitudes of the largest wavelengths (in the broadband cases) to the initial diffuse interface thickness, as well as the fact that the mixing layer itself is much more diffuse by the time these large wavelengths start to saturate and grow nonlinearly. This poses an additional challenge for conducting DNS with broadband perturbations, as an initial diffuse thickness is required in order to fully resolve the interface at early time. As can be seen in the grid convergence study for these DNS cases, presented below, the current initial diffuse thickness ($\delta = \lambda_{\text{min}}/4$) already makes it quite challenging to fully resolve the initial impulse.
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(a) $Re_0 = 122 \ (m = 0)$.

(b) $Re_0 = 261 \ (m = -1)$.

(c) $Re_0 = 526 \ (m = -2)$.

(d) $Re_0 = 1051 \ (m = -2)$.

Figure 6.10 – Contours of volume fraction $f_1$ for the DNS cases at time $\tau = 11.1$. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
Figure 6.11 – Contours of volume fraction $f_1$ for the DNS cases at time $\tau = 46.2$. The major ticks on both axes correspond to a grid spacing of $\Delta x = 1$ m.
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Figures 6.12–6.16 demonstrate grid convergence in the integral width, molecular mixing fraction, total fluctuating kinetic energy and domain-integrated enstrophy and scalar dissipation rate for the four DNS cases. Each of the different Reynolds number cases are shown to be suitably converged for each of these integral quantities at the finest grid resolution considered, even during the early-time period prior to the shock exiting the domain.

Grid convergence
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Figure 6.13 – Convergence of molecular mixing fraction for the air–SF₆ DNS cases.

Comparisons with ILES

The following figures compare the integral quantities shown in Figures 6.12–6.14 obtained from the various DNS cases with their respective ILES counterparts. Figure 6.17 shows the comparison of integral width between each of the DNS and ILES cases. In each case the effect of finite Reynolds number is to reduce the integral width in comparison to the ILES result, with the higher $Re_0$ cases closer to their respective ILES results, particularly at later times. This is because the growth of $W$ is dominated by the longer wavelengths at these times, which are less affected by viscosity.
than smaller wavelengths. This is true even after the longest initial wavelength has saturated, especially in the $m = -2$ simulations, even though there are negligible amounts of secondary instabilities induced.

In general, care must be taken when using the integral width $W$ to estimate $\theta$ for a finite Reynolds number case, especially when this is used to impute the value of $\theta$ for some other measure of the layer width, such as the visual width $H$ or the peak-to-peak width $h$. This is because $W$ is a measure of both width and mix, therefore at low Reynolds number diffusive mixing may be a significant contributing factor rather than
just a reduction in the physical width of the layer. Nonetheless, nonlinear regression
is used as before to fit a model of the form $W = \beta (\tau - \tau_0)^\theta$ to the data. Doing so
gives a value of $\theta = 0.33$ for the $Re_0 = 122$ (narrowband) case over the time period
from peak mix velocity to the end of the simulation at $\tau = 58$. This is very close to
the value of 0.34 that was obtained from the ILES data, suggesting that most of the
reduction in $W$ comes from a reduction in the prefactor $\beta$, which is equal to 0.19 in
the DNS and 0.24 in the ILES. For the $Re_0 = 261$ ($m = -1$) case, $\theta = 0.49$ prior to
saturation of the longest wavelength, which is close to both the ILES result of 0.47
over this period and the theoretical value of $1/2$. For the period of time after this to the end of the simulation a value of $\theta = 0.47$ was obtained, although this is not really long enough to capture the behaviour after saturation has occurred. For the $Re_0 = 526$ and $Re_0 = 1051$ ($m = -2$) cases, values of $\theta = 0.72$ and $\theta = 0.70$ were obtained over the period of time prior to saturation of the longest wavelength, both of which are slightly higher than the value of 0.69 for the ILES case. For the period of time after this to the end of the simulation values of $\theta = 0.49$ were obtained for both DNS cases. Note that estimates of an instantaneous value of $\theta$ for the DNS cases
Figure 6.17 – Comparison of integral width between the ILES and DNS cases

Figure 6.18 – Comparison of molecular mixing fraction between the ILES and DNS cases

would require making modifications to the simple buoyancy-drag model to account for the effects of viscosity. These estimates could also be made more accurate by including a varying effective length scale, as in the studies of Youngs and Thornber [48, 49].

Figure 6.18 shows the comparison of molecular mixing fraction $\Theta$ between each of the DNS and ILES cases, for which the effects of finite Reynolds number are much more apparent. The observations made for Figure 6.10 and Figure 6.11 regarding homogeneity of the mixing layer are also quantified here, with both the minimum and late-time value of $\Theta$ decreasing with increasing $Re_0$ (and decreasing $m$). The difference between the value of $\Theta$ in the DNS cases compared with their respective ILES case is also greatest at the point of minimum mix and then decreases as the simulation progresses. Figure 6.19 compares the total fluctuating kinetic energy between each of
the DNS and ILES cases. Following the same trend as in Figure 6.18, the DNS data become increasingly close to the respective ILES results as $Re_0$ is increased. The lack of any significant secondary instabilities means that there is still a large gap between the TKE in the ILES cases and that in the DNS cases however. For the $Re_0 = 122$ ($m = 0$) case the flow field is so diffuse that there are substantial differences with the TKE in the equivalent ILES case even right after shock passage. Also note that the shock exits the domain earlier in the $Re_0 = 1051$ case due to the reduced domain size, hence the earlier discontinuous drop in TKE. Finally, the latest time shown here is still too early to give a good estimate for $n$, the late-time decay rate of TKE. The DNS cases would likely need to be run to much later dimensionless times without significant influence of viscosity (i.e. at higher Reynolds numbers so that significant secondary motions are produced) in order to give a good estimate for $n$.

6.4 Conclusions

This chapter has presented simulations of an idealised shock tube experiment between air and sulphur hexafluoride that build upon the previous results and analysis presented in Chapters 3–5. In particular, the effects of additional long wavelength modes in the initial perturbation were explored by comparing the results obtained using a narrowband surface perturbation (similar to the one presented in Chapter
4) and two broadband perturbations (similar to those in Chapter 5). The narrowband perturbation consisted of initial wavelengths ranging from $\lambda_{\text{min}} = L/32$ up to $\lambda_{\text{max}} = L/16$ with spectral exponent $m = 0$, while for the broadband perturbations $\lambda_{\text{min}}$ was the same but $\lambda_{\text{max}}$ was set to $L/2$ and the spectral exponents were $m = -1$ and $m = -2$ respectively. Preliminary results, suitably non-dimensionalised to allow for comparison with the experiments of Jacobs et al. [8], were presented using various integral quantities for both the ILES and DNS cases, showing that there are substantial differences in late-time growth rates of the mixing layer width and decay rates of fluctuating kinetic energy for the different initial perturbations. Furthermore, these results provide some possible explanations for different behaviours that have been observed in shock tube experiments with multi-mode initial perturbations, such as the ones presented in Jacobs et al. [8] and Krivets et al. [6], and are summarised as follows.

For the ILES cases, the additional long wavelength modes in the broadband perturbations lead to substantial increases in the width of the mixing layer, as well as the growth rate. Using nonlinear regression, the growth rate exponent of the mixing layer width was estimated to be $\theta = 0.34$ in the narrowband case. For the $m = -1$ broadband case, $\theta$ was estimated to be 0.47 during the period where the growth rate is dominated by the just-saturating mode and reduced to $\theta = 0.41$ in the period after the longest initial wavelength had saturated. For the $m = -2$ broadband case, $\theta$ was found to be 0.69 and 0.44 over these equivalent periods. Similarly for the total fluctuating kinetic energy, the additional long wavelength modes in the broadband perturbations were found to give reduced decay rates, which were estimated at late time to be $n = -1.2$, $n = -0.85$ and $n = -0.65$ for the $m = 0$ (narrowband), $m = -1$ and $m = -2$ (broadband) cases respectively. These were also shown to approximately satisfy the relation $n = 3\theta - 2$, indicating that the decay of TKE is close to self-similar.

For the DNS cases four different initial Reynolds numbers were considered; $Re_0 = 122$ ($m = 0$), $Re_0 = 261$ ($m = -1$), $Re_0 = 526$ ($m = -2$) and $Re_0 = 1051$ ($m = -2$), the results for which were compared with their respective ILES counterparts. In terms of integral width, the effects of finite Reynolds number were significant for the $Re_0 = 122$
case but became negligible as $Re_0$ was increased, despite there being no noticeable secondary instabilities induced (even in the $Re_0 = 1051$ case). In all cases the effects of viscosity on the growth rate exponent $\theta$ were marginal at most. Much greater differences were observed in the molecular mixing fraction however, which was much larger in all of the DNS cases due to the homogenising effects of diffusion, as well as for the TKE, which was much smaller due to the lack of secondary motions.

As has already been emphasised, these results are preliminary and do not represent a complete analysis of these cases. It is anticipated that much more insight can be gained by applying the same methods as those used in Chapter 4, and indeed this will be performed in future work. A particular focus will be on differences in the normalised dissipation rates (and other important quantities for modelling) that exist when there are unsaturated long wavelength modes present and which are dominating the growth of the layer. As always, DNS data at higher Reynolds numbers helps provide additional insight and for the narrowband perturbation comparable Reynolds numbers to those simulations in Chapter 4 may be obtained by simply increasing the wavelengths in the perturbation relative to the size of the domain (i.e. use $\lambda_{\text{min}} = L/8$ and $\lambda_{\text{max}} = L/4$). For the broadband perturbations, there are significantly greater challenges to obtaining higher Reynolds numbers that are imposed by the greater range of length scales in the initial perturbation, as well as the desire for all initial amplitudes to remain linear. The initial diffuse thickness of the interface that is required in order to be able to fully resolve the initial impulse also has detrimental effects, mainly that it suppresses the growth of secondary instabilities and hence the transition to turbulence.

Nonetheless, it is likely that the current broadband cases will still be useful for estimating the effects of additional long wavelength modes at higher Reynolds numbers, especially when used in conjunction with higher Reynolds number narrowband simulations. This is similar to how the lower Reynolds number simulations in Chapter 4 were still useful for estimating trends at higher Reynolds numbers. There are also several options for at least partially overcoming the obstacles mentioned here that should be explored further. One of these is the use of higher grid resolutions (i.e. $4096^2$ cross-
section) at very early times and then filtering these results onto coarser grids as time progresses and resolution requirements decrease. This would allow for both higher initial Reynolds numbers and smaller initial diffuse interface thicknesses while also remaining fully resolved. For a finite-volume algorithm on Cartesian grids this filtering process is easy to perform while also remaining conservative; it is simply a box filter applied to the cell averages. A more effective, but also more time-intensive, version of this would be to implement some form of adaptive mesh refinement. Finally, the use of interface sharpening/tracking could also help with resolving the initial impulse for smaller initial diffuse interface thicknesses. This sharpening/tracking could then be terminated once the interface is able to be fully resolved on the computational grid.
Chapter 7

Conclusions & Further Work

7.1 Summary of current research

The main aim of this thesis was to make significant contributions to improving the understanding of turbulent mixing driven by the Richtmyer–Meshkov instability using high-fidelity numerical simulations. This was motivated by the importance of turbulent mixing in applications such as inertial confinement fusion, high-speed combustion and various astrophysical flows, where the extreme nature of these types of flows makes gathering detailed and accurate experimental data either difficult or impossible. The general approach taken in this thesis has been to use a series of well-designed numerical simulations of canonical flows to inform the theory and modelling of shock-induced turbulent mixing in the applications mentioned above. In particular, the focus has been on the effects of Reynolds number on the transition to turbulence as well as the influence of initial conditions, both of which are key issues in accurately modelling turbulent mixing in these types of applications. Where appropriate, this has been analysed using the technique of implicit large eddy simulation. However, in general, directly simulating the governing equations without any modelling assumptions is required for generating the level of detailed insight into the flow physics that is needed for model development. This is particularly true for transitional flows and was therefore the main approach used in this thesis.
Given the extremely resource-intensive nature of DNS, the initial focus was on ensuring that the numerical method used was capable of efficiently simulating mixtures of arbitrary gases, given the well-documented deficiencies of the standard four-equation mass fraction model. This lead to the development of the five-equation number fraction model, which was presented in Chapter 3. For the 1D test problems considered, both the new five-equation model and the standard four-equation model were shown to be second-order accurate. However, the five-equation model was approximately one order of magnitude more accurate for a given grid resolution on problems where the ratio of specific heats varies with mixture composition. Unlike other quasi-conservative models, the new model is suitable for DNS (and explicit LES) and was shown to be up to $40 \times$ as efficient as the standard four-equation model on a 2D single-mode RMI test case.

As a first step towards using DNS to analyse the transition to turbulence in RMI-induced flows, an appropriate test case needed to be defined. This was performed in Chapter 4, where an existing benchmark case for ILES was adapted to be suitable for DNS. This test case, based on the standard problem from the $\theta$-group collaboration, consisted of a narrowband initial surface perturbation in a heavy-light configuration, a $M = 1.84$ shock and a post-shock Atwood number of $A^+ = 0.487$. A methodology for assessing the level of grid convergence was also developed, based on domain-integrated and spectral quantities that involve gradients of the solution and are therefore biased towards contributions from the smallest scales of motion. It was shown that satisfactory convergence in these quantities was also consistent with resolving the Kolmogorov scale. Comparisons were made with the results of a previous ILES calculation of the same test case, showing that the decay rate of TKE was greater in the DNS and that less TKE was transferred to the transverse components, resulting in greater anisotropy. However, the overall agreement in the motion of the large scales between the DNS and ILES was found to be very good and resulted in negligible differences in the growth rate exponent $\theta$.

Following the initial analysis and comparison with ILES, a full Reynolds number sweep was performed using this initial condition. For integral quantities such as the
molecular mixing fraction and normalised mixed mass, the observed Reynolds number trends were used to estimate the high Reynolds number limit of features such as the point of minimum mix and late time asymptotic value. Only minor variation with Reynolds number was observed in the integral width, and a decomposition into separate bubble and spike widths showed that both quantities grow with the same exponent $\theta$ at late time. An analysis of the Reynolds number dependence for various statistics of the velocity and scalar fields was also presented. For the velocity field statistics, the decay rates of turbulent kinetic energy and dissipation rate were shown to decrease with increasing Reynolds number, while the spatial distribution of both of these quantities was shown to be biased towards the spike side of the layer. This was also true of the distribution of the various measures of anisotropy considered, and was shown to be due to highly energetic spikes that had escaped the main mixing layer. A decomposition of the turbulent kinetic energy spectra into incompressible and compressible components showed that, at early time, there are important contributions to the energy budget at low to intermediate wavenumbers due to compressibility.

For the scalar field statistics there was less variation with Reynolds number, particularly at later times, and the two fluids were shown to be less mixed on the bubble side of the layer. The Reynolds number dependence of the normalised dissipation rates was also analysed, and fitting an appropriate functional form to the data allowed for the estimation of the high Reynolds number asymptotic value for both of these quantities. Finally, an evaluation of the mixing transition criterion for unsteady flows was performed, showing that even for the highest Reynolds number case the turbulence in the flow is not fully developed. However, by considering the theoretical rate at which the ratio of inner-viscous and diffusion layer length scales should vary, the critical Reynolds number at which fully developed turbulence should be obtained was able to be estimated from the current data.

In concurrence with performing DNS of the idealised narrowband initial condition to analyse Reynolds number effects, a separate body of work was conducted investigating the influence of initial conditions using ILES and which was presented in Chapter 5. In particular, broadband initial perturbations were considered which contain a much
larger range of initial wavelengths and are therefore also more representative of the initial conditions encountered in practical applications. Different families of initial conditions were generated by varying the bandwidth of initial modes and the slope of the initial power spectra and a good collapse of the data for various integral quantities was obtained between the different cases when suitably non-dimensionalised. The values of the growth rate exponent $\theta$ were shown to compare favourably with theoretical predictions for the infinite bandwidth limit. The decay rates of TKE were also shown to be much lower than in the narrowband case, since the flow at low wavenumbers is largely irrotational and therefore does not dissipate as quickly as in a fully developed mixing layer. Furthermore, it was shown that because of the presence of slowly growing unsaturated modes in these cases, a commonly employed empirical relation between the growth rate exponent $\theta$ and the TKE decay rate $n$ that is derived using dimensional analysis does not hold. The results of this chapter provided good validation of theoretical approaches that analyse the growth of the mixing layer in terms of linear growth rates of individual modes in the perturbation, as well as highlighting where this analysis fails to accurately capture the behaviour of the mixing layer.

The final piece of work presented in this thesis combined the methodologies of both Chapter 4 and Chapter 5 to conduct ILES and DNS calculations of an idealised shock tube experiment. Specifically, the effects of additional long wavelength modes in the initial surface perturbation were explored by comparing the results obtained using a narrowband initial condition and two broadband initial conditions. The results from the ILES cases showed that substantial differences are produced in the late-time growth rate of the mixing layer width and the decay rate of TKE when additional long wavelength, low amplitude modes are included in the initial perturbation. These differences persisted well after the saturation time of the longest initial wavelength in the broadband perturbations. The results also provided some possible explanations for the different growth rate exponents that have been observed in shock tube experiments with multi-mode initial conditions.

