

Direct Numerical Simulation of Shear-Induced Transitional Mixing and its Interplay with Combustion

MOUSTAFA ALI

B.Eng (Hons)

Supervisor: Professor Matthew Cleary
Associate Supervisor: Professor Ben Thornber

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School of Aerospace Mechanical and Mechatronic Engineering
Faculty of Engineering
The University of Sydney
Australia

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Declaration of Originality

I hereby declare that this thesis is my own work and contains no material that has been previously submitted nor accepted for any other award or degree at the University of Sydney or any other institution of higher education.

I also declare that the intellectual content of this thesis is the product of my own work and that any assistance or support received during its preparation has been acknowledged in the following text.

Moustafa Ali

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Abstract

This thesis investigates the dependence of turbulent mixing on fundamental primary shear instabilities, a critical factor in a wide range of energy and propulsion applications, including hypersonic propulsion and nuclear fusion. Understanding how varying turbulent mixing states unfold is essential for controlling process output, stability, and efficiency. Shear instabilities, particularly Kelvin-Helmholtz Instabilities (KHI), play a dominant role in turbulence generation, making them a natural focus for this investigation. This study explores the influence of initial perturbation parameters, specifically the perturbation wavelength bandwidth and free-stream velocities, on turbulent mixing and the subsequent flow evolution.

The study leverages high-fidelity direct numerical simulations (DNS) to investigate the impact of these perturbation parameters which were chosen because they appear directly in the eigenvalue representation of the KHI. Unlike conventional approaches that initiate simulations with fully turbulent conditions, by modelling the KHI in an eigenvalue-eigenvector framework and implementing this framework to the flow initialisation, the present study assesses turbulent mixing as a dynamic system, providing insights into how variations in initial conditions influence the evolution of the flow. This offers a more accurate representation of the natural transition from laminar to turbulent flow.

The results reveal that turbulence and mixing scales are heavily influenced by the initial shear instability characteristics, including the initial shear instability wavelength bandwidth. The study finds that the relative dimensions of the instability, rather than its absolute values, are crucial for understanding the growth of large-scale flow structures. Notably, a Strouhal number-like normalization unveils a self-similar collapse during both transitional and asymptotic stages of the large-scale flow evolution. However, the onset of fully developed turbulence is not solely dependent on achieving a high Reynolds number; instead, it requires an adequate

energy-transferring mechanism seeded by the initial perturbation. This insight challenges traditional Reynolds number thresholds for turbulence onset and offers a more rigorous criterion supported by spectral and Reynolds stress analyses.

Furthermore, the research examines the effects of these perturbations on mixing scales in reacting flows. The study shows that while large mixing scales are more sensitive to free-stream velocities, finer mixing scales extend the dependency on perturbation wavelength. This dual sensitivity underscores the complexity of turbulent mixing.

The thesis also delves into the implications of these findings for flame structure and stability. It uncovers significant variability in flame behaviour due to differences in initial perturbation characteristics.

This research not only deepens the understanding of turbulent mixing but also provides a valuable dataset for future model development in transitional reacting flows. The findings highlight the importance of considering initial perturbations in turbulence studies and pave the way for more accurate predictions and control strategies of turbulent mixing in advanced energy and propulsion technologies.

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Nomenclature

List of Acronyms

BC	Base Case
CFL	Courant-Friedrich-Levy
CMC	Conditional Moment Closure
CPU	Central Processing Unit
DNS	Direct Numerical Simulation
FFT	Fast Fourier Transform
FLAMENCO	Flow Analysis and Modelling Environment with Combustion
HIFiRE	Hypersonic International Flight Research Experimentation
HLLC	Harten, Lax, and Leer Contact Reimann Solver
HMa	High Mach Number Case
HPC	High Performance Computing
HRe	High Reynolds Number
IC	Internal Combustion
ILES	Implicit Large Eddy Simulation
JANAF	Joint Army Navy Airforce
KHI	Kelvin-Helmholtz Instability
LD	Large Domain Case
LES	Large Eddy Simulation
LRe	Low Reynolds Number
MARS	Multivariate Adaptive Spline Regression
MPI	Message Passing Interface
MUSCL	Monotonic Upstream Centered Scheme for Conservation Laws
NCI	National Computational Infrastructure
PCA	Principal Component Analysis

PDF	Probability Density Function
RAM	Random Access Memory
RANS	Reynolds Averaged Navier Stokes
RDE	Rotating Detonation Engine
RMI	Richtmyer-Meshkov Instability
RMS	Root Mean Square
RTI	Rayleigh-Taylor Instability
TB	Terabyte
TVD	Total Variation Dimishing Runge-Kutta Scheme

List of Symbols

ω	Wavenumber Vector
χ	Scalar Dissipation
δ_h	Streamwise Velocity Threshold Thickness
δ_m	Initial Momentum Thickness
δ_Z	Mixing Zone Thickness
δ_{ω_I}	Integration-Based Vorticity Thickness
δ_ω	Vorticity Thickness
δ_{ij}	Kronecker Delta
$\delta_{m,0}$	Initial Momentum Thickness
$\dot{\omega}_T$	Heat Release Rate
η	Kolmogorov Length Scale
κ	Wavenumber
κ_0	Minimum Wavenumber
λ	Mixture-Averaged Thermal Conductivity
λ_i	Taylor Length Scale Component
$\lambda_{min,0}$	Minimum Wavelength of Initial KHI
$\mathcal{F}$	Fourier Transform Operator
$\mathcal{K}$	Turbulent Kinetic Energy
$\mathcal{L}$	Large Eddy Length Scale
μ	Dynamic Viscosity

ν	Kinematic Viscosity
ω_1	Transverse Vorticity Component
ω_y	Streamwise Wavenumber
ω_z	Spanwise Wavenumber
$\overline{r_z}$	Mechanical-to-Scalar Mixing Time Scale Ratio
Φ	Velocity Potential
Φ_0	Initial KHI Eigenvalue
i	Velocity RMS Component/ Heat Diffusion
ρ	Density
σ	Root Mean Square
τ_c	Chemical Time Scale
τ_d	Diffusive Time Scale
τ_t	Turbulence Time Scale
τ_{ij}	Viscous Stress Tensor
θ'	Divergence of Velocity Fluctuation
$\underline{\kappa}$	Radial Wavenumber
ε	Turbulent Kinetic Energy Dissipation
φ_{ij}	Velocity Spectrum Tensor
ξ	Mixture Fraction
ξ_{st}	Stoichiometric Mixture Fraction
ζ	Amplitude Perturbation
A_{ij}	Two-Point Correlation
D	Molecular Diffusivity
Da	Local Damkohler Number
Da_q	Quenching Damkohler Number
Da_t	Large Turbulent Eddy Damkohler Number
E	Total Non-Chemical Energy
$E_i i$	One-Dimensional Energy Spectrum
E_{ij}	Two-Dimensional Radial Energy Spectrum
FI	Flame Index

g	Gravitational Acceleration
h	Sensible Enthalpy
I_i	Integral Length Scale Component
L_χ	Normalised Integrated Scalar Dissipation
L_x	Transverse Domain Length
L_y	Streamwise Domain Length
L_z	Spanwise Domain Length
Ma	Mach Number
N_x	Number of Cells in Cross-Stream Direction
N_y	Number of Cells in Streamwise Direction
N_z	Number of Cells in Spanwise Direction
P	Thermodynamic Pressure
$P_\phi(\Xi)$	ϕ Weighted Probability, Conditioned on Ξ
PA	Product Alignment Index
Pr	Prandtl Number
Re	Outer-Scale/ Visual Thickness Reynolds Number
$Re_{\lambda i}$	Directional Taylor Reynolds Number
Re_t	Turbulent Reynolds Number
Re_{δ_h}	Threshold Thickness Reynolds Number
Re_{δ_z}	Mixing Zone Thickness Reynolds Number
s'_{ij}	Fluctuating Rate-of-Strain Tensor
Sc	Schmidt Number
St	Strouhal Number
T	Thermodynamic Temperature
t	Time
u_i	Velocity Field Component
V_{ki}	Diffusion Velocity
x	Cross-stream/ Transverse Direction
y	Streamwise/ Longitudinal Direction
Y_i	Species Mass Fraction