In addition to ILES, DNS of the same computational setup was also performed for
four different initial Reynolds numbers. A preliminary analysis of the results of these simulations focused on comparisons with those from the ILES cases, with similar trends observed to those in Chapter 4 regarding differences in integral properties. It was also observed that, for equivalent values of the initial Reynolds number, the broadband DNS cases of Chapter 6 exhibited far fewer motions due to secondary instabilities than the narrowband DNS cases in Chapter 4. In explaining why this occurs, several aspects were highlighted that demonstrate the additional challenges for obtaining fully developed turbulence in a DNS with broadband initial conditions, relative to purely narrowband ones. However, through the use of both DNS and ILES to capture the low and high Reynolds number limiting behaviour, the results for narrowband and broadband perturbations may be combined to provide a clearer picture of what corrections should be applied to account for the effects of low Reynolds number or overly idealised initial conditions. More importantly, the new computational setup that has been developed allows for the generation and analysis of data that can be verified experimentally. This has the potential to lead to the use of experiments to identify shortcomings in the numerical approach, which in turn would allow for improved confidence in the ability of numerical simulations to accurately model the more complicated aspects of shock-induced turbulent mixing.

7.2 Recommendations for future research

Based on the research presented in this thesis, the following recommendations for future work on the topics covered here can be made. These are divided into two broad areas; numerical modelling of compressible multispecies flows and the physics of shock-induced turbulent mixing.

7.2.1 Numerical modelling of compressible multispecies flows

From the review of the literature on numerical modelling of RMI performed in Chapter 2, two novel approaches were identified that seem worthy of further investigation.
7.2 Recommendations for future research

The first involves the use of a velocity perturbation for initialising an RMI calculation. While this is not novel in and of itself, it has the potential to be used in novel ways due to the fact that a shock wave does not need to be explicitly calculated. For low to moderate shock Mach numbers, where the post-shock flow is approximately incompressible and therefore sufficiently smooth, using a velocity perturbation would allow for the application of a spectral method. For a planar configuration, the inhomogeneous direction could be handled in a number of ways, for example by using an appropriate basis function (i.e., Chebyshev polynomials) or by using a triply-periodic domain and initialising a second, unperturbed interface far away from the primary one. The second approach worthy of further investigation is the use of interface tracking in combination with a diffuse interface model for situations where the interface thickness is small with respect to the grid size. As an example, the volume-of-fluid interface reconstruction method has the potential to be combined with the new five-equation model that was presented in Chapter 3. Chapter 6 demonstrates such a situation where this could be useful; by allowing for smaller initial diffuse interface thicknesses while still sufficiently resolving the initial impulse.

With regards to modifications to the current numerical method, the test cases in Appendix C highlight that some form of adaptive mesh refinement may be quite beneficial for improving the convergence of DNS cases. While increasing the resolution of the inviscid and viscous flux approximations for the same formal order of accuracy gave mixed results, increasing the overall formal order of accuracy of the numerical method may provide greater improvements, especially when used in conjunction with adaptive mesh refinement. In the longer term, the development of a unified hyperbolic model for mixtures of viscous, compressible, miscible fluids would also be of great interest. Appendix B presents some early work in this direction. This appears to be the most straightforward way to applying state-of-the-art arbitrarily high-order accurate methods to DNS of compressible turbulent mixing problems. It would also allow for exploring regimes where the conventional multicomponent Navier–Stokes equations fail to accurately capture reality, for example when finite relaxation times begin to become important.
7.2 Recommendations for future research

7.2.2 Physics of shock-induced turbulent mixing

Starting with the obvious, it is important to continue to achieve increasingly high Reynolds numbers in DNS of RMI-induced turbulence. The ultimate aim here is to eventually reach the minimum state Reynolds number, at which point the dynamics of the energy-containing scales are completely independent of the dissipation mechanism in the flow. A DNS at this Reynolds number could, in theory, be used to construct the ideal sub-grid model for that specific flow at any arbitrarily higher Reynolds number of practical interest. The path towards achieving a fully resolved simulation at the minimum state Reynolds number will be driven by algorithmic progress, such as the suggestions given above, as well as increases in computing efficiency through increasingly powerful/specialised hardware and better utilisation of it. In addition to higher Reynolds numbers, another focus should be on extending the present dataset to other Schmidt, Atwood and Mach numbers. This has already begun with the simulations presented in Chapter 6, and should be motivated by gas combinations and Mach numbers of practical interest (for example, air and hydrogen in a scramjet combustor).

The other major theme of the research presented in this thesis has been the influence of initial conditions, in particular the effects of long wavelength, largely irrotational modes on the growth of the mixing layer. While these broadband initial conditions are more representative of those in real RMI flows, they are still somewhat idealised. It is possible to extend the methodology presented here to incorporate initial conditions with multiple distinct spectral ranges and analyse the effects of this. Another potentially fruitful line of investigation would be to extend the just-saturated mode theory to include some of the effects of nonlinearity (i.e. by using a more complex expression for the growth rate of each individual mode) and then validate this against simulations with nonlinear amplitudes. The effects of viscosity may also be incorporated into this theory through modifications to the growth rate of each individual mode, which can be calculated using the results of 2D single-mode DNS cases. Similarly, given the challenges of conducting DNS of broadband perturbations, it would be useful to find ways in which results from narrowband perturbations can be related
to results from broadband perturbations for quantities such as integral width and TKE.

![Figure 7.1](image)

**Figure 7.1** – A priori assessment of the Smagorinsky sub-grid closure model, comparing the actual dissipation rate with the modelled dissipation rate based on the filtered DNS flow field.

Finally, there is plenty of scope for using the current DNS and ILES datasets to calibrate various reduced-order models. Following Thornber et al. [105], where the budgets of transport equations for the mean momentum, mean mass fraction, turbulent kinetic energy and mass fraction variance were examined using data from the $\theta$-group collaboration [30], the same analysis should be performed using the broadband ILES dataset presented in Chapter 5. It would also be simple to include the terms that were neglected in those budgets (since the ILES calculations were nominally inviscid).
and apply them to the DNS dataset from Chapter 4 as well. To conclude, an example will be given of how the current DNS data may be used to assess the efficacy of common LES subgrid closure models for compressible flows. Taking the solution at the latest time \( t = 0.10 \) s in the \( Re_0 = 1826 \) narrowband DNS case from Chapter 4 and applying a box filter with a filter width of \( \bar{\Delta} = 64\Delta \), the filtered dissipation rate is compared with the dissipation rate calculated by applying the Smagorinsky closure model to the filtered velocity field [29]. A scatter plot is shown in Figure 7.1, including the line of best fit to the data. Without going into unnecessary detail, it is clear than the modelled dissipation is in general not sufficient, since this line of best fit is well below the line \( y = x \) that indicates the ideal contribution from the sub-grid closure model. Assessments of this kind provide a way for determining appropriate modifications to existing sub-grid closure models and highlight the importance of achieving the highest possible Reynolds number in a DNS, so that any modifications that are made are applicable to flows of practical interest.
7.2 Recommendations for future research
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Appendix A

Application of the Five-Equation Model to a Mixture of Air and CH$_4$

This appendix considers two fundamental test cases in one-dimension, in order to demonstrate the advantage of the new five-equation model (referred to here as the volume fraction model) over the standard four-equation model for simulating multispecies flows$^1$. By considering the simple case of (approximately) incompressible diffusion between two quiescent gases, the availability of an analytical solution allows us to assess the accuracy of both approaches by performing formal grid convergence studies. Galilean invariance of the governing equations also allows us to analyse the effects of advection by performing the same grid convergence study but with an additional velocity applied to the interface.

A.1 Diffusion of air and methane

The first test case considers the diffusion of air and methane on a domain of $0 \leq x \leq 1$ m, with reflective boundary conditions applied and grid sizes ranging from 32 to 2048

The ideal gas equation of state is used for both gases, which have a fixed ratio of specific heats of $\gamma_{\text{air}} = 1.4$ and $\gamma_{\text{CH}_4} = 1.32$ respectively. The initial pressure and temperature are $p = 100000$ Pa and $T = 300$ K, and the molecular weights are taken to be $W_{\text{air}} = 28.964$ g/mol and $W_{\text{CH}_4} = 16.0425$ g/mol, resulting in a density ratio of 1.805. The analytical solution for the volume fraction distribution is given by

$$f_1 = \frac{1}{2} \left[ 1 - \text{erf} \left( \frac{x - x_0}{\sqrt{4Dt + h_0^2}} \right) \right], \quad (A.1)$$

where $x_0 = 0.5$ m, $h_0 = 0.02$ m and the diffusion coefficient is artificially fixed to be $D = 0.01$ m$^2$/s. The velocity field is initialised by assuming that the volume-weighted velocity is initially zero, which is equivalent to stating that the divergence of the mass-weighted velocity field must be zero. The grid convergence study is performed by comparing the computed and analytical volume fraction profiles for each grid resolution. The expected order of accuracy of the algorithm is second order. Table A.1 gives the errors norms for the five-equation volume fraction model, while
Table A.2 gives the errors norms for the four-equation mass fraction model. As can be seen in Table A.1 and Table A.2, the mass fraction model is actually more accurate for this particular test case. There are two reasons for why this is the case. Firstly, the majority of the errors that arise in the mass fraction approach are produced when the material interface is advected through the computational mesh [158, 153]. Secondly, the current discretisation is derived for advection-dominated flows, as there is no feedback of the source terms (i.e. viscosity, diffusion) back onto the inviscid flux component. This affects the volume fraction model more severely as part of the diffusion of species volume fraction is calculated in the inviscid flux subroutine and the remainder calculated in the viscous flux subroutine. Even though the amount of diffusion in this test case has been amplified by a few orders of magnitude, this is still not an ideal approach and future work should be aimed at mitigating such errors by discretising the advection and source terms together in a unified framework.
Table A.3 – Error norms for Case 2 at $t = 0.5$ s for the volume fraction model.

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>$L^1$</th>
<th>$L^\infty$</th>
<th>$O(L^1)$</th>
<th>$O(L^\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>3.28E-03</td>
<td>5.04E-03</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>64</td>
<td>2.04E-04</td>
<td>3.31E-04</td>
<td>4.01</td>
<td>3.93</td>
</tr>
<tr>
<td>128</td>
<td>7.55E-05</td>
<td>1.48E-04</td>
<td>1.43</td>
<td>1.16</td>
</tr>
<tr>
<td>256</td>
<td>1.98E-05</td>
<td>3.77E-05</td>
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<td>1.97</td>
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<tr>
<td>512</td>
<td>5.01E-06</td>
<td>9.35E-06</td>
<td>1.98</td>
<td>2.01</td>
</tr>
<tr>
<td>1024</td>
<td>1.28E-06</td>
<td>2.34E-06</td>
<td>1.97</td>
<td>2.00</td>
</tr>
<tr>
<td>2048</td>
<td>3.42E-07</td>
<td>5.88E-07</td>
<td>1.90</td>
<td>1.99</td>
</tr>
</tbody>
</table>

Figure A.1 displays the error norms contained in Table A.1 and Table A.2 as a log-log plot, showing that second-order accuracy is obtained for both the mass fraction and volume fraction models. The slightly lower order of convergence shown for both models at the finest grid resolution is because the analytical solution is for incompressible mixing, whereas very small compressibility effects are becoming resolved in the simulations.

A.2 Advection-diffusion of air and methane

The second test case considers the same process of diffusion of air and methane, but this time with an additional mean velocity of 4 m/s applied, with the domain now $0 \leq x \leq 2$ m and the boundary conditions changed to periodic. In other words, the previous case has been mirrored about $x = 1$ m and is advected until the interface returns to its starting position at $t = 0.5$ s. The initial conditions are the same as for Case 1, and the grid sizes used in the convergence study are also doubled so as to maintain the same grid spacing. Table A.3 gives the errors norms for the volume fraction model, while Table A.4 gives the errors norms for the mass fraction model. With the additional advection of the interface the advantage of the five-equation model becomes clear, with the results close to an order of magnitude more accurate. This highlights the motivation for developing the new model, as usually some advection will be present in a turbulent mixing calculation. The results shown in Table A.3 and Table A.4 and visualised in Figure A.2 show that for the same error,
the volume fraction model can be run on somewhere between a half to a quarter of the grid resolution. Even though the five-equation model is roughly $1.25\sim 1.5\times$ more computationally expensive, this result indicates that it can still produce equivalent results for somewhere between 10% to 40% of the cost of the mass fraction model in one dimension (assuming a CFL restriction on the time step size).

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>$L^1$</th>
<th>$L^\infty$</th>
<th>$O(L^1)$</th>
<th>$O(L^\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>32</td>
<td>7.91E-03</td>
<td>1.74E-02</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>64</td>
<td>2.15E-03</td>
<td>4.32E-03</td>
<td>1.88</td>
<td>2.01</td>
</tr>
<tr>
<td>128</td>
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<td>2.86E-04</td>
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<td>2.00</td>
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<tr>
<td>512</td>
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<td>2.00</td>
<td>2.00</td>
</tr>
<tr>
<td>1024</td>
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<td>2.00</td>
</tr>
<tr>
<td>2048</td>
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<td>1.99</td>
<td>2.00</td>
</tr>
</tbody>
</table>

**Table A.4** – Error norms for Case 2 at $t = 0.5$ s for the mass fraction model.

**Figure A.2** – Comparison of error norms for the mass fraction (MF) and volume fraction (VF) models for Case 1.
Appendix B

A First-Order Hyperbolic Reformulation of the Four-Equation Model

In this appendix, a reformulation of the compressible multicomponent Navier–Stokes equations that govern the behaviour of mixtures of miscible gases is introduced\(^1\). The resulting equation set is a first-order hyperbolic system containing stiff source terms, which recovers the conventional parabolic theory of viscosity, conduction and diffusion as a first-order approximation in the relaxation limit. An important advantage of this approach versus other first-order reformulations of the Navier–Stokes equations is that the wave speeds remain finite as some relaxation parameter tends to zero. The complete system of equations is presented in one-dimension for binary mixtures of viscous, heat conducting gases.

The motivation for this model is the same as for the five-equation model introduced in Section 3.3, namely the desire to conduct direct numerical simulations of flows that contain shock waves, material interfaces and fine-scale turbulent structures. As outlined in Chapter 2, this combination of flow features poses significant conflict-

\(^1\)The work presented in this appendix has been published in Groom, M., Thornber, B., Roman- ski, E. (2018). Hyperbolic governing equations for miscible and viscous compressible fluids, In Proceedings of the 10th International Conference on Computational Fluid Dynamics, Barcelona, Spain.
B.1 First-order hyperbolic formulation of continuum mechanics with binary diffusion

ing requirements on the numerical method, which must be both robust enough to capture the various discontinuities in the flow but still have good fidelity in the high wavenumber range. In particular for DNS, the numerical method should preferably be high-order accurate in multiple dimensions as this will greatly increase the efficiency of the computation \[214\]. Numerical methods that satisfy all of these requirements are most easily designed for systems of hyperbolic conservation laws, as the theory of hyperbolic partial differential equations is much more advanced than for more general systems \[97\].

B.1 First-order hyperbolic formulation of continuum mechanics with binary diffusion

Recently, a unified first-order hyperbolic formulation of continuum mechanics has been proposed in \[215, 216\], which is in theory capable of describing the entire spectrum of viscous flows and even elastic and plastic deformations in solids. The main features of this model that are desirable from both a mathematical and physical standpoint are that it is a consistent, overdetermined system that is compatible with the first and second laws of thermodynamics and is symmetric hyperbolic, which implies that it is well-posed and causal \[216\]. Dissipative processes are modelled as algebraic source terms with a characteristic relaxation time for each process. Since these terms do not depend on any space derivatives, the characteristic speeds of the system remain finite regardless of whatever value the relaxation time takes, unlike other relaxation approaches that are used in hyperbolic reformulations of the Navier-Stokes equations \[217, 171\]. Through formal asymptotic expansion it can be shown that this purely hyperbolic description of viscous dissipation and thermal conduction includes Newton’s law of viscosity and Fourier’s law of conduction as a first order approximation in the stiff relaxation limit. The work presented in the following sections builds on this model by adding a hyperbolic description of binary diffusion of gaseous mixtures to the existing framework.
A first-order hyperbolic system is also advantageous for various numerical reasons as well, as it will be less sensitive to irregularities in the computational mesh when simulating complex geometries. It will also allow for a higher order of accuracy scheme for a given stencil and will be subject to a less restrictive stability condition ($O(\Delta x)$ vs. $O(\Delta x^2)$). In cells where the time step in a conventional Navier-Stokes code would be viscous limited (such as in a boundary layer), the time step in a first-order hyperbolic model would only be subject to a CFL condition, giving a $O(1/\Delta x)$ speedup in computational efficiency [217]. Hyperbolicity also means that a wide range of numerical methods are available (e.g. finite volume [97], discontinuous Galerkin [218], residual distribution [219], active flux [220]), allowing the use of the best suited numerical method for the problem at hand. Thus methods that were developed for the inviscid part of the Navier-Stokes equations, such as upwind fluxes and limiters, can be directly applied to the entire hyperbolic model, enabling a simple and uniform discretisation.

Given the many advantages outlined above to having a first-order hyperbolic formulation of viscous fluid dynamics, it is therefore of great interest to investigate whether the formulation can be extended to include diffusion in the miscible, multi-component case. For the sake of simplicity only binary diffusion will be considered here. Given the nature of the model, it is only necessary to consider mass diffusion and heat conduction in the initial formulation, the terms relating to viscosity can be included afterwards for the complete description. The derivation is structured as follows; starting from a master system of generating equations (inspired by a single entropy approximation of the equations governing multiphase flow), source terms are introduced such that the production of entropy is non-negative. Following this, the link with the classical theory of binary diffusion is established by considering the kinetic coefficients of these source terms in the relaxation limit. The derivation is completed by presenting the new system of equations in terms of the parameters of state.
B.1 First-order hyperbolic formulation of continuum mechanics with binary diffusion

B.1.1 Generating system of conservation laws for binary mixtures

In this section a master system for compressible and miscible binary mixtures is formulated, from which the governing equations are generated. The form of the master system is inspired by the equations of multiphase flow, specifically the single entropy approximation presented in [221] where the mixture is characterised by a single entropy $s$. As in the multicomponent Navier-Stokes equations, both species are assumed to be in pressure and temperature equilibrium. In one dimension, the parameters of state that describe the mixture are

$$\{\rho, Y_1, u, \dot{w}, J, s\}$$

The definitions of $\rho$, $Y_1$ and $u$ are the same as in the conventional theory, however two new state parameters are introduced to incorporate mass diffusion and heat conduction as per the theory of thermodynamically compatible systems [222]. The thermal impulse $J$ has been introduced previously in [216], while $\dot{w}$ is an artificial variable (of similar form to the relative velocity $w$ used in multiphase models) that is defined such that its energy gradient in state space, $\frac{\partial E}{\partial \dot{w}}$, is equal to the diffusion flux (denoted here by $\mathcal{J}$). Assuming that the total energy $E$ is a function of $\rho, Y_1, u, \dot{w}, J$ and $s$, the generating system in one dimension is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \right) = 0,$$  \hspace{1cm} (B.1a)

$$\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x} \left( \rho Y_1 u + E_{\dot{w}} \right) = 0,$$  \hspace{1cm} (B.1b)

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + \rho^2 E_\rho \right) = 0,$$  \hspace{1cm} (B.1c)

$$\frac{\partial \rho \dot{w}}{\partial t} + \frac{\partial}{\partial x} \left( \rho \dot{w} u + E_{Y_1} \right) = 0,$$  \hspace{1cm} (B.1d)

$$\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x} \left( \rho J u + E_s \right) = 0,$$  \hspace{1cm} (B.1e)

$$\frac{\partial \rho s}{\partial t} + \frac{\partial}{\partial x} \left( \rho s u + E_J \right) = 0,$$  \hspace{1cm} (B.1f)
where $E_\xi$ denotes the partial derivative $\frac{\partial E}{\partial \xi}$. The fact that the total energy $E$ is not an unknown but rather a potential that depends on the remaining unknowns is an important feature of this system, as it means that solutions of the above system of equations also satisfy the additional conservation law

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x} \left( \rho E + p \right) u + E_{Y_1} E_{\tilde{w}} + E_s E_j = 0,$$  \hspace{1cm} (B.2)

which describes the conservation of total energy (note that by definition $p = \rho^2 E_{\rho}$).

The requirement that $E$ is a potential and that all of the constitutive terms in the fluxes (and source terms when they are introduced later) in Equation (B.1) are generated from this potential means that the overdetermined system (B.1)–(B.2) is consistent [216]. Moreover, if the energy potential is a convex function then Equation (B.1) can be transformed into a symmetric hyperbolic form (see [221] for details), which implies that it is well-posed.

B.1.2 Introduction of source terms

Source terms are now introduced into the master system to represent the dissipative processes of diffusion and conduction. This is done with adherence to the following requirements; the total energy conservation law must not be affected, production of entropy must be non-negative and the Onsager principle of symmetric kinetic coefficients is assumed to hold. Taking this into account, the governing equations with dissipation are given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} \left( \rho u \right) = 0,$$  \hspace{1cm} (B.3a)

$$\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x} \left( \rho Y_1 u + E_{\tilde{w}} \right) = 0,$$  \hspace{1cm} (B.3b)

$$\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + \rho^2 E_{\rho} \right) = 0,$$  \hspace{1cm} (B.3c)

$$\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x} \left( \rho \tilde{w} u + E_{Y_1} \right) = -\theta_{11} E_{\tilde{w}} - \theta_{12} E_j,$$  \hspace{1cm} (B.3d)

$$\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x} \left( \rho J u + E_s \right) = -\theta_{21} E_{\tilde{w}} - \theta_{22} E_j,$$  \hspace{1cm} (B.3e)
where \( \theta_{ij} \geq 0 \) are the kinetic coefficients (note that \( \theta_{12} = \theta_{21} \)), interpreted here as relaxation parameters where the eigenvalues of the matrix \( \theta = [\theta_{ij}] \) characterise the rate of relaxation of the heat flux and species mass flux. The entropy production \( Q \) should be non-negative and is derived such that the total energy conservation law remains unchanged. This gives

\[
Q = \frac{1}{E_s} \left( \theta_{11} E_{\tilde{w}}^2 + 2 \theta_{12} E_{\tilde{w}} E_J + \theta_{22} E_J^2 \right) \geq 0,
\]

(B.4)

thus meeting all of the requirements for the introduction of source terms into the master system. Since the energy conservation law has remained unchanged and the production of entropy is non-negative, then the master system with source terms included satisfies both the first and second laws of thermodynamics respectively.

### B.1.3 Closure relations

The remaining task now is to define closure relations for the master system so that the governing equations can be generated. The total energy must be defined such that the governing equations that are generated have physical meaning, and is distributed as follows:

\[
E(\rho, Y_1, u, \tilde{w}, J, s) = E_1(\rho, Y_1, s) + E_2(\tilde{w}, J) + E_3(u),
\]

(B.5)

where \( E_1 \) is the internal energy, \( E_2 \) is the non-equilibrium energy and \( E_3 = \frac{1}{2}u^2 \) is the kinetic energy per unit mass. The internal energy \( e = E_1 \) is defined as the mass-weighted average of the internal energies of each species, which are defined through an equation of state of the form \( \epsilon_l = \epsilon_l(\rho_l, s) \). Therefore

\[
e(\rho, Y_1, s) = Y_1 \epsilon_1(\rho_1, s) + Y_2 \epsilon_2(\rho_2, s).
\]

(B.6)

Note that the partial density \( \rho_l = \frac{\rho Y_l}{z_l} \) depends on the volume fraction \( z_l \) and thus \( e = e(\rho, Y_1, z_1, s) \). However, given the assumption of pressure and temperature equilibrium...
(i.e. $p_1 = p_2$ and $T_1 = T_2$) then $z_l$ can be determined from $Y_1$ as it will be equivalent with the mole fraction $X_l = \frac{W_l}{W} Y_k$ [90], where $W_l$ is the molecular weight of species $l$ and $W$ is the molecular weight of the mixture. The non-equilibrium energy is defined as

$$E_2(\tilde{w}, J) = \frac{\alpha^2 J^2}{2} + \frac{\beta^2 \tilde{w}^2}{2},$$

where $\alpha$ and $\beta$ are parameters yet to be determined. With these definitions, the energy gradients in state space may now be determined. Following Romenski et al. [223], they are given by

$$E_\rho = \frac{z_1 p_1 + z_2 p_2}{\rho^2} = \frac{p}{\rho^2} \quad E_{Y_1} = \eta_1 - \eta_2 \quad E_s = T \quad E_{\tilde{w}} = \beta^2 \tilde{w} \quad E_J = \alpha^2 J$$

where $\eta_l = \epsilon_l + \frac{p_l}{\rho_l} - sT$ is the chemical potential for species $l$, meaning that the gradient $E_{Y_1}$ is just the difference in species enthalpies.

#### B.2 Determination of kinetic coefficients in the relaxation limit

The introduction of kinetic coefficients into the master system allows for a hyperbolic approximation of the parabolic theory for diffusive heat and mass transfer by considering the stiff relaxation limit i.e. for small relaxation times. In the model thermal and mass diffusion are coupled (due to the $\theta_{12} = \theta_{21}$ coefficient) and therefore an explicit relaxation time for each process cannot be defined, however it is sufficient to consider the eigenvalues of the matrix $\Theta$ which characterise the rate of relaxation. These are assumed to be much larger than the characteristic rate of transfer of each process. Therefore in the relaxation limit the time derivative and the convective term in the equations for $\tilde{w}$ and $J$ can be neglected, resulting in:

$$\begin{bmatrix}
\theta_{11} & \theta_{12} \\
\theta_{21} & \theta_{22}
\end{bmatrix}
\begin{bmatrix}
E_{\tilde{w}} \\
E_J
\end{bmatrix} = \left[- \frac{\partial E_{Y_1}}{\partial x}, - \frac{\partial E_s}{\partial x}\right]$$

(B.9)
Therefore

\[ E_w = -\chi_{11} \frac{\partial E_{Y_1}}{\partial x} - \chi_{12} \frac{\partial E_s}{\partial x}, \]
\[ E_J = -\chi_{21} \frac{\partial E_{Y_1}}{\partial x} - \chi_{22} \frac{\partial E_s}{\partial x}, \]  
(B.10)

where the matrix \( \chi = [\chi_{ij}] \) is given by

\[
\begin{bmatrix}
\chi_{11} & \chi_{12} \\
\chi_{21} & \chi_{22}
\end{bmatrix}
= \begin{bmatrix}
\theta_{11} & \theta_{12} \\
\theta_{21} & \theta_{22}
\end{bmatrix}^{-1}.
\]  
(B.11)

The aim now is to relate the derivatives \( E_w \) and \( E_J \) to the diffusive and thermal fluxes. For conventional parabolic theory these will depend on gradients of \( Y_1, T \) and \( p \) in the most general case [61], therefore the derivative \( \frac{\partial E_{Y_1}}{\partial x} \) is written as follows:

\[
\frac{\partial E_{Y_1}}{\partial x} = E_{Y_1} \frac{\partial Y_1}{\partial x} + E_{Y_1 T} \frac{\partial T}{\partial x} + E_{Y_1 p} \frac{\partial p}{\partial x}.
\]  
(B.12)

Noting that \( E_s = T \), Equation (B.10) becomes

\[
E_w = -\chi_{11} E_{Y_1} \frac{\partial Y_1}{\partial x} - \left( \chi_{11} E_{Y_1 T} + \chi_{12} \right) \frac{\partial T}{\partial x} - \chi_{11} E_{Y_1 p} \frac{\partial p}{\partial x},
\]
\[
E_J = -\chi_{21} E_{Y_1} \frac{\partial Y_1}{\partial x} - \left( \chi_{21} E_{Y_1 T} + \chi_{22} \right) \frac{\partial T}{\partial x} - \chi_{21} E_{Y_1 p} \frac{\partial p}{\partial x}.
\]  
(B.13)

These need to be related to the conventional parabolic description, which given by

\[
J = -\rho D \left( \frac{\partial Y_1}{\partial x} + \frac{k_T}{T} \frac{\partial T}{\partial x} + \frac{k_p}{p} \frac{\partial p}{\partial x} \right),
\]
\[
q = \left( \frac{k_T}{T} \frac{\partial \eta}{\partial Y_1} - \frac{T}{T} \frac{\partial \eta}{\partial T} + \eta \right) J - \kappa \frac{\partial T}{\partial x}.
\]  
(B.14)

Now, given that \( E_{Y_1} = \eta = \eta_1 - \eta_2 = h_1 - h_2 \) where the species enthalpy \( h_l = \epsilon_l (\rho_l, s) + \frac{\rho_l}{\rho} \), it can be evaluated as follows:

\[
\frac{\partial}{\partial x} (h_1 - h_2) = \left( \frac{\rho c_1^2}{\rho_1 z_1} + \frac{\rho c_2^2}{\rho_2 z_2} \right) \frac{\partial Y_1}{\partial x} - \left( \frac{\rho Y_1 \epsilon_1^2}{\rho_1 z_1} + \frac{\rho Y_2 \epsilon_2^2}{\rho_2 z_2} \right) \frac{\partial z_1}{\partial x} + \left( \frac{Y_1 \epsilon_1^2}{\rho_1 z_1} - \frac{Y_2 \epsilon_2^2}{\rho_2 z_2} \right) \frac{\partial p}{\partial x}
\]
\[
= \left( \frac{c_1^2}{Y_1} + \frac{c_2^2}{Y_2} \right) \frac{\partial Y_1}{\partial x} - \left( \frac{c_1^2}{z_1} + \frac{c_2^2}{z_2} \right) \frac{\partial z_1}{\partial x} + \left( \frac{c_1^2}{\rho} - \frac{c_2^2}{\rho} \right) \frac{\partial p}{\partial x},
\]  
(B.15)
where $c_l$ is the speed of sound in species $l$, defined as $c_l^2 = \frac{\partial p_l}{\partial \rho_l}$. Using the assumption of pressure and temperature equilibrium, the volume fraction $z_l = \frac{W_l Y_l}{W}$, which gives

$$\frac{\partial z_1}{\partial x} = \frac{W^2}{W_1 W_2} \frac{\partial Y_1}{\partial x}$$  \hspace{1cm} \text{(B.16)}$$

where $W$ is the mixture molecular weight, given in Equation (3.17). Since $\rho = \rho Y_1 + \rho Y_2 = \rho_1 z_1 + \rho_2 z_2$ then the derivative $\frac{\partial \rho}{\partial x}$ can be written as

$$\frac{\partial \rho}{\partial x} = (\rho_1 - \rho_2) \frac{\partial z_1}{\partial x} + z_1 \frac{\partial \rho_1}{\partial x} + z_2 \frac{\partial \rho_2}{\partial x}.$$  \hspace{1cm} \text{(B.17)}$$

To evaluate the derivative $\frac{\partial \rho}{\partial x}$ an equation of state must be defined for each species. Assuming both gases are ideal gives

$$\rho_l = \frac{p W_l}{R T},$$  \hspace{1cm} \text{(B.18)}$$

where $R$ is the universal gas constant. Thus $\frac{\partial \rho}{\partial x}$ may be written as

$$\frac{\partial \rho_l}{\partial x} = \frac{W_l}{RT} \frac{\partial p}{\partial x} - \frac{W_l p}{RT^2} \frac{\partial T}{\partial x},$$  \hspace{1cm} \text{(B.19)}$$

Therefore Equation (B.15) may be evaluated to be

$$\frac{\partial}{\partial x} (h_1 - h_2) = \left[ \frac{(c_1^2 Y_1 + c_2^2 Y_2)}{Y_1 Y_2} - \frac{(W_1 c_1^2 Y_1 + W_2 c_2^2 Y_2)}{Y_1 Y_2} + \frac{(c_1^2 - c_2^2)(\rho_1 - \rho_2) W^2}{\rho W_1 W_2} \frac{\partial Y_1}{\partial x} + \frac{(c_1^2 - c_2^2) \frac{\partial p}{\partial x}}{p} - \frac{(c_1^2 - c_2^2) \frac{\partial T}{\partial x}}{T} \right] \frac{\partial Y_1}{\partial x} + \left[ \frac{(c_1^2 - c_2^2) \frac{\partial T}{\partial x}}{p} - \frac{(c_1^2 - c_2^2) \frac{\partial T}{\partial x}}{T} \right] \frac{\partial Y_1}{\partial x}$$

$$= E_{Y_1 Y_1} \frac{\partial Y_1}{\partial x} + E_{Y_1 T} \frac{\partial T}{\partial x} + E_{Y_1 p} \frac{\partial p}{\partial x}.$$  \hspace{1cm} \text{(B.20)}$$

This allows for the terms $E_{Y_1 Y_1}$, $E_{Y_1 T}$ and $E_{Y_1 p}$ to be determined, which means that the coefficients $\chi_{ij}$ can be evaluated through use of Equation (B.13).
B.2 Determination of kinetic coefficients in the relaxation limit

Noting that \( E_{Y_1} = \eta \) and \( E_s = T \), the thermal flux is

\[
q = E_{Y_1} E_{\bar{w}} + E_s E_J \\
= \eta E_{\bar{w}} + T E_J \\
= -\eta \chi_{11} \frac{\partial \eta}{\partial x} - \eta \chi_{12} \frac{\partial T}{\partial x} - T \chi_{21} \frac{\partial \eta}{\partial x} - T \chi_{22} \frac{\partial T}{\partial x}.
\]

Also, given that \( E_{\bar{w}} = J \) then \( q \) can be written as:

\[
q = \left( \eta + \frac{\chi_{21} T}{\chi_{11}} \right) J - \frac{\chi_{11} \chi_{22} - \chi_{12} \chi_{21}}{\chi_{11}} T \frac{\partial T}{\partial x},
\]

which means that the thermal conductivity coefficient \( \kappa \) is equal to

\[
\kappa = \frac{\chi_{11} \chi_{22} - \chi_{12} \chi_{21}}{\chi_{11}} T.
\]

Given that the mass flux \( J \) takes the form

\[
J = -\chi_{11} \eta_{Y_1} \frac{\partial Y_1}{\partial x} - (\chi_{12} - \chi_{11} \eta_T) \frac{\partial T}{\partial x} - \chi_{11} \eta_p \frac{\partial p}{\partial x}
\]

\[
= -\rho D \left( \frac{\partial Y_1}{\partial x} + \frac{k_T}{T} \frac{\partial T}{\partial x} + \frac{k_p}{p} \frac{\partial p}{\partial x} \right),
\]

then \( \chi_{11}, \chi_{12} = \chi_{21} \) and \( \chi_{22} \) can be found as follows:

\[
\chi_{11} = \frac{\rho D}{\eta_{Y_1}} \quad \chi_{12} = \left( \frac{k_T}{T} \eta_{Y_1} - \eta_T \right) \chi_{11} \quad \chi_{22} = \frac{\kappa}{T} + \frac{\chi_{12} \chi_{21}}{\chi_{11}}
\]

where \( \eta_{Y_1} = E_{Y_1 Y_1}, \eta_T = E_{Y_1 T} \) and \( \eta_p = E_{Y_1 p} \) are found using Equation (B.20). Thus
the kinetic coefficients $\theta_{ij}$ are given by

$$
\begin{bmatrix}
\theta_{11} & \theta_{12} \\
\theta_{21} & \theta_{22}
\end{bmatrix} =
\begin{bmatrix}
\chi_{11} & \chi_{12} \\
\chi_{21} & \chi_{22}
\end{bmatrix}^{-1}
\begin{bmatrix}
\frac{\rho D}{\eta Y_1} \\
\left(\frac{k^*}{T} \eta Y_1 - \eta_T\right) \frac{\rho D}{\eta Y_1} \\
\left(\frac{k^*}{T} \eta Y_1 - \eta_T\right)^2 \frac{\rho D}{\eta Y_1} + \left(\frac{k^*}{T} \eta Y_1 - \eta_T\right) \frac{\rho D}{\eta Y_1}
\end{bmatrix}^{-1}
$$

This completes the analysis of the stiff relaxation limit. The generating system can now be used to formulate governing equations in terms of the state parameters, as all thermodynamic forces have been expressed in terms of derivatives of the total energy $E$, and all of the model kinetic coefficients have been defined.