z Spanwise Direction

List of Subscripts

1 Cross-stream Direction

2 Streamwise Direction

3 Spanwise Direction

F Fuel Stream

O Oxidiser Stream

x Cross-stream Direction

y Streamwise Direction

z Spanwise Direction

LFA Laminar Flamelet Assumption

CHAPTER 1

Introduction

1.1 Background and Motivation

Turbulence, a multi-scale complex phenomenon, strongly influences the physics of almost all practical fluid flows, including those with chemical reactions. Reacting flows are of great interest to the energy, defence, and transport sectors, and their extensive research, particularly in the framework of the underlying turbulence, has driven substantial advancements in these sectors. For instance, taking the internal combustion (IC) engine, which provides close to 25% of the world's energy [1], extensive research of the relevant flow and chemistry dynamics has helped support major advances in IC engine designs both in terms of efficiency and in reducing toxic emissions, which have fallen a 1000-fold over the last four decades [1]. The pursuit of these cutting-edge improvements has driven researchers to improve the fundamental understanding of the underlying physical phenomena that govern such applications. Combustion in reacting flows requires adequate mixing of fuel and oxidizer. This particularly makes having a premixed fuel and oxidizer mixture prior to combustion advantageous; however, in many reacting flow applications, such convenience is not feasible, and there is no way around starting with separate fuel and oxidiser streams. This mixing requirement in non-premixed reacting flows relies on fully established turbulence where mixing is most rapid [2]. Consequently, up to this stage, most research focus on reacting flows has been on fully turbulent regimes [3], which historically served as the most critical and commonly encountered flow regimes in classical applications. In comparison, much less focus has been given to the laminar to turbulent transition.

Nowadays, with the impending necessity for more efficient energy systems that are more environmentally friendly, unconventional fuels and engine designs are garnering more interest. An important element of increasing combustion efficiency is the more thorough mixing of fuels and oxidiser as that results in more complete fuel oxidation, which reduces the formation of by-products of combustion that reduce process efficiency and pollute the environment. With optimal mixing requiring fully turbulent flow regimes, designing combustion systems for rapid and controlled flow turbulence development is pivotal to support more efficient engine realizations. This requires a deeper appreciation of the dependence of the developing turbulence on the seeding flow perturbations that manifest as a result of system design and affect the ensuing transitional process [4], [5].

Turbulence is generated from fundamental flow instabilities. These initially manifest as large-scale structures - for instance, the large vortices resulting from shear instabilities. Combustion occurs at the molecular scale and is only triggered once these large-scale instabilities break and cascade down into smaller eddies that initiate the microscale mixing required. Nevertheless, attaining a state of flow turbulence, with a steady influx of small-scale eddies from the onset of the flow instabilities, involves an intermediary complex multi-stage transitional flow regime [6]. This regime starts with receptivity mechanisms as the disturbed flow assimilates the instabilities. This is followed by transient growth that is well characterized by linear stability theory and hence is often referred to as linear growth in literature (as it is well described through linearization of the governing equations), although it usually actually involves non-linear (e.g. exponential) growth of the initial instability modes. The following process involves a range of nonlinear interactions of these growing instabilities, and the final stage of transition is the breakdown of the larger flow structures as the flow starts developing a self-similar turbulent state. What makes studying transition difficult is that transitional mechanisms are heavily dependent on the nature of the flow and its configuration, as there are many different ways to trigger turbulence in a flow. Therefore, transitional flows are complex and not statistically universal as the fully turbulent limit.

In conventional applications, this transitional flow regime is short-lived due to the range of different flow instabilities subjected to the flow simultaneously and is often neglected. This

complicates the study of transitional flows compared to more widely studied turbulent and laminar flows. For example, in the fundamental flow over a flat plate, as shown in Figure 1.1, the conventional approach is to define a critical Reynolds number midway between the laminar and turbulent regimes and use that to categorize the flow as either entirely laminar or turbulent while neglecting the transitional regime altogether. Moreover, most conventional combustion applications involve low-speed flow regimes where the fluid has sufficient time to become turbulent in the confines of the engine. This time is commonly referred to as residence time. To help gain an appreciation of the duration of transitional regimes, Figure 1.1 highlights the flow development from shear instabilities in a simple boundary layer from flow over a flat plate. For this fundamental flow, the fluid must travel 30 times the distance from the onset of the instability in the boundary layer to become turbulent and span a wide range of eddies. This distance is required to increase the flow Reynolds number, a non-dimensional parameter that depicts the ratio of inertial to dissipative viscous forces and is commonly used to characterize the onset of turbulence.