### B.3 Governing equations in terms of parameters of state

For implementation in a numerical method it is more convenient to write the governing equations in terms of the parameters of state defined in Section B.1.1. Prior to this, a hyperbolic formulation of viscosity will be added to the model by deriving a one-dimensional form of the evolution equations for the distortion tensor in [215, 216]. These equations can be added to this existing equation set without affecting any of the previous derivations, thus providing a complete hyperbolic description of a viscous binary mixture in one dimension which will be written in terms of the state parameters for numerical implementation.
B.3 Governing equations in terms of parameters of state

### B.3.1 One-dimensional equations for distortion

One-dimensional equations for the distortion tensor $A$ can be derived from the three-dimensional equations presented in [216] and read as

$$
\frac{\partial A_{11}}{\partial t} + \frac{\partial uA_{11}}{\partial x} = -\frac{\Psi_{11}}{\phi}, \\
\frac{\partial A_{22}}{\partial t} + u\frac{\partial A_{22}}{\partial x} = -\frac{\Psi_{22}}{\phi}, \\
\frac{\partial A_{33}}{\partial t} + u\frac{\partial A_{33}}{\partial x} = -\frac{\Psi_{33}}{\phi},
$$

where $\Psi_{ik} = E_{A_{ik}}$ and $\phi$ is some function of the strain dissipation time $\tau$. These equations are obtained under the assumption that the fluid flows with velocity $u$ only in the $x$-direction and hence $A_{ij} = 0$, $i \neq j$. Assuming that $A_{22} = A_{33}$ due to isotropy, and denoting $A_1 = A_{11}$, $A_2 = A_{22}$ gives

$$
\frac{\partial A_1}{\partial t} + \frac{\partial uA_1}{\partial x} = -\frac{\Psi_{11}}{\phi}, \\
\frac{\partial A_2}{\partial t} + u\frac{\partial A_2}{\partial x} = -\frac{\Psi_{22}}{\phi},
$$

As per Dumbser et al. [216], the relaxation terms on the right-hand side are given in matrix form as

$$
\Psi = \frac{\partial E}{\partial A} = c_s^2 A \text{dev}(G), \quad G = AA^T,
$$

where $c_s$ is the shear sound velocity, that is, the characteristic velocity of propagation of transverse perturbations. Since $A_{ij} = 0$, $i \neq j$ then $G$ is given by

$$
G = \begin{bmatrix}
A_1^2 & 0 & 0 \\
0 & A_2^2 & 0 \\
0 & 0 & A_3^2
\end{bmatrix},
$$

(B.30)
and the deviatoric part of $G$ is given by

$$\text{dev}(G) = G - \frac{1}{3} \text{Tr}(G) = \begin{bmatrix} \frac{2}{3}(A_1^2 - A_2^2) & 0 & 0 \\ 0 & -\frac{1}{3}(A_1^2 - A_2^2) & 0 \\ 0 & 0 & -\frac{1}{3}(A_1^2 - A_2^2) \end{bmatrix},$$  \hspace{1cm} (B.31)$$

Therefore the energy gradients are

$$\Psi_{11} = c_s^2 A_1 \frac{2}{3}(A_1^2 - A_2^2),$$

$$\Psi_{22} = -c_s^2 A_2 \frac{1}{3}(A_1^2 - A_2^2).$$  \hspace{1cm} (B.32)$$

The strain relaxation source term $\phi$ is defined following [216]:

$$\phi = \tau c_s^2 \frac{1}{3} \text{det}(A) \frac{\partial E}{\partial A} = \tau c_s^2 \frac{1}{3} (A_1 A_2^2 - A_2 A_1^2).$$  \hspace{1cm} (B.33)$$

**B.3.2 Modification of the momentum equation**

The inclusion of equations for the distortion tensor also requires that a shear stress tensor is added to the momentum equations. Since the fluid is assumed to flow only in the $x$-direction, there is only one momentum equation

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p - \sigma_{11})}{\partial x} = 0$$  \hspace{1cm} (B.34)$$

Following [216], the shear stress tensor $\sigma$ is computed as

$$\sigma = -\rho A^T \frac{\partial E}{\partial A} = -\rho c_s^2 G\text{dev}(G).$$  \hspace{1cm} (B.35)$$

Thus, in matrix form $\sigma$ is given by

$$\sigma = \begin{bmatrix} -\rho c_s^2 A_1^2 \frac{2}{3}(A_1^2 - A_2^2) & 0 & 0 \\ 0 & \rho c_s^2 A_2^2 \frac{1}{3}(A_1^2 - A_2^2) & 0 \\ 0 & 0 & \rho c_s^2 A_2^2 \frac{1}{3}(A_1^2 - A_2^2) \end{bmatrix},$$  \hspace{1cm} (B.36)$$
B.3 Governing equations in terms of parameters of state

and therefore

\[ \sigma_{11} = -\rho c_s^2 A_1^2 \frac{2}{3} (A_1^2 - A_2^2). \] (B.37)

B.3.3 Complete system of equations

The full set of state parameters describing the mixture in one spatial dimension is now

\[ \{ \rho, Y_1, u, A_1, A_2, \tilde{w}, J, s \}. \]

The total energy is defined as per Equation (B.5), with the definition of the non-equilibrium energy extended to include the components of the distortion tensor

\[ E_2(A_1, A_2, \tilde{w}, J) = \frac{c_s^2}{4} G_{ij}^{TF} G_{ij}^{TF} + \frac{\alpha^2}{2} J^2 + \frac{\beta^2}{2} \tilde{w}^2 \]

\[ = \frac{c_s^2}{6} (A_1^2 - A_2^2)^2 + \frac{\alpha^2}{2} J^2 + \frac{\beta^2}{2} \tilde{w}^2 \] (B.38)

where \( G_{ij}^{TF} = \text{dev}(G) \) is the trace-free part of \( G \). The parameter \( c_s \) cannot be determined explicitly, but via a formal asymptotic expansion of the tensor \( G \) in terms of the small parameter \( \tau \), it can be shown that (to first order in \( \tau \)) the conventional dynamic viscosity coefficient \( \mu = C_0 \tau c_s^2 \), where \( C_0 \) is some additional constant. In order to recover both parameters, experimental measurements of high frequency sound propagation are required (see [216] for further details). Similarly, the parameters \( \alpha \) and \( \beta \) are not known explicitly, but the products \( \epsilon \alpha^2 \) and \( \epsilon \beta^2 \) can be connected to the conventional transport coefficients for thermal and mass diffusion, where \( \epsilon \) is some small relaxation parameter (each process will have a characteristic relaxation time but these cannot be defined explicitly due to coupling as noted in Section B.2). This is not trivial to do and will be performed in future work.

Therefore the complete set of equations in one dimension, including the effects of viscosity, diffusion and conductivity, is given by

\[ \frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} = 0, \] (B.39a)

\[ \frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x} \left( \rho Y_1 u + \beta^2 \tilde{w} \right) = 0, \] (B.39b)
\[
\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + p + \rho c_s^2 A_1^2 \frac{2}{3} (A_1^2 - A_2^2) \right) = 0, \tag{B.39c}
\]
\[
\frac{\partial A_1}{\partial t} + \frac{\partial u A_1}{\partial x} = - \frac{2(A_1^2 - A_2^2)}{\tau(A_1 A_2)^{\frac{3}{2}}}, \tag{B.39d}
\]
\[
\frac{\partial A_2}{\partial t} + u \frac{\partial A_2}{\partial x} = - \frac{A_2(A_1^2 - A_2^2)}{\tau(A_1 A_2)^{\frac{3}{2}}}, \tag{B.39e}
\]
\[
\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x} \left( \rho \tilde{w} u + h_1 - h_2 \right) = -\theta_{11}\beta^2 \tilde{w} - \theta_{12}\alpha^2 J, \tag{B.39f}
\]
\[
\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x} \left( \rho J u + T \right) = -\theta_{21}\beta^2 \tilde{w} - \theta_{22}\alpha^2 J, \tag{B.39g}
\]
\[
\frac{\partial \rho s}{\partial t} + \frac{\partial}{\partial x} \left( \rho s u + \alpha^2 J \right) = Q, \tag{B.39h}
\]

where now the entropy production \( Q \) is
\[
Q = \frac{1}{E_5} \left( \frac{1}{\phi} (\psi_{11}^2 + \psi_{22}^2) + \theta_{11} E_{\tilde{w}}^2 + 2\theta_{12} E_{\tilde{w}} E_s + \theta_{22} E_J^2 \right) \geq 0. \tag{B.40}
\]

For numerical implementation it is better to solve the following set of equations:
\[
\frac{\partial \rho Y_1}{\partial t} + \frac{\partial}{\partial x} \left( \rho Y_1 u + \beta^2 \tilde{w} \right) = 0 \tag{B.41a}
\]
\[
\frac{\partial \rho Y_2}{\partial t} + \frac{\partial}{\partial x} \left( \rho Y_2 u - \beta^2 \tilde{w} \right) = 0 \tag{B.41b}
\]
\[
\frac{\partial \rho u}{\partial t} + \frac{\partial}{\partial x} \left( \rho u^2 + p + \rho c_s^2 A_1^2 \frac{2}{3} (A_1^2 - A_2^2) \right) = 0 \tag{B.41c}
\]
\[
\frac{\partial A_1}{\partial t} + \frac{\partial u A_1}{\partial x} = - \frac{2(A_1^2 - A_2^2)}{\tau(A_1 A_2)^{\frac{3}{2}}}, \tag{B.41d}
\]
\[
\frac{\partial A_2}{\partial t} + u \frac{\partial A_2}{\partial x} = - \frac{A_2(A_1^2 - A_2^2)}{\tau(A_1 A_2)^{\frac{3}{2}}}, \tag{B.41e}
\]
\[
\frac{\partial \rho \tilde{w}}{\partial t} + \frac{\partial}{\partial x} \left( \rho \tilde{w} u + h_1 - h_2 \right) = -\theta_{11}\beta^2 \tilde{w} - \theta_{12}\alpha^2 J \tag{B.41f}
\]
\[
\frac{\partial \rho J}{\partial t} + \frac{\partial}{\partial x} \left( \rho J u + T \right) = -\theta_{21}\beta^2 \tilde{w} - \theta_{22}\alpha^2 J \tag{B.41g}
\]
\[
\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x} \left( \rho E u + (p + \rho c_s^2 A_1^2 \frac{2}{3} (A_1^2 - A_2^2)) u + \beta^2 (h_1 - h_2) \tilde{w} + \alpha^2 T J \right) = 0 \tag{B.41h}
\]

This system of equations cannot be written in a fully conservative form when the equations for the distortion tensor are included, however recent advances in path-conservative methods for non-conservative systems provide a suitable approach for
discretisation [224]. Indeed, when considering multispecies (or more generally multi-phase) systems it is necessary to discretise the colour function in a non-conservative manner in order to preserve pressure equilibrium across an isolated contact surface [85], hence the fact that the distortion tensor equations are non-conservative is less of a hindrance to numerical implementation than may first appear. Another difficult aspect of this system when considering an appropriate numerical method to use is the stiffness of the source terms. One option is to use Strang time splitting [225], which allows a stiff ODE integrator to be used for the source terms, however a more efficient and promising approach is the family of high order one-step ADER schemes [172–175]. Future work will address the application of these methods to the current system of equations.

The work presented here forms a small part of a much greater goal; the formulation of a three-dimensional, hyperbolic, two-velocity, two-temperature model for viscous, miscible and compressible fluids and its numerical implementation within a high-order, multidimensional finite volume framework. The next steps towards this goal should be the numerical implementation of the current set of equations and a comparison with the conventional governing equations using a rigorous set of one-dimensional test cases. Once this has been achieved, this model may be used to assist in determining the necessary parameters and coefficients of a more general single entropy model for two-phase flow (similar in form to that presented in [221]), which is a better candidate for extension to multiple dimensions and numerical implementation with very high-order methods.
Appendix C

Assessment of Further Improvements to the Numerical Method

C.1 Introduction

This appendix considers some extensions to the existing numerical method outlined in Chapter 3, which are assessed using a series of two-dimensional low Mach test cases. These are all still within the same method of lines framework and are described in turn in the following sections. The general approach taken here is to pursue incremental modifications that increase the resolution of the numerical method rather than increase the formal order of accuracy, which would require major structural changes to the code. In other words, the approximation error is reduced by reducing the coefficient of the leading-order error term, rather than increasing the exponent of the leading-order error.

At coarse grid resolutions this can still give results that are competitive, when considered in terms of computational cost for a given error, with formally higher-order accurate schemes. This is particularly true for nonlinear problems involving discontinuities, as stability becomes a crucial consideration and the various means of enforcing
stability result in highly nonlinear error terms. At fine grid resolutions and for smooth problems, higher-order accurate methods are typically much more computationally efficient [214, 226]. For complex turbulent flows, the higher wavenumber modes in the solution are not as well resolved and thus the accuracy of the numerical method at coarser grid resolutions remains an important factor. This is particularly true for the broadband simulations presented in Chapter 5, where the aim is to maximise the range of modes that can be accurately computed. Thus the main aim any modification, including those proposed below, should be to increase the efficiency of the numerical method at coarser grid resolutions on relevant test problems, while also ensuring that the efficiency at finer grid resolutions is not affected or is improved too.

C.1.1 Low Mach correction for the HLLC Riemann solver

Rather than modify the reconstructed velocities at the interface, it is possible apply a low Mach correction within the Riemann solver instead, see for example Thornber and Drikakis [227] for a simple modification to the Roe solver that substantially reduces the dissipation at low Mach number. Recently, Xie et al. [10] proposed a low Mach correction for the HLLC Riemann solver. The correction involves modifying the pressure in the star region for the momentum fluxes, such that the modified numerical flux in the star region is

\[
\mathbf{F}^*_K = \begin{bmatrix}
\rho^*_K S^* \\
\rho^*_K S^*[u_k + n_z(S^* - q_K)] + n_z p^{***} \\
\rho^*_K S^*[v_k + n_y(S^* - q_K)] + n_y p^{***} \\
\rho^*_K S^*[w_k + n_z(S^* - q_K)] + n_z p^{***} \\
S^*(\rho^*_K e^*_K + p^*)
\end{bmatrix},
\]  

(C.1)

where \(p^{***} = f p^* + (1 - f)p^*\) and \(p^* = \theta p^* + (1 - \theta)(p_L + p_R)/2\). The scaling function \(\theta = \min(\max(M_L, M_R), 1)\), which is the same function as the one used in Thornber et al. [9], while the pressure weight function \(f = \min(p_R/p_L, p_L/p_R)^3\). \(q_K = u n_z + v n_y + w n_z\) is the velocity normal to the cell interface and \(n = [n_x, n_y, n_z]^t\).
is the unit vector normal to this interface. While the method was only presented at first-order in Xie et al. [10], it is trivial to extend to higher order accuracy by using the left and right extrapolated values at the interface from a high-order spatial discretisation. Note that only the correction at low Mach numbers from Xie et al. [10] is applied; a separate correction for high Mach number deficiencies was also presented but is not considered here. In the sections below, the existing low Mach correction of Thornber et al. [9] is referred to as LM1 while the new method of Xie et al. [10] is referred to as LM2.

### C.1.2 Alternate choices of reconstructed variables

Recently, Williams [228] showed that by choosing an appropriate set of reconstructed variables for the mass fraction model, when pressure and temperature equilibrium exists between two neighbouring cells it is also maintained at the interface between them. The choice of which variables to reconstruct is guided by the consideration that they be thermodynamically consistent when monotonicity bounds are enforced, therefore preserving pressure and temperature equilibrium at an interface if it exists in both cells. The standard set of reconstructed primitive variables used in the mass fraction model is \([\rho, u, p, Y_i]^t\), which was the set used in Section 3.3, as enforcing monotonicity bounds (i.e. limiting) on these variables ensures the positivity of mass fractions along with the requirement that \(\sum Y_i = 1\). However, limiting these variables at an interface does not automatically maintain pressure and temperature equilibrium, which explains the poor performance of the mass fraction model relative to the new five-equation model in Case 1 and Case 3 of Section 3.3.

Three alternative sets of primitive variables were proposed by Williams [228] that avoid this issue. The first of these is \([n, u, p, Y_i]^t\) where \(n\) is the number density, which is the set implemented here due to the minimal changes required. The second set is \([\rho_i, u, p, f_i]^t\), which is the same set of primitive variables that are reconstructed in the five-equation model, while the third set is \([s_i, u, p, f_i]^t\) where \(s_i\) are the phase entropies and \(f_i\) are the volume fractions calculated under the assumption of thermodynamic
C.1 Introduction

equilibrium. By limiting these variables at an interface instead of the standard choice, pressure and temperature equilibrium is maintained while also retaining all of the other favourable properties of the original scheme. Williams [228] showed that a substantial improvement is achieved on the 1D Diffusion test case (Case 3 of Section 3.3) when any of these alternative sets of reconstructed variables are used in place of the conventional set. Once the reconstruction procedure has been performed, these variables are converted back to the conventional set of primitive and conserved variables and then passed to the Riemann solver. In the sections below, the mass fraction model with the reconstructed variables \([n, u, p, Y_i]\) is referred to simply as the mass fraction (MF) model, while the inviscid and viscous five-equation models are referred to as the volume fraction (VF) model.

C.1.3 Fourth-order viscous fluxes

One straightforward way of potentially increasing the resolution of the numerical scheme is to evaluate the viscous flux \(F^{(v)}(U, U')\) using fourth-order central differences rather than second-order. It is important to ensure that the finite difference formulas used are based on cell averages rather than point values. This is achieved by integrating over each cell the Taylor series expansions used to derive the finite difference formula for a given stencil. At second-order accuracy this gives the same formula regardless of whether cell averages or point values are used, however different coefficients are derived when higher-order accurate finite differences (i.e. larger stencils) are considered. Following Guzik et al. [229], the solutions variables \(U\) are interpolated at the \(i + 1/2\) interface of cell \(i\) to fourth-order accuracy as

\[
U_{i+1/2} = \frac{7}{12} (U_i + U_{i+1}) - \frac{1}{12} (U_{i-1} + U_{i+2}),
\]

where \(U_i\) denotes the cell-averaged quantity in cell \(i\). Similarly, the first derivative \(U'\) is given by

\[
U'_{i+1/2} = \frac{15}{12} (U_{i+1} - U_i) - \frac{1}{12} (U_{i+2} - U_{i-1}).
\]
The same procedure is repeated in each direction when extending to multiple di-
mensions, with the transverse velocity derivatives (e.g. $\frac{\partial u}{\partial y}$, $\frac{\partial v}{\partial x}$) also evaluated at fourth-order [229].

The fourth-order calculation of the viscous fluxes was used in the double vortex
test case in Section C.2.2, however the results relative to the standard second-order
approach were not sufficiently improved to warrant its inclusion on the later test
cases.

C.1.4 Fifth-order TENO reconstruction

While TVD reconstruction schemes are able to stably capture discontinuities, they
degenerate to first-order accuracy and provide excessive numerical dissipation near
extrema and other critical points in smooth regions of flow. This lead to the develop-
ment of essentially non-oscillatory interpolation (ENO) schemes [230], which retain
high-order accuracy for a given stencil in smooth flow while also producing virtually no
oscillations at discontinuities (i.e. the magnitude of the oscillations decays as $O(\Delta x^k)$
where $k$ is the order of accuracy). ENO schemes can be viewed as a trade-off between
less robust discontinuity capturing for increased resolution of complex smooth flow
structures and are thus potentially quite useful for computing turbulence induced by
RMI. They choose the least oscillatory stencil from a set of candidate stencils at a
given cell and use this to reconstruct the solution variables at the cell interface. An
important extension is the concept of weighted essentially non-oscillatory (WENO)
schemes, which take a weighted average of all candidate stencils so as to increase the
order of accuracy and improve upon some of the shortcomings of the original ENO
method in smooth flow regions. By applying appropriate weights to each candidate
stencil an essentially non-oscillatory interpolation is maintained, although in general
WENO methods are less robust at discontinuities than their ENO counterparts.

Recently, a new class of schemes known as targeted essentially non-oscillatory (TENO)
schemes was proposed [231], which aims to combine the best of both approaches. Un-
like WENO schemes, each candidate stencil is either applied with its optimal weight
or eliminated entirely if it contains oscillations above a certain threshold. The set of candidate stencils for a given method is also selected by assembling upwind-biased stencils of incremental width, as in the original ENO approach, rather than all candidate stencils having the same width as in WENO schemes. This approach reduces numerical dissipation to that of the underlying linear scheme while also allowing for more robust capturing of discontinuities.

In this section, the fifth-order TENO scheme is implemented as a potential alternative to the existing fifth-order MUSCL reconstruction method. The scheme is given as follows, noting that while the original presentation in Fu et al. [231] was for reconstruction of numerical fluxes for a conservative finite-difference method, it is straightforward to adapt to a finite-volume setting. Following Balsara et al. [174], WENO reconstruction on a structured mesh for a finite-volume scheme is most efficiently formulated in modal space with a Legendre polynomial basis. The fifth-order scheme consists of three stencils; \( S_0 = \{u_{i-1}, u_i, u_{i+1}\} \), \( S_1 = \{u_{i-2}, u_{i-1}, u_i\} \) and \( S_2 = \{u_i, u_{i+1}, u_{i+2}\} \) for some quantity \( u \). The reconstructed polynomial on each stencil is given by

\[
u_j(x) = u_i P_0(x) + u'_j P_1(x) + u''_j P_2(x),
\]

where \( P_0(x) = 1 \), \( P_1(x) = x \) and \( P_2(x) = x^2 - \frac{1}{12} \) are the zeroth, first and second Legendre polynomials. The first and second moments on each stencil \( S_j \) are given by

\[
u'_j = \begin{cases} 
(u_{i+1} - u_{i-1})/2 & \text{if } j = 0, \\
(3u_i - 4u_{i-1} + u_{i-2})/2 & \text{if } j = 1, \\
(-3u_i + 4u_{i+1} - u_{i+2})/2 & \text{if } j = 2,
\end{cases}
\]

\[
u''_j = \begin{cases} 
(u_{i+1} - 2u_i + u_{i-1})/2 & \text{if } j = 0, \\
u_i - 2u_{i-1} + u_{i-2})/2 & \text{if } j = 1, \\
(u_i - 2u_{i+1} + u_{i+2})/2 & \text{if } j = 2.
\end{cases}
\]
The smoothness measures for each stencil can then be written as
\[
\beta_j = \left( u_j' \right)^2 + \frac{13}{3} \left( u_j'' \right)^2.
\tag{C.6}
\]

The nonlinear weights are formulated following Fu et al. [231] as
\[
\gamma_j = \left( C + \frac{\tau}{\beta_j + \epsilon} \right)^q,
\tag{C.7}
\]
with \( C = 1 \), \( q = 6 \) and \( \epsilon = 10^{-40} \). \( \tau \) is the global smoothness indicator, given by
\( \tau = |\beta_2 - \beta_1| \). An ENO-like stencil selection is enforced by applying a sharp cutoff function
\[
\delta_j = \begin{cases} 
0 & \text{if } \chi_j < C_T, \\
1 & \text{if } \chi_j \geq C_T,
\end{cases}
\tag{C.8}
\]
where
\[
\chi_j = \frac{\gamma_j}{\sum \gamma_j}.
\tag{C.9}
\]
are the normalised nonlinear weights. For the fifth-order scheme, the optimal linear weights are \( d_0 = 6/10 \), \( d_1 = 1/10 \) and \( d_2 = 3/10 \) (note that when extrapolating to \( x_{i-1/2} \), \( d_1 \) and \( d_2 \) are swapped). These are re-normalised to be
\[
w_j = \frac{\delta_j d_j}{\sum \delta_j d_j},
\tag{C.10}
\]
so that contributions from stencils containing discontinuities vanish. Finally, the quantity \( u \) is extrapolated to the \( x_{i+1/2} \) interface by
\[
u_{i+1/2} = u_i + u' P_1 (1/2) + u'' P_2 (1/2),
\tag{C.11}
\]
where \( u' = \sum w_j u_j' \) and \( u'' = \sum w_j u_j'' \). Similarly, the value of \( u \) at the \( x_{i-1/2} \) interface is given by
\[
u_{i-1/2} = u_i + u' P_1 (-1/2) + u'' P_2 (-1/2).
\tag{C.12}
All that remains now is to specify the cutoff value $C_T$. Fleischmann et al. [232] used a value of $C_T = 10^{-5}$ was used when simulating the single-mode Rayleigh–Taylor instability to introduce a strong degree of scale separation. In Fu et al. [233], an adaptive procedure was introduced where $C_T$ is varied between $10^{-5}$ and $10^{-10}$ depending on the presence of discontinuities in each stencil. This procedure is also adopted here.

If the reconstruction procedure outlined above is performed directly on the conserved or primitive variables, spurious oscillations may still be introduced near discontinuities due to the interaction of different characteristic fields [232]. These oscillations can be significantly reduced by decomposing the cell-averaged conserved variables into characteristic variables and reconstructing these instead. The reconstructed characteristic variables at the interface are then projected back to physical variables which are passed to the Riemann solver. This procedure is computationally expensive but often necessary for ensuring positivity of density and pressure, as well as boundedness of mass fractions, in complex flows involving shock waves. An unfortunate downside of this approach is that it was found to become unstable at low Mach numbers when a low Mach correction was included. This did not occur when the characteristic projection was not included, suggesting that there is an interaction effect that is currently not well understood and requires further investigation. Results using TENO reconstruction are given for the isentropic vortex test case in Section C.2.1 without a low Mach correction applied, showing that such a correction is still necessary for efficient computation of low Mach vortical flows. For this reason, it is not included in any of the other test cases.
C.2 Test cases

C.1.5 Third-order timestepping

The accuracy of the timestepping can also be improved by using the third-order TVD Runge-Kutta method of Gottlieb and Shu [148]:

\[
\begin{align*}
U^{(1)}_i &= U^n_i + \Delta t L (U^n_i), \\
U^{(2)}_i &= \frac{3}{4} U^n_i + \frac{1}{4} U^{(1)}_i + \frac{1}{4} \Delta t L (U^{(1)}_i), \\
U^{n+1}_i &= \frac{1}{3} U^n_i + \frac{2}{3} U^{(2)}_i + \frac{2}{3} \Delta t L (U^{(2)}_i).
\end{align*}
\] (C.13)

This requires additional storage compared to the second-order method as well as an additional sub-iteration, making it approximately 1.5× more expensive for the same timestep size. The CFL restriction is the same as the second-order method, which is given in Equation (3.26). The third-order timestepping method gives only marginal improvements when paired with the existing fifth-order MUSCL reconstruction, however it was found to be necessary for maintaining stability when using the fifth-order TENO reconstruction method in low Mach number flow (see Section C.2.1 below).

C.2 Test cases

The proposed modifications to the numerical method are evaluated using a series of two-dimensional test cases. Of particular relevance to simulations of RMI is the performance in vortical flows at low Mach number, therefore the first two test cases compare the ability of both low Mach corrections, as well as the fifth-order TENO reconstruction without a low Mach correction applied, to simulate a single- and multi-species vortex. The final test case is a 2D single-mode RMI calculation between Air and SF$_6$, a particularly challenging gas combination. This is used to compare both low Mach corrections as well as the new set of reconstructed variables in the mass fraction model. A description of each test case is given in the following subsections, as well as an assessment of the performance of the various modifications relative to the baseline numerical scheme.
C.2 Test cases

C.2.1 Isentropic vortex

The performance of the low Mach correction of Xie et al. [10] relative to existing correction of Thornber et al. [9], both using the standard fifth-order MUSCL (M5) reconstruction, is assessed using a low Mach variant of the isentropic vortex test case of Shu [234]. These two methods are referred to as M5+LM1 and M5+LM2 below. A third comparison is also made with results produced using fifth-order TENO reconstruction without a low Mach correction (due to instability issues when combined with the characteristic projection) and third-order Runge-Kutta time stepping. This is useful for demonstrating the importance of a low Mach correction for the efficient simulation of low Mach number vortical flows using upwind methods.

Specifically, this test case is useful for determining stability in the limit of $M \to 0$ as well as measuring the irreversible dissipation of kinetic energy, which should be as small as possible while still remaining positive in order to satisfy the second law of thermodynamics. Both of these criteria are very important for the simulation of RMI flows and compressible turbulence more generally, particularly when performing implicit large eddy simulations where the dissipation is provided entirely by the numerical method.

The setup is as follows. The two-dimensional Euler equations are solved on the square domain $[0, 10] \times [0, 10] \text{m}^2$ with periodic boundary conditions. The initial condition is a vortex centred on the point $(x_0, y_0) = (5, 5) \text{m}$ and is defined by the following isentropic perturbation of the mean flow;

$$u = u_0 - \frac{\beta}{2\pi} \exp \left( \frac{1}{2} (1 - r^2) \right) (y - y_0), \quad v = v_0 + \frac{\beta}{2\pi} \exp \left( \frac{1}{2} (1 - r^2) \right) (x - x_0),$$

$$T = T_0 - \frac{(\gamma - 1)\beta^2}{8\gamma \pi^2} \exp(1 - r^2), \quad (C.14)$$

where $r^2 = (x - x_0)^2 + (y - y_0)^2$ and $\beta = 5$ is the vortex strength. The mean flow is $(u_0, v_0) = (1, 1) \text{m/s}$ and the background density is $\rho_0 = 1 \text{ kg/m}^3$. The background pressure is given by

$$p_0 = \frac{\rho_0(u_0^2 + v_0^2)}{\gamma M_0^2}, \quad (C.15)$$
where $M_0$ is the Mach number of the mean flow. The background temperature $T_0$ is computed using the ideal gas equation of state and the density of the perturbation is computed from the isentropic relation $p/\rho^\gamma = C$ for some constant $C$. This case has an exact solution, which is simply the advection of the initial condition at the mean flow velocity.

Three different Mach numbers are considered; $M_0 = 0.1$, $M_0 = 0.01$ and $M_0 = 0.001$. The numerical solution is computed up to time $t = 10$ s, at which point the vortex has returned to its initial position. All cases here use a time step size given by $\text{CFL} = 0.375$ (the simulations with MUSCL reconstruction use the standard second-order Runge-Kutta time stepping). At time $t = 10$, the $L^1$ and $L^\infty$ errors with respect to the initial condition in both velocity and density are computed. The cumulative, irreversible dissipation of kinetic energy, which is given by $\epsilon \Delta t = T \Delta s$ [103], is also computed at each timestep as

$$\epsilon \Delta t = \int T \frac{R}{\gamma - 1} \log \left( \frac{p/\rho^\gamma}{p_0/\rho_0^\gamma} \right) \, dx \, dy.$$

(C.16)

$M_0 = 0.1$

Table C.1 and Table C.2 give the errors with respect to the exact solution at time $t = 10$ s for the low Mach correction of Thornber et al. [9] and Xie et al. [10] respectively, while Table C.3 gives the errors when using the fifth-order TENO method without a low Mach correction. Note that the velocity error norms are actually the average of the error norms computed for the $u$ and $v$ velocity components. The rate of convergence for each of the error norms is also given. In general, the rate of convergence is less than second-order for the M5 cases, and equal to or greater than second order for the TENO cases. In simulations of the original problem of Shu [234] where $M_0 = 1.2$ (not included here), second-order convergence has been obtained with the existing numerical method described in Chapter 3, indicating that this low Mach variant is a significantly more challenging test case.

Figure C.1 plots the $L^1$ and $L^\infty$ norms obtained from simulations with M5 reconstruction and both low Mach corrections as well as with TENO reconstruction.
the coarsest grid resolution it can be seen that M5 reconstruction with the low Mach correction of Thornber et al. [9] gives superior results in terms of velocity, while TENO reconstruction gives slightly better results in terms of density. For all other grid resolutions, TENO reconstruction gives more accurate results. Figure C.1 also shows the computational efficiency of each method, measured in terms of CPU time for a given error. By this measure the M5+LM1 method performs the best on the coarsest grid, with TENO reconstruction performing better on all of the finer grids. Between the two M5 based methods, the low Mach correction of Xie et al. [10] is more accurate in terms of the velocity field for grid resolutions of $32^2$ and greater, while for grid resolutions of $64^2$ and greater it is also more accurate in the density field as well. The convergence is also more uniform for this method and is closer to the expected second-order accuracy.