Emphasis here is on how the Reynolds number needs to increase 30-fold from the initial Reynolds number at the onset of the instability. Even more emphasis is on that it is the length scale (distance downstream of the plate) element of the Reynolds number that dictates the transition criteria in this case. Technically, in this application, the fluid length scales correlate more with the boundary layer thickness that more directly drives the flow eddies. However, since the boundary layer thickness can be shown to correlate directly with the square root of the downstream distance, which is more convenient to measure, the latter is reserved as the length scale for the Reynolds number definition of flows over a flat plate. Since turbulence spans a wide range of length and time scales, a Reynolds number can be defined differently depending on the scale choice. Some specific Reynolds number definitions can be universally used to characterize the onset of turbulence due to their relevant velocity and length scales more conveniently calculated or measured than others in a wide range of different flow setups as extensively studied and discussed by Dimotakis [3], [8], [9].

The fact that an appropriate length scale drives Reynolds number growth implies that it is not always the case flows can readily attain critical values of these Reynolds numbers within the

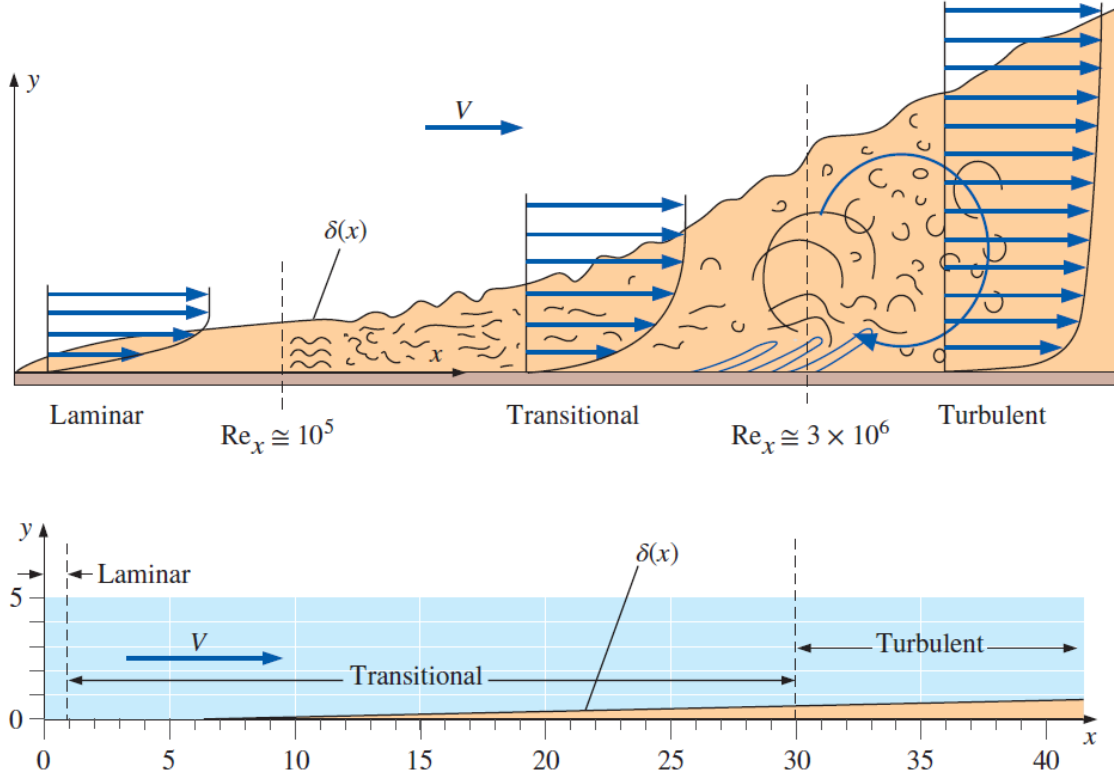


FIGURE 1.1. Schematic (not-to-scale) of boundary layer development over a smooth flat plate, reproduced from Figures 10-81 and 10-82 in [7]

confines of the physical system, even if their initial velocities are high as the relevant length scale remains low. For instance, surprisingly, the Reynolds number based on momentum thickness inside hypersonic boost-glide weapons and scramjets alike can be as low as 1000 in the free stream and even lower near walls, both leading to and inside the combustion chamber [10]. Assuming the visual thickness, a commonly used term in literature to denote a large length scale used in Reynolds number benchmarks for established turbulence, is $8 \times$ the momentum thickness (based on the assumptions of Rogers & Mosers and Dimotakis in [11]), this results in visual thickness Reynolds number of 8000 which is below 20 000- the established turbulence threshold quoted by Dimotakis [9]. This can be surprising to some because engineers are conditioned to think about Reynolds numbers in terms of velocity based on how it is taught in fundamental fluid mechanics and applied in industry. The most common and popular application of fluid mechanics is pipe flows, in which the length scale

in developed flows is the pipe diameter, which is fixed, leaving the average velocity to be the main turbulence-controlling variable!