The reasons for the superior overall performance of TENO reconstruction at this Mach number, as well as of the LM2 correction relative to the LM1 correction, can be explained by looking at slices of $\rho$, $u$ and $v$ across different grid resolutions. Figure C.2 plots density across a slice taken at $y = 5$ m for each grid resolution at the final time. On the coarsest grid, the LM1 correction resolves more of the perturbation, but produces a more oscillatory density field than that obtained using TENO recon-
C.2 Test cases

Table C.3 – Error norms and convergence rates for the isentropic vortex test case at $M_0 = 0.1$ using fifth-order TENO reconstruction.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$L^u_{\infty}$</th>
<th>$L^u_1$</th>
<th>$L^\rho_{\infty}$</th>
<th>$L^\rho_1$</th>
<th>$O(L^u_{\infty})$</th>
<th>$O(L^u_1)$</th>
<th>$O(L^\rho_{\infty})$</th>
<th>$O(L^\rho_1)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$16^2$</td>
<td>2.74E+00</td>
<td>2.93E-01</td>
<td>1.40E-02</td>
<td>1.80E-03</td>
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</tr>
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<td>$32^2$</td>
<td>2.36E-01</td>
<td>4.77E-02</td>
<td>1.28E-03</td>
<td>3.83E-04</td>
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<td>3.45E+00</td>
<td>2.23E+00</td>
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<td>2.70E-05</td>
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</tr>
<tr>
<td>$256^2$</td>
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<td>5.35E-05</td>
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</tr>
</tbody>
</table>

struction. At higher grid resolutions the behaviour of the two low Mach corrections is very similar, while both lag behind the results produced using TENO reconstruction. Figure C.3 shows the $y$ velocity across the same slice, showing similar behaviour; the M5+LM1 simulations resolve more of the perturbation at low grid resolutions, while at higher grid resolutions the performance of the two low Mach corrections is again very similar. Interestingly the M5 reconstruction with the LM1 correction actually produces a sharper velocity gradient on the $16 \times 16$ grid than the TENO reconstruction without a low Mach correction.

The main differences arise when examining the $x$ component of velocity, which is plotted in Figure C.4. Across the slice at $y = 5$ m, the perturbation in $u$ should actually be zero. However the values stored at the nodes located along this slice are actually the cell-averaged quantities in the cells located directly above $y = 5$ m which are non-zero. Since the cell size decreases with each successive grid refinement, these cell-averages also decrease. Therefore, Figure C.5 shows plots of $u$ across the same slice but with the data scaled relative to the initial condition on the coarsest grid. This makes it possible to visualise the relative degree of convergence with respect to the exact solution on each grid. From this it can also be seen that the convergence in $u$ using the LM2 correction is substantially better than that of the LM1 correction, which produces a much more non-uniform velocity field with much greater errors. The same behaviour is observed at different slices across the domain, for example when plotting $v$ over the slice $x = 5$ m (not shown). The cause is likely due to the fact that the LM1 correction approaches a central difference in all three velocity components in the limit of $M \to 0$, which potentially violates the TVD property. This is no doubt exacerbated by the present test case, where the vortex propagates diagonally through the computational mesh and represents a worst-case
Figure C.1 – Error norms vs. (a) number of cells per dimension and (b) CPU wall time for the isentropic vortex test case at $M_0 = 0.1$. Shown are the $L^1$ and $L^\infty$ norms for velocity (solid lines) and density (dotted lines), as well as the fiducial line for second-order accuracy (dash-dot).

scenario for the numerical method to resolve. Relative to both M5 based methods, the TENO reconstruction does a significantly better job of resolving the transverse velocity component along this slice, which results in it producing lower overall errors in velocity relative to the exact solution.

These differences in the smoothness and resolution of the velocity field can also be used to explain the behaviour of cumulative dissipation of kinetic energy, shown in Figure C.6. On the $16 \times 16$ grid, the M5+LM1 method produces less dissipation
than either the M5+LM2 method or the TENO method, while on the $32 \times 32$ grid it still produces less dissipation than the M5+LM2 method, with the TENO method now the least dissipative. For finer grids however, the M5+LM1 method becomes anti-dissipative (i.e. negative) and at the finest grid resolution the absolute value of dissipation is the greatest of any method. The M5+LM2 method on the other hand remains positively dissipative for all of the grids considered, likely due to the much smoother velocity field in those simulations, as does the TENO method which is much less dissipative again than the M5+LM2 method on the finest grids. This has important ramifications for ILES, in which the dissipation of kinetic energy is provided entirely by the numerical method. It is therefore highly desirable that the method be dissipative, albeit as little as possible, as this helps ensure that the results
C.2 Test cases

Figure C.4 – $x$ component of velocity vs. $x$ position across a slice at $y = 5\ m$ for the isentropic vortex test case at $t = 10\ s$ and $M_0 = 0.1$. Note that the data have been scaled relative to the $16^2$ initial condition.

Figure C.5 – $x$ component of velocity vs. $x$ position across a slice at $y = 5\ m$ for the isentropic vortex test case at $t = 10\ s$ and $M_0 = 0.1$. Note that the data have been scaled relative to the $16^2$ initial condition.

satisfy the second law of thermodynamics.

Based on the results of this subsection, it would appear that TENO reconstruction implemented in a method of lines finite-volume algorithm and without a low Mach correction applied is quite competitive, and perhaps even preferable, when compared with the standard MUSCL based approach plus a low Mach correction. This is likely due to the smaller differences between left and right velocities reconstructed at an interface using this method, which are responsible for the excessive dissipation at low Mach numbers in upwind schemes [103]. However, the M5+LM1 method still gives better overall results on the coarsest grid resolution considered, showing that a low Mach correction remains important for accurately simulating coarsely resolved flow features. In the next subsection, it will be shown that as the Mach number of the
flow is further reduced, a low Mach correction becomes increasingly important for efficiently generating results at finer and finer grid resolutions too.

**M₀ = 0.01**

Table C.4 and Table C.5 give the errors with respect to the exact solution at time \( t = 10 \) s for the M5+LM1 and M5+LM2 methods respectively when \( M₀ = 0.01 \), while Table C.6 gives the errors for the fifth-order TENO method without a low Mach correction. The rate of convergence is generally less than second-order for the M5+LM1 method, fairly close to second-order for the M5+LM2 method and greater than second-order for the TENO method. Note that the errors in density are lower than in the \( M₀ = 0.1 \) case as the density (and pressure) fluctuations are now a factor of 100 smaller. In general, the errors in velocity are quite similar to those in the \( M₀ = 0.1 \) case for both of the M5 methods, but are larger for the TENO method due to the lack of a low Mach correction.

Figure C.7 plots the \( L^1 \) and \( L^∞ \) norms obtained from the \( M₀ = 0.01 \) simulations with M5 reconstruction and both low Mach corrections, as well as TENO reconstruction without a low Mach correction. Compared to the \( M₀ = 0.1 \) case, the M5+LM2 method is more accurate relative to the M5+LM1 method in terms of velocity errors,
**Table C.4** – Error norms and convergence rates for the isentropic vortex test case at $M_0 = 0.01$ using fifth-order MUSCL reconstruction and the low Mach correction of Thornber et al. [9].

<table>
<thead>
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<th>$L^1_\rho$</th>
<th>$L^\infty_\rho$</th>
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<td>6.85E-01</td>
<td>1.57E+00</td>
<td>1.10E+00</td>
</tr>
<tr>
<td>128^2</td>
<td>1.37E-01</td>
<td>4.84E-02</td>
<td>1.43E-05</td>
<td>2.36E-06</td>
<td>2.24E+00</td>
<td>1.59E+00</td>
<td>1.70E+00</td>
<td>1.33E+00</td>
</tr>
<tr>
<td>256^2</td>
<td>6.41E-02</td>
<td>2.95E-02</td>
<td>6.03E-06</td>
<td>1.03E-06</td>
<td>7.16E-01</td>
<td>1.62E+00</td>
<td>1.29E+00</td>
<td>1.20E+00</td>
</tr>
</tbody>
</table>

**Table C.5** – Error norms and convergence rates for the isentropic vortex test case at $M_0 = 0.01$ using fifth-order MUSCL reconstruction and the low Mach correction of Xie et al. [10].

<table>
<thead>
<tr>
<th>N</th>
<th>$L^1_u$</th>
<th>$L^\infty_u$</th>
<th>$L^1_\rho$</th>
<th>$L^\infty_\rho$</th>
<th>$O(L^1_u)$</th>
<th>$O(L^\infty_u)$</th>
<th>$O(L^1_\rho)$</th>
<th>$O(L^\infty_\rho)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16^2</td>
<td>3.68E+00</td>
<td>4.78E-01</td>
<td>1.69E-03</td>
<td>1.00E-04</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>32^2</td>
<td>9.08E-01</td>
<td>1.35E-01</td>
<td>5.30E-04</td>
<td>6.69E-05</td>
<td>2.02E+00</td>
<td>1.83E+00</td>
<td>1.68E+00</td>
<td>5.85E-01</td>
</tr>
<tr>
<td>64^2</td>
<td>1.95E-01</td>
<td>4.88E-02</td>
<td>1.07E-04</td>
<td>2.48E-05</td>
<td>2.22E+00</td>
<td>1.46E+00</td>
<td>2.31E+00</td>
<td>1.43E+00</td>
</tr>
<tr>
<td>128^2</td>
<td>3.31E-02</td>
<td>1.40E-02</td>
<td>1.79E-06</td>
<td>1.75E-06</td>
<td>2.56E+00</td>
<td>1.80E+00</td>
<td>2.58E+00</td>
<td>1.72E+00</td>
</tr>
<tr>
<td>256^2</td>
<td>5.54E-03</td>
<td>3.80E-03</td>
<td>3.06E-06</td>
<td>1.74E-06</td>
<td>2.58E+00</td>
<td>1.89E+00</td>
<td>2.55E+00</td>
<td>2.11E+00</td>
</tr>
</tbody>
</table>

but less accurate in terms of density errors (which have been multiplied by a factor of 100 in the figure). The LM1 method also still gives superior results in both velocity and density on the coarsest grid. The accuracy of the TENO method has also now decreased relative to the other two methods and in terms of velocity it is the least accurate of the three methods on the coarsest grid. When viewed in terms of computational efficiency the comparison is even less favourable, with the TENO method being the least efficient of the three methods in terms of velocity on grid resolutions up to at least $32 \times 32$. In terms of density the comparison is slightly better but the M5+LM1 method is still more efficient on coarse grids, with the TENO method only becoming more efficient on grid resolutions somewhere between $32 \times 32$ and $64 \times 64$.

Figure C.8 plots density across a slice taken at $y = 5$ m for each grid resolution at the final time. At this lower Mach number the M5+LM1 method is clearly superior, particularly at coarse grid resolutions where the errors in the density field for the M5+LM2 method are larger than the perturbation itself and the TENO method is very dissipative. When looking at the pressure field however, which is shown in Figure C.9, the performance of the M5+LM2 method is much better while the M5+LM1 and TENO methods gives results that are identical to the density field. In fact, the M5+LM2 method gives better results than the other two methods for pressure at grid
### Table C.6 – Error norms and convergence rates for the isentropic vortex test case at $M_0 = 0.01$ using fifth-order TENO reconstruction.

<table>
<thead>
<tr>
<th>N</th>
<th>$L_1$</th>
<th>$L_\infty$</th>
<th>$L_1$</th>
<th>$L_\infty$</th>
<th>$O(L_1^1)$</th>
<th>$O(L_\infty^1)$</th>
<th>$O(L_1^\infty)$</th>
<th>$O(L_\infty^\infty)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>6.96E+00</td>
<td>7.98E-04</td>
<td>2.75E-05</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>32</td>
<td>1.41E+00</td>
<td>1.33E-05</td>
<td>2.10E+00</td>
<td>1.44E+00</td>
<td>1.44E+00</td>
<td>1.05E+00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>64</td>
<td>8.11E-02</td>
<td>3.90E-06</td>
<td>4.12E+00</td>
<td>4.23E+00</td>
<td>3.38E+00</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>128</td>
<td>4.73E-03</td>
<td>4.52E-07</td>
<td>6.93E-08</td>
<td>4.70E+00</td>
<td>3.11E+00</td>
<td>4.21E+00</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>256</td>
<td>8.71E-04</td>
<td>5.34E-05</td>
<td>1.01E-07</td>
<td>2.44E+00</td>
<td>2.17E+00</td>
<td>2.53E+00</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

resolutions of $32^2$ and greater.

Figure C.10 shows the $y$ velocity across the same slice, showing a virtually identical solution for both M5 based methods to that which was obtained at $M_0 = 0.1$, while the solution for the TENO method is substantially more dissipative at coarser grid resolutions. The ability of the M5+LM1 method to resolve velocity gradients is now even greater relative to the TENO method at this Mach number. For the scaled $x$ velocity component, shown in Figure C.11, the results are quite similar for the M5+LM2 method while for the M5+LM1 and TENO methods they are worse than at $M_0 = 0.1$, with the solution for the M5+LM1 method tending to become more and more oscillatory as the grid resolution is refined and the solution for the TENO method being more dissipative at coarse grid resolutions.

Finally, the cumulative dissipation of kinetic energy at $M_0 = 0.01$ is shown in Figure C.12. The results for the M5 based methods are largely the same as for the $M_0 = 0.1$ case, with the M5+LM1 method initially being the least dissipative but becoming anti-dissipative for grid resolutions of $64^2$ and greater. The dissipation for the M5+LM2 method is also slightly larger than at $M_0 = 0.1$ but remains positive for all grid resolutions considered here, while the dissipation for the TENO method has substantially increased at this Mach number and is roughly equal to that of the M5+LM2 method on coarse grids.

### M0 = 0.001

Figure C.13 plots the $L^1$ and $L^\infty$ norms obtained from the $M_0 = 0.001$ simulations with M5 reconstruction and both low Mach corrections, as well as TENO reconstruction without a low Mach correction, while Figure C.14 shows the cumulative
dissipation of kinetic energy. For the sake of brevity, the solution plots are not shown here as they merely showed the continuation of the same trends discussed earlier. The main takeaway here is that the results on coarse grids are nowhere near as favourable for the TENO method at these lower Mach numbers. As will be shown later in Section C.2.3, this Mach number range also corresponds to the Mach numbers observed in the fine-scale turbulent structures of RMI, hence the results here at coarse grid resolutions are highly relevant. For this reason, TENO reconstruction is not used in
any of the further test cases. It should be noted that it is possible to use TENO reconstruction for the primitive variables instead, in which case the it is able to be combined with a low Mach correction. This would make the method much more efficient and competitive at all Mach numbers for this particular test case. Issues arise however when simulating problems involving shock waves, particularly the interaction of shock waves with another discontinuity such as a material interface in multiple dimensions, which necessitates the use of reconstruction in characteristic variables. Future work should investigate why the combination of a characteristic projection and a low Mach correction becomes unstable, as rectifying this would likely result in a method that improves upon the existing computational approach on more challenging test problems.
A simple modification to the low Mach correction of Thornber et al.

Given the results of the previous subsections, there is a sense that the LM2 correction produces a smoother velocity field than the LM1 correction but at the expense of transferring these errors to the density field instead. While this is arguably preferable behaviour anyway, it is also not correct as in fact both the LM1 and LM2 corrections can be shown to give almost identical results for the velocity field after a simple modification is applied to the LM1 correction which also retains its superior behaviour for the density field as well. Following Simmonds et al. [235], the low Mach correction of Thornber et al. [9] is applied only to the normal velocity component at each interface. For example, on a Cartesian mesh only $u_L, u_R$ are corrected when the reconstruction
is performed in the $i$ direction, and only $v_L$, $v_R$ in the $j$ direction etc. This has the effect of increasing the overall dissipation of the numerical method, in particular for the transverse velocity components, which in this case is desirable as it reduces the error with respect to the exact solution. Figure C.15 shows the velocity components, density and pressure for the modified LM1 correction at $M_0 = 0.01$. The gradients in $v$ are not as sharp at coarse grid resolutions as for the original method, however the overall velocity field is much smoother which is evident in the plot of $u$. Comparing these plots with those for the LM2 correction in Figures C.11 and C.10 shows that the velocity fields produced by both methods are almost identical. The pressure field for both methods is also more or less the same, however the density field for the modified LM1 correction is much more satisfactory and mirrors the behaviour of the pressure field. Table C.7 gives the errors with respect to the exact solution at time $t = 10$ s for the modified LM1 correction at $M_0 = 0.01$. Compared to the LM2 correction, the velocity errors are virtually identical while the density errors are greatly improved and closely follow those obtained using the original LM1 correction. The cumulative dissipation of kinetic energy for the modified LM1 correction is not shown here but is also virtually the same as for the LM2 correction and remains positive on every grid.
C.2 Test cases

(a) Grid convergence.

(b) Efficiency.

Figure C.13 – Error norms vs. (a) number of cells per dimension and (b) computational effort, for the isentropic vortex test case at $M_0 = 0.001$. Shown are the $L^1$ and $L^\infty$ norms for velocity (solid lines) and density (dotted lines), as well as the fiducial line for second-order accuracy (dash-dot). Note that the density error norms have been multiplied by $10^4$.

C.2.2 Dual-mode Kelvin–Helmholtz instability

The performance of the numerical methods used in the previous section are now assessed at low Mach number with an additional viscous flux using the double vortex test case from Shanmuganathan et al. [100]. This test case models a vortex-pairing process in two dimensions, initiated by the Kelvin-Helmholtz instability with a dual-mode velocity perturbation. The ability of numerical methods to accurately capture
the evolution of such a process is critical to efficiently simulating transition to turbulence in more complex flows, such as RMI. The initial conditions are as follows. A shear layer between two streams of fluid is initialised with \( U_1 = -1.32 \times 10^{-2} \) m/s the velocity of the upper stream and \( U_2 = 1.32 \times 10^{-2} \) m/s the velocity of the lower stream. The domain has dimensions \( L \times L \) where \( L = 0.06 \) m. The Mach number is given by \( M = \frac{\Delta u}{\sqrt{\gamma p/\rho}} \), where \( \Delta U = U_2 - U_1 \) and is adjusted by varying the background pressure. The initial density is \( \rho = 1000 \) kg/m\(^3\), the Reynolds number is \( Re = L\Delta U/\nu = 1600 \) and the Prandtl number is set to 1. The unperturbed velocity in the \( x \) direction is

\[
  u = -\frac{\Delta U}{2} \tanh \left( \frac{y}{2\Theta_0} \right), \tag{C.17}
\]
where the initial momentum thickness is $\Theta_0 = 0.0003$ m. Velocity perturbations $u'$ and $v'$ are added to the flow and are given by

$$
\frac{u'}{v'} = -\frac{\partial \psi}{\partial y}, \quad \frac{v'}{u'} = \frac{\partial \psi}{\partial x},
$$

(C.18)

with the stream function $\psi$ defined as

$$
\psi = A_1(y)\frac{V_1}{k_1} \cos(k_1 x) \exp(-k_1 |y|) + A_2(y)\frac{V_2}{k_2} \cos(k_2 x) \exp(-k_2 |y|).
$$

(C.19)
The wave numbers of the two modes are $k_1 = 2\pi/L$ and $k_2 = 4\pi/L$, while the amplitudes are

$$A_i = \frac{1 - \exp(-2k_i[L/2 - |y|])}{1 - \exp(-k_i L)},$$

(C.20)

and the velocity amplitudes are $V_1 = 0.025\Delta U$ and $V_2 = 0.05\Delta U$.

The boundary conditions are periodic in the $x$ direction and reflective in the $y$ direction. The simulations are run until time $t = 6$ s, at which point the final structure has a wavelength approximately equal to $L$. The shear layer width is quantified using the momentum thickness $\Theta$, given by

$$\Theta = \int \frac{(U_1 - \bar{u})(\bar{u} - U_2)}{(U_1 - U_2)^2} \, dy,$$

(C.21)

where $(\ldots)$ indicates a plane average taken in the $x$ direction. A passive scalar is also included in the simulations, for which the diffusive flux is nominally zero, effectively giving an infinite Schmidt number (note that some numerical diffusion is still present however). This is useful for visualisation of the vortex and also gives another way of assessing the width of the shear layer through the integral width $W$. The integral width behaves in a similar manner to the momentum thickness and should satisfy $W = \sqrt{2\Theta}$ in a self-similar shear layer [100]. Four different Mach numbers are considered; $M = 0.2$, $M = 0.02$, $M = 0.002$ and $M = 0.0002$. The following subsections compare the performance of the (original) low Mach correction of Thornber et al. [9], referred to as LM1, with the low Mach correction of Xie et al. [10], referred to as LM2, using fifth-order MUSCL reconstruction. The viscous fluxes in this test case are approximated using fourth-order central differences and the second-order TVD Runge-Kutta method is used for time stepping.

**M=0.2**

Figure C.16 and Figure C.17 show the momentum thickness and integral width respectively vs. time for both the LM1 and LM2 corrections. The behaviour for both measures is qualitatively the same and therefore the same discussion applies to both
At the lowest grid resolution (16 × 16 cells), the LM2 correction gives results that are closer to the converged solution (512 × 512 cells). At the next level of grid refinement (32 × 32 cells), the results for both methods are more or less equivalent, while for the 64 × 64 grid resolution the LM1 correction is now closer to the converged solution in both Θ and W. This behaviour seems to suggest that when a viscous flux is included, there is a threshold grid resolution below which oscillations in the pressure/velocity field (as observed for the isentropic vortex test case) produced using the LM1 correction hinders convergence and above which the reduced dissipation (relative to the LM2 correction) improves convergence to the true solution.

**M=0.02**

Figure C.18 shows the momentum thickness vs. time for both the LM1 and LM2 corrections at M = 0.02. The behaviour is virtually identical to that of the M = 0.2 case, which is to be expected as the solution is approximately incompressible, and therefore the conclusions about both corrections are the same. Figure C.19 shows contours of the passive scalar mass fraction at time t = 6 s on the coarsest grid (16 × 16), while Figure C.20 shows the same contours on the 64 × 64 grid. Three
contour lines are shown, equal to $Y_1 = 0.25$, $Y_1 = 0.5$ and $Y_1 = 0.75$ respectively. The high resolution reference solution, computed on a $512 \times 512$ grid, is also shown in Figure C.21.

At the $16 \times 16$ grid resolution, the LM2 correction appears to capture the overall shape of the vortex better, in line with the observations made for Figure C.18 that the momentum thickness is closer to that of the converged solution. This is also in contrast with the results on the coarsest grid for the isentropic vortex case, where the LM1 correction produced a more accurate, although also more oscillatory, solution.

A potential explanation for this behaviour is that the LM1 correction still produces these oscillations in the inviscid part of the algorithm on coarse grids, which causes the viscous fluxes to be overestimated due to artificially large gradients. This has the effect of providing excess dissipation to the solution, dampening the overall growth of the instability.

On the $64 \times 64$ grid, the large-scale structure of the vortex is the same for both methods, with only small differences in the fine-scale structure at the centre of the roll-up. At this grid resolution the LM1 correction also gave a slightly better prediction of the momentum thickness, reversing the trend seen at lower grid resolutions. The explanation here is that any oscillations produced by the inviscid part of the algorithm...
are small enough such that they do not result in overestimation of the viscous fluxes. Instead, the lower overall dissipation of the method helps improve convergence with respect to the true solution. This could have important consequences when performing DNS of turbulent mixing, which will be explored further in the next section. The conclusions of this section for the LM2 method relative to the LM1 correction are also expected to hold for the modified version of the LM1 correction given in Section C.2.1.

**M = 0.002 and M = 0.0002**

Figure C.22 shows the momentum thickness vs. time for both the LM1 and LM2 corrections at $M = 0.002$, while Figure C.23 shows the same plot at $M = 0.0002$. As the trends are identical to the previous section, no further discussion is warranted here.

Finally, Figure C.24 compares the momentum thickness calculated using second-order central differences for the viscous flux vs. fourth-order central differences. On a grid resolution of $16 \times 16$ the improvement when using fourth-order differences is already minimal, and on the $64 \times 64$ grid the results are essentially the same, yet they are not fully converged with respect to the true solution. This suggests that the
accuracy of the numerical method is not limited by that of the viscous flux calculation, similar to how minimal improvements are seen when third-order time stepping is used instead of second-order. For this reason, only second-order differences are used for the viscous flux calculation in the rest of this appendix.

C.2.3 Single-mode Richtmyer–Meshkov instability

The final test case is a 2D, single-mode calculation of RMI between Air and SF$_6$. The setup is similar to the test case presented in Section 3.3.6. A single-mode sinusoidal perturbation of wavelength $\lambda = 2\pi$ m and amplitude $a = 0.5$ m is initialised at a mean position of $x_0 = 6.5$ m, with an initial diffuse thickness of $\delta = \lambda/4$ m. A $M = 1.5$ shock wave is initialised at $x_s = 4.5$ m in the light gas (air). The computational domain has dimensions $L_x \times L_y = 3\pi \times 2\pi$ m$^2$.

The initial background state of the unshocked gases is $p_0 = 101325$ Pa and $T_0 = 298.15$ K. The molecular weight of both gases is $W_{\text{air}} = 28.83$ g/mol and $W_{\text{SF}_6} = 146.07$ g/mol, while the ratio of specific heats is $\gamma_{\text{air}} = 1.4$ and $\gamma_{\text{SF}_6} = 1.09$. The Prandtl
number of both gases is $Pr_{\text{air}} = 0.71$ and $Pr_{\text{SF}6} = 0.90$ and the diffusivity is calculated by assuming that the Lewis number of both species is unity. The viscosities of both species at this temperature are calculated from the Chapman-Enskog viscosity model to be $\mu_{\text{air}} = 1.836 \times 10^{-5}$ Pa-s and $\mu_{\text{SF}6} = 1.535 \times 10^{-5}$ Pa-s. These are modified to set the initial Reynolds number $Re_0 = \frac{\bar{\rho}\dot{a}_0}{\bar{\mu}}$, but are kept in the same proportion to each other. For example, to set an initial Reynolds number of $Re_0 = 4096$, the average viscosity is $\bar{\mu} = (\mu_{\text{air}} + \mu_{\text{SF}6})/2 = (0.6232 + 0.5210)/2 = 0.5721$ Pa-s. The post-shock densities are $\rho_1^+ = 2.67 \text{ kg/m}^3$ and $\rho_2^+ = 17.3 \text{ kg/m}^3$, giving a mean post-shock density of $\bar{\rho}^+ = 10.0 \text{ kg/m}^3$, while the initial impulse is $a_0 = 37.3 \text{ m/s}$ (using the Vandenboomgaarder formula and including the correction for initial diffuse thickness as in Section 6.2).

**ILES**

To test the ability of the low Mach correction within the HLLC Riemann solver to resolve turbulent fluctuations compared to the existing numerical method, implicit large
eddy simulations are performed at a grid resolution of $768 \times 512$. The performance of the mass fraction model with the improved choice of reconstructed variables relative to that of the volume fraction model is also assessed. Therefore three simulations are performed in total; the first with the volume fraction model and the low Mach correction of Thornber et al. [9], the second with the volume fraction model and the low Mach correction of Xie et al. [10] and the third with the mass fraction model and the low Mach correction of Thornber et al. [9]. These are denoted VF-LM1, VF-LM2 and MF-LM1 in the following discussion.

A visualisation of the three simulations at time $t = 0.25$ s is given in Figure C.25 in the form of a simulated density Schlieren. The density Schlieren formula used is the same as that given in Chapter 4. Comparing between each simulation, the VF-LM1 case has slightly more fine-scale structure in the roll-ups at the head of the spike than the other two cases. There is also a small perturbation at the tip of the spike in the VF-LM1 and MF-LM1 cases that is not present in the VF-LM2 case. In all cases there is some fine-scale structure present ahead of the bubble front, which is likely due to a combination of acoustic waves from the shock deformation.
and subsequent straightening, post-shock numerical instability and bulk deposition of vorticity. Figure C.26 shows the flow field at an earlier time of $t = 0.05$ s for the VF-LM1 case, with the fine-scale structure between the interface and the shock much more clearly visible. Evidently some of these structures become entrained by the spike as it develops, resulting in the faint density gradients on either side of the centre line of the spike that are visible in Figure C.25.

To illustrate where the low Mach correction is most active, and therefore where the greatest differences between the LM1 and LM2 corrections should occur, contours of Mach number are plotted in Figure C.27 for the VF-LM1 case at $t = 0.25$ s. Aside from the upper part of the spike stem, which is borderline compressible, the rest of the flow field is incompressible and in general the Mach number is smaller in regions of finer fluctuations. In particular, the Mach number in the roll-ups is 0.1 or less and therefore the results of the previous two test cases are directly applicable here. Furthermore, in 3D cases run to late time, the Mach number can decrease by up to three orders of magnitude [105], which would further exacerbate the differences between methods observed here. The slightly greater amount of fine-scale structure present in these roll-ups for the VF-LM1 case is perhaps not solely due to the fact...
that the LM1 method is better able to resolve velocity gradients in low Mach flow, but also potentially due to the method not providing enough dissipation in these regions.

Switching attention to the comparison between the volume fraction and mass fraction models, the first comparison to make is whether the mass fraction model still produces spurious pressure/temperature oscillations with the new choice of reconstructed variables. Figure C.28 shows plots of the temperature field for the VF-LM1 and MF-LM1 cases, with there being negligible difference between the two models in terms of the maximum and minimum temperatures observed. This is in stark contrast to the results of the similar case presented in Chapter 3 and clearly demonstrates the benefits of maintaining strict thermodynamic consistency between limited properties at a cell interface. Figure C.29 shows plots of the pressure field for the two cases, focusing on the head of the spike in particular. There are some differences in the locations of the vortices between the two methods, in particular the primary vortex of each roll-up. The core of each primary vortex in the VF-LM1 case is also stronger by almost 2000 Pa.

As noted in Williams [228], pressure perturbations still occur when using the mass fraction model to calculate mixing between dissimilar materials at different tempera-
C.2 Test cases

Figure C.24 – Momentum thickness vs. time for the double vortex test case at $M = 0.02$ using second-order and fourth-order approximations for the viscous flux. Dashed lines correspond to a grid resolution of $16 \times 16$ and solid lines correspond to a grid resolution of $64 \times 64$.

For the purposes of this appendix, the most important aspect when assessing the various modifications to the numerical method is whether they improve the performance of a DNS calculation. To this end, direct numerical simulations are performed of the 2D single-mode case at an initial Reynolds number of $Re_0 = 4096$. Of particular
C.2 Test cases

Comparisons are made between the LM1 and LM2 corrections using the volume fraction model, as well as with the LM1 correction using the mass fraction model with the new choice of reconstructed variables. All three methods use second-order central differences for the viscous fluxes and second-order time stepping. The results produced on coarse grids ($24 \times 16$ cells up to $192 \times 128$ cells) are compared to a converged solution on a grid resolution of $1536 \times 1024$. These coarse grid solutions are informative for more complex perturbations that involve a wide range of initial length scales, such as the broadband perturbations considered in Chapters 5 and 6, where inevitably the smallest length scales will not be as well resolved as the largest ones. Thus it is desirable that the numerical method produces results that are as close to the true solution as possible on coarse (i.e. under-resolved) grids, while also converging uniformly as the grid resolution is refined. For the comparisons made here
C.2 Test cases

Figure C.26 – Simulated density Schlieren $\Phi$ at $t = 0.05$ s for the VF-LM1 case, where yellow corresponds to $\Phi = 1$ and blue corresponds to $\Phi = 0$. The major ticks on both axes correspond to a grid spacing of $\Delta x = \Delta y = 1$ m.

The differences between each approach are relatively small, as will be shown below, however this same criteria should be used when assessing any novel numerical method for these types of applications, with the additional consideration of computational cost as well.

Figure C.31 shows volume fraction and simulated density Schlieren contour plots for the reference solution, obtained using the VF model and LM1 correction on a grid resolution of $1536 \times 1024$. When compared with the plots shown in Figure C.25 there is significantly less fine-scale structure present in the solution, including in the region ahead of the bubble front. The volume fraction contour plots show good qualitative similarity with the 2D single-mode experiments of Jacobs and Krivets [180], particularly for the earlier times shown in Figure C.32. The main differences are confined to the roll-ups, which go on to develop significantly more fine-scale structure in the experiments than in the DNS.

Higher Reynolds numbers than the present case could easily be obtained if the aim was to match a single-mode experiment, however here the main interest is the Reynolds
number of a single mode which can be resolved using a moderate number of cells per wavelength (i.e. \( N \leq 128 \)). This is assessed using the integral width, molecular mixing fraction, total fluctuating kinetic energy and domain integrated instantaneous enstrophy and scalar dissipation rate, the definitions of which are given in Section 4.3.1. The results computed using the LM1 and LM2 corrections with the VF model, as well as the LM1 correction with the MF model, on grids of size \( 24 \times 16 \), \( 48 \times 32 \), \( 96 \times 64 \) and \( 192 \times 128 \) are compared with a converged reference solution computed on a \( 1536 \times 1024 \) grid. In the figures below, the numbers in the legend refer to the cross-sectional resolution.

Figure C.33 shows the evolution of integral width in time for the three different methods on each of the various grids. The results for the VF-LM1, VF-LM2 and MF-LM1 methods are all essentially the same on the \( 192 \times 128 \) grid and are approximately converged with respect to the reference solution. The results on the coarser grids are also quite similar, with the only real difference seen at the coarsest grid, where the VF-LM2 method performs the best, followed by the VF-LM1 method and then the MF-LM1 method. All methods appear to be in or close to asymptotic convergence with
Figure C.28 – Contours of temperature for the VF-LM1 and MF-LM1 cases at time $t = 0.25$ s. The major ticks on both axes correspond to a grid spacing of $\Delta x = \Delta y = 1$ m.

C.2 Test cases

respect to the reference solution. Figure C.34 shows the molecular mixing fraction vs. time, for which the performance of each algorithm is also very similar. The only noticeable difference is again at the coarsest grid resolution, where the MF-LM1 method gives slightly better results (although this could be due to cancellation of errors). All three methods are essentially converged on the $192 \times 128$ grid.

Figure C.35 shows the temporal evolution of TKE for each of the three methods. In each case, the initial deposition of kinetic energy by the shock wave ($t < 0.025$ s) is not quite resolved on the $192 \times 128$ grid but this does not seem to affect the subsequent behaviour, which is well-resolved at this grid resolution. The small discontinuity present at $t \approx 0.04$ s is due to the shock wave leaving the domain, which induces
C.2 Test cases

Figure C.29 – Contours of pressure at the head of the spike for the VF-LM1 and MF-LM1 cases at time $t = 0.25$ s. The major ticks on both axes correspond to a grid spacing of $\Delta x = \Delta y = 1$ m.

some spurious oscillations behind it that temporarily contribute to the total kinetic energy budget. These post-shock oscillations are greater for this gas combination in the light-heavy configuration than for the heavy-light $At = 0.5$ cases in Chapter 4 and Chapter 5. This is mainly due to the slow speed of sound in SF$_6$, through which the transmitted shock travels. Comparing between the different methods, in both the VF-LM1 and MF-LM1 cases the TKE is over-predicted (once the shock has existed the domain) at the coarsest grid resolution, while it is under-predicted by the VF-LM2 method which is also slightly closer to the reference solution. Convergence is obtained (for $t > 0.04$ s) for all cases on grids of size $96 \times 64$ and greater.

Figure C.36 shows the domain integrated enstrophy $\Omega$ vs. time for each case. For this metric the solution does not appear to converge at early time during the initial passage of the shock wave, likely due to the gradients in the induced post-shock instabilities that increase as the mesh size is decreased (although the overall amplitude of the fluctuations decreases). Nevertheless, beyond $t = 0.05$ s (once the shock has exited
C.2 Test cases

Figure C.30 – Advection of an initially discontinuous contact surface between air and SF₆.

The domain) good convergence is obtained in the reference solution and the results on the 192 × 128 grid are also approximately converged. At the coarsest grid resolution, the VF-LM1 and MF-LM1 methods outperform the VF-LM2 algorithm, likely due to better resolution of velocity gradients from the reduced dissipation of the (original) LM1 method. This is also observed on the 48 × 32 grid, although the difference is not as great. Finally, Figure C.37 shows the domain integrated scalar dissipation rate χ vs. time. For this metric (as well as Ω), asymptotic convergence does not start until a grid resolution of 48 × 32. The data on the 192 × 128 grid are also almost converged, with the greatest differences with respect to the reference solution at the latest time. The performance of all three algorithms is quite similar, with no noticeable differences to report.

Overall the performance of each of the three algorithms considered here is quite similar. For all of the 3D DNS calculations in this thesis, the (original) LM1 method is chosen over the LM2 method due to its slightly better resolution of the enstrophy on coarse grids. For cases where the ratio of specific heats varies with mixture composition, such as in Chapter 6, the VF model is chosen over the MF model for its slightly better resolution of the integral width and TKE on coarse grids. These decisions are all made without any considerations of computational effort, since here the dif-
C.2 Test cases

(a) Volume fraction. 
(b) Simulated density Schlieren.

Figure C.31 – Contour plots of volume fraction $f_1$ and simulated density Schlieren $\Phi$ at $t = 0.25$ s for the high-resolution DNS case, where yellow corresponds to $f_1 = \Phi = 1$ and blue corresponds to $f_1 = \Phi = 0$. The major ticks on both axes correspond to a grid spacing of $\Delta x = \Delta y = 1$ m.

...ferences are minimal. In general though, when considering the performance of other algorithms (e.g. TENO reconstruction) for these types of flows, the computational efficiency should be the metric that guides the decision. This test case is also used for estimating grid resolution requirements for 3D DNS cases, or equivalently Reynolds numbers for a given grid resolution that can be adequately resolved. This makes it quite useful for predicting how beneficial a given modification to the algorithm will be for a practical case.
C.3 Conclusions

This appendix has presented an assessment of various improvements to the existing numerical method using a series of two-dimensional test cases. The extensions to the numerical method that were considered include an alternate form of low Mach correction, a novel choice of reconstructed variables, higher-order viscous fluxes and time stepping as well as targeted ENO reconstruction. It was shown that for nominally inviscid flows at low Mach number, the low Mach correction of Xie et al. [10] produced a less oscillatory velocity field, although at the expense of being more dissipative, and is equivalent to applying the low Mach correction of Thornber et al. [9] to only the normal velocity components. The fifth-order MUSCL method with a low Mach correction was also shown to give superior performance compared to the fifth-order TENO method without a low Mach correction on coarse grids. Negligible gains in accuracy were observed when using the fourth-order approximation for the viscous fluxes or third-order Runge-Kutta time stepping. The new choice of primitive...
variables that are used in the reconstruction phase of the mass-fraction algorithm also substantially improved its performance relative to the five-equation model on the 2D single-mode RMI test case, although pressure perturbations are still produced when dissimilar materials at different temperatures mix. Based on the results of these test cases, it was determined that the optimal solver settings to use for DNS of 3D RMI were the original low Mach correction, due to its reduced dissipation, along with the standard fifth-order MUSCL reconstruction, second-order time stepping and second-order central differences for the viscous flux. For inviscid computations, there is a stronger case to be made for using the alternate low Mach correction of Xie et al. \[10\] as the original low Mach correction of Thornber et al. \[9\] was shown to be anti-dissipative on the isentropic vortex test case, hence this method is used for the ILES.
To conclude, a few more comments will be made regarding the use of the current algorithm for DNS of compressible turbulent mixing. Firstly, it appears that the new choice of reconstructed variables in the MF model substantially improves its performance relative to the VF model for these types of flows, such that a lot of the conclusions made in Chapter 3 are no longer as strong. This is not to say that there is no longer an advantage to using the VF model, as retaining individual species temperatures is useful for calculating the mixing of dissimilar materials at different temperatures. It may just be that it is most advantageous relative to the MF model when performing an LES calculation, particularly explicit LES, or in under-resolved DNS.
Secondly, the convergence using the current algorithm, in any of its variants considered here, appears to eventually become limited by the fact that the inviscid and viscous fluxes are calculated independently of each other in the method of lines framework. In other words, they are only coupled at each sub-iteration of the Runge-Kutta method, the calculation of the inviscid flux does not take into account the viscous terms and vice versa. This is a kind of predictor-corrector approach, where the flux in the absence of viscous terms is calculated by the Riemann solver and is then corrected using central differences of the viscous terms. Thus methods that do not perform as well in DNS on coarse grids eventually ‘catch up’ on finer grids, see for example the convergence of enstrophy in Figure C.36, such that the grid resolution becomes the limiting factor in obtaining full convergence. It was also shown in Section C.2.2 that using a more sophisticated method for calculating the viscous flux has a similar effect, where improvements that may occur on coarse grids diminish relative to the second-order method as the grid resolution is increased.

This would indicate that greater gains in efficiency (for DNS) may come from incorporating some form of adaptive mesh refinement into the current algorithm, as there appears to be diminishing returns to focusing on more sophisticated methods for calculating the inviscid and viscous fluxes. Note that for ILES the case for using such methods, for example TENO reconstruction, becomes stronger as there the goal is to include as much fine-scale structure as possible. Even then, computational efficiency must ultimately be what determines whether such methods are viable or not. For
DNS however, the amount of fine-scale structure (i.e., the number of local maxima and minima) is set by the Reynolds number and at a certain point adding more cells across each of these structures becomes the only real way to achieve convergence with respect to the true solution. The use of adaptive mesh refinement would at least mean that these cells are allocated in an efficient manner. Increasing the formal order of accuracy of the scheme, i.e., using a more sophisticated method to approximate the integral in Equation (3.37), may also yield greater improvements. However, the greatest improvement may come from using a method for calculating the flux that directly incorporates the contribution from the source terms, such as an ADER method [236, 237, 172–175]. For viscous flows, this would require the governing equations to be reformulated as a set of hyperbolic PDEs with potentially stiff source terms [216]. Appendix B contains some preliminary results in this direction for multicomponent flows.
Appendix D

An Investigation of Anisotropy in the 3D Multimode Richtmyer–Meshkov Instability

This appendix examines anisotropy in the Richtmyer-Meshkov instability (RMI) for a given three-dimensional, narrowband, multimodal perturbation, and whether anisotropy persists at later times when the mixing layer is tending towards self-similar growth\(^1\). In particular, the degree to which viscous dissipation and molecular diffusion affect anisotropy is investigated by comparing the results of a low Reynolds number DNS with a high Reynolds number ILES for the same initial condition and numerical framework, as well as ILES of a quarter-scale initial condition, implemented in the University of Sydney high-order finite-volume code Flamenco. Various measures of anisotropy are considered, including ratios of the components of domain integrated turbulent kinetic energy and enstrophy, ratios of directional Taylor-scale Reynolds numbers and Lumley’s anisotropy tensor. The results from the standard ILES case show that the flow field is persistently anisotropic in the shock-parallel direction at the latest time considered, while comparisons with the DNS results show that anisotropy

is moderately increased at low Reynolds number although tending towards the high Reynolds number results at later times. For the quarter-scale ILES it can be seen that at very late times the layer is relaxing towards isotropy although a significant amount of anisotropy remains at the latest time, indicating that any eventual return to isotropy occurs over a very long time scale.

D.1 Introduction

An area where there is less clear agreement between various numerical as well as experimental studies of RMI is on the level of anisotropy that persists after the passage of the shock wave, an important consideration for the development of models for these types of flows. Tritschler et al. [166] found that for low Reynolds number DNS of RMI at three different Mach numbers the decay rates of turbulent kinetic energy and enstrophy, as well as probability density functions of the velocity and its longitudinal and transverse derivatives, are in good agreement with values for decaying isotropic turbulence. However various high Reynolds number LES studies simulating RMI induced mixing layers to late time have shown that there is persistent anisotropy in the TKE components, with the component in the shock direction typically having 30-60% higher energy [31, 82, 30]. Similar observations have also been made experimentally [192].

Other studies have used different measures of isotropy, for example Lombardini et al. [184] considered an anisotropy measure of the velocity power spectra for a range of different Mach numbers and found that at late time there was substantial, although not complete, isotropisation particularly at higher wavenumbers. The same study also used the ratio of Taylor-scale Reynolds numbers (which is based on both TKE and dissipation rate) as an anisotropy measure, and found that this ratio tended to a value of $\approx 1.5$ at late time for all Mach numbers considered. It is also likely that the level of anisotropy depends on initial conditions, as evidenced by gas curtain experiments [238] and studies that have looked at the effects of different RMS slopes of the initial interface such as Grinstein et al. [239], who quantified anisotropy using the diagonal
components of Lumley’s anisotropy tensor. Mohaghar et al. [188] also investigated
anisotropy using this measure and found that significant anisotropy exists prior to
reshock in both single-mode and multi-mode cases.

Given the differing results and conclusions with regards to anisotropy in RMI-induced
mixing, the focus of the appendix is to compare four measures of anisotropy for
the results of three numerical simulations; a high Reynolds number ILES and a low
Reynolds number DNS of the same initial condition, as well as an ILES of a scaled
version of the initial condition so as to allow for a much later non-dimensional time to
be simulated. The ILES results have been documented previously in Thornber et al.
[30] (although not for all of the quantities considered here), whilst the DNS results
were presented in Chapter 4.

D.2 Quantities of interest

Four different measures are used to quantify the anisotropy of the mixing layer as
it evolves in time. The first is the ratio of components of Favre-averaged turbulent
kinetic energy, which is given by

$$\text{TKE}(t) = \text{TKX} + \text{TKY} + \text{TKZ} = \int \frac{1}{2} \rho u''_i u''_i dV \quad (D.1)$$

where $u''_i = u_i - \bar{u}_i$ and $\bar{u}_i = \rho u''_i / \rho$ is a Favre average. A plane average taken over
the homogeneous directions is used to calculate the ensemble average $\bar{\phi}$ of a quantity
$\phi$. The ratio is then given by:

$$\text{TKR} = \frac{2 \times \text{TKX}}{\text{TKY} + \text{TKZ}} \quad (D.2)$$

where a value of TKR = 1 corresponds to complete isotropy of the turbulent kinetic
energy components. The second measure used is similar to the first but with com-
ponents of enstrophy used in place of components of TKE. The enstrophy is defined
D.2 Quantities of interest

\[ \Omega(t) = \Omega_x + \Omega_y + \Omega_z = \int \rho \omega_i \omega_j dV \] (D.3)

where \( \omega_i \) is the vorticity. As with the first measure, a value of \( 2 \times \Omega_x / (\Omega_y + \Omega_z) = 1 \) corresponds to complete isotropy of the enstrophy components. The third measure is a variable-density variant of Lumley’s anisotropy tensor, defined by:

\[ b_{ij} = \frac{\langle \rho u_i'' u_j'' \rangle}{\rho} - \frac{1}{3} \delta_{ij} \] (D.4)

where \( \langle \ldots \rangle \) indicates a plane average. The diagonal elements of the tensor are bounded between \(-1/3\) and \(2/3\), with \( b_{ii} = -1/3 \) corresponding to no turbulent kinetic energy in the \( i \)th direction and \( b_{ii} = 2/3 \) corresponding to all of the turbulent kinetic energy in that direction, while a value of 0 indicates isotropy. Given that the tensor is calculated for each \( y - z \) plane, the results presented here are averaged over all \( y - z \) planes that satisfy the following condition:

\[ 4 \langle Y_1 \rangle \langle Y_2 \rangle \geq 0.9 \] (D.5)

where \( Y_l \) is the mass fraction of fluid species \( l \). Planes that satisfy Equation (D.5) are referred to as the inner mixing zone [4]. The last measure considered here is the ratio of directional Taylor-scale Reynolds numbers, defined by:

\[ \text{Re}_{\lambda_i} = \frac{\langle u_i''^2 \rangle}{\langle \nu \rangle} \left| \frac{\partial u_i''}{\partial x_i} \right|^2 \] (D.6)

Defining the transverse Taylor-scale Reynolds number as \( \text{Re}_{\lambda_{yz}} = (\text{Re}_{\lambda_y} + \text{Re}_{\lambda_z})/2 \), the ratio of interest is given by \( \text{Re}_{\lambda_x}/\text{Re}_{\lambda_{yz}} \) where a value of 1 corresponds to isotropy. As with the anisotropy tensor, the results presented here are for \( \text{Re}_{\lambda_x}/\text{Re}_{\lambda_{yz}} \) averaged over the inner mixing zone.
D.3 Results

The evolution of the ratio of TKE components in non-dimensional time (defined as $\tau = t\bar{W}_0/\bar{\lambda}$) is shown in Figure D.1. In the standard case, after an initial peak due to the compression by the shock there is a second peak in both the DNS and ILES data at time $\tau = 0.1845$, with values of 5.113 and 4.573 respectively. Beyond this peak there is a rapid decrease in anisotropy that flattens out into a slow decay, with the DNS data appearing to be converging to the ILES. At the latest point in time the values of this anisotropy measure are 1.701 and 1.423 for the DNS and ILES respectively, with the ILES data seemingly approaching an asymptotic value. However, by examining the behaviour at much later non-dimensional time using the quarter-scale ILES data, it can be observed that the results for the standard case are still in some initial transient stage and are not approaching a steady state. For times later than $\tau \approx 40$ there is a slow but steady decay in anisotropy of TKE components, and although at the latest time there is still 33.6% more fluctuating energy in the $x$-direction this value is still decreasing, presumably asymptotically approaching isotropy.

In a similar vein as Figure D.1, Figure D.2 shows the evolution of the ratio of enstrophy components with non-dimensional time. During the initial compression of the layer
D.3 Results

Figure D.2 – Ratio of enstrophy components. Left: Standard case. Right: Quarter-scale case.

This ratio is close to 0 as the majority of the vorticity that is deposited baroclinically is confined about the transverse directions (i.e. rotation normal to the plane). The reason for the sharp jump in this ratio at time $\tau = 0.2091$ is due to the shock exiting the domain, at which point there is a large drop in $\Omega_y$ and $\Omega_z$. Interestingly in the standard case the ratio of enstrophy components peaks at a value greater than 1 before declining, this occurs at time $\tau = 0.8365$ for the DNS and time $\tau = 0.5535$ for the ILES. The behaviour after this point is also qualitatively different, with the ILES data asymptoting towards a value of 1 whereas the DNS data is continuing to decrease below 1 at the latest time considered. This is due to the $x$-direction component of enstrophy having a greater decay rate than the transverse components at late times in the DNS. For the later non-dimensional times simulated in the quarter-scale ILES, the ratio of enstrophy components is steadily approaching 1 (the final value is 0.9870), indicating an eventual return to isotropy.

Figure D.3 shows the diagonal elements of the anisotropy tensor while Figure D.4 shows the ratio of Taylor-scale Reynolds numbers, both averaged across the inner mixing zone, as they evolve in time. The trends observed here are almost identical to those observed for the ratio of TKE components; after the high anisotropy at compression there is a steady decrease in anisotropy towards what appears to be a
D.4 Conclusions

Anisotropy in the narrowband RMI has been examined by comparing four different measures of anisotropy for three separate simulation databases, an ILES and a DNS of the same nominal case as well as an ILES of a quarter-scale version of the same case to evaluate the behaviour at much later non-dimensional time. The results show that anisotropy is moderately increased at low Reynolds number initially, prior to an

steady-state, with the DNS data close to converging to the ILES data at the end of the standard case. The results of the quarter-scale case show that there is an continual return towards isotropy that occurs over a very long period of time. It is useful to compare the values of these two measures with the values for the ratio in TKE components, as this will bring greater insight to the results of previous papers where only presented a single measure has been presented. For the latest time considered in the quarter-scale case the ratio of TKE components is 1.336, which corresponds to a ratio of Taylor-scale Reynolds numbers of 1.281 and values of 0.0536, -0.0287 and -0.0249 for the respective diagonal components of the anisotropy tensor.

Figure D.3 – Diagonal elements of the anisotropy tensor. Left: Standard case. Right: Quarter-scale case. DNS data is given by the solid lines and ILES data by the dashed lines.
apparent return to the high Reynolds number limit at later times. At very late time there is a definite trend towards isotropy although this is not achieved within the period of time considered in the simulation, indicating that the narrowband RMI is persistently anisotropic over a very large time scale. These results may have important ramifications for models of these flows that assume isotropy over a time scale on the same order as that considered here.