The visual thickness-based threshold Reynolds number value, which has been established to characterize the onset of developed turbulence, has been frequently contested in literature, with several research groups claiming that the onset of turbulence is achieved at even higher visual thickness Reynolds number [11]–[13]. Therefore, it is quite likely that mixing in high-speed propulsion and hypersonic applications relies heavily on uncharacterized transitional rather than fully turbulent flow regimes, particularly in the combustion stages [10]. This might be initially surprising given the high speeds of the flows involved (in the order of 1000-3000 m/s), but compressibility effects in high-speed propulsion impede the growth of mixing layers [14] which restricts the length scales that affect Reynolds number growth associated with mixing which is detrimental to combustion and heat diffusion/dissipation. This is why, historically, aerospace applications have utilized compressor configurations in turbojets and turbofans that decelerate the airflow to subsonic speeds to allow for longer residence time in combustion chambers such that adequate fuel-oxidiser mixing and deflagration (combustion in subsonic flows) occurs. This time is needed to allow the different flow scales to loop through the transitional mechanisms outlined by Kachanov[6], from receptivity to breakdown, growing the relevant Reynolds numbers in the process.

With the compelling need to advance hypersonic propulsion technology, whether for defence or to support space exploration and efficient satellite deployment efforts, restricting combustion to deflagration is no longer convenient and serves as a bottleneck to pioneering more efficient and robust propulsion technology. Detonation - supersonic combustion, therefore, becomes an attractive alternative in these high-speed propulsion applications. Furthermore, there is a clear motivation in these applications for combustion to be non-premixed. For instance, there is a strong push for air-breathing propulsion systems [10]. Current rocket-based propulsion systems dedicate 40-65% of their total pre-launch gross weight to carry the oxidiser needed to ascend through Earth's atmosphere. Air-breathing engines that remove the need to carry such significant oxidiser weight and readily capture air from the atmosphere during ascent pose a lucrative solution to improve propulsion efficiency substantially.

This is also the case in all scramjet engine designs, including in the recent HIFiRE (Hypersonic International Flight Research Experimentation) Projects, where the oxidiser and fuel streams are always initially separate, and combustion is predominantly non-premixed [15]. Therefore, it is clear that high-speed propulsion engines must effectively utilize non-premixed supersonic combustion, which is problematic. As previously discussed, the supersonic flow regimes inside the combustion chamber exhibit strong compressibility effects with multiple interacting shockwaves that impede mixing layer growth, turbulence onset, and fuel-oxidiser mixing. Therefore, the extent of reactions that can occur is limited, as is the chemical energy that can be harnessed from the fuel. This is particularly troublesome as these applications must overcome significant internal and external drag forces [10] that require more energy released from combustion. Additionally, these resilient transitional flows exhibit strong flow-chemistry coupling in the combustors, destabilising combustion and reducing thrust reliability. For instance, in 2011, the X-51A scramjet catastrophically malfunctioned due to this exact reason. This is why the transitional flow-chemistry coupling challenge has been identified as a critical hurdle to overcome for advancing supersonic combustion applications, along with navigating the challenges posed by the significant thermomechanical and aerodynamic loads that are endured in these applications, particularly on the external surfaces [10].

Another prospective high-speed propulsion system that is set to replace traditional rocket propulsion is the rotating detonation engine (RDE) concept [16], which can also utilize an air-breathing setup. The combustion chamber of an RDE is thin and annular in shape, with detonation waves continuously circulating around the chamber, perpendicular to the incoming separate flows of fuel and oxidizer, as shown in Figure 1.2. Air enters the engine via a supersonic intake and mixes in the annular refill zone with the separately injected fuel. Instabilities at the interface between initially separate and non-turbulent fuel and air streams drive the mixing process, as shown in Figure 1.2 (C). Provided the mixture is within detonation limits (which are generally fuel, oxidiser, pressure, temperature, and geometry dependent), one or more detonation waves, characterized by leading shock coupled with a trailing combustion zone, traverse the refill region and generate very high pressure and temperature gas which can be expanded through a nozzle for thrust or a turbine for power.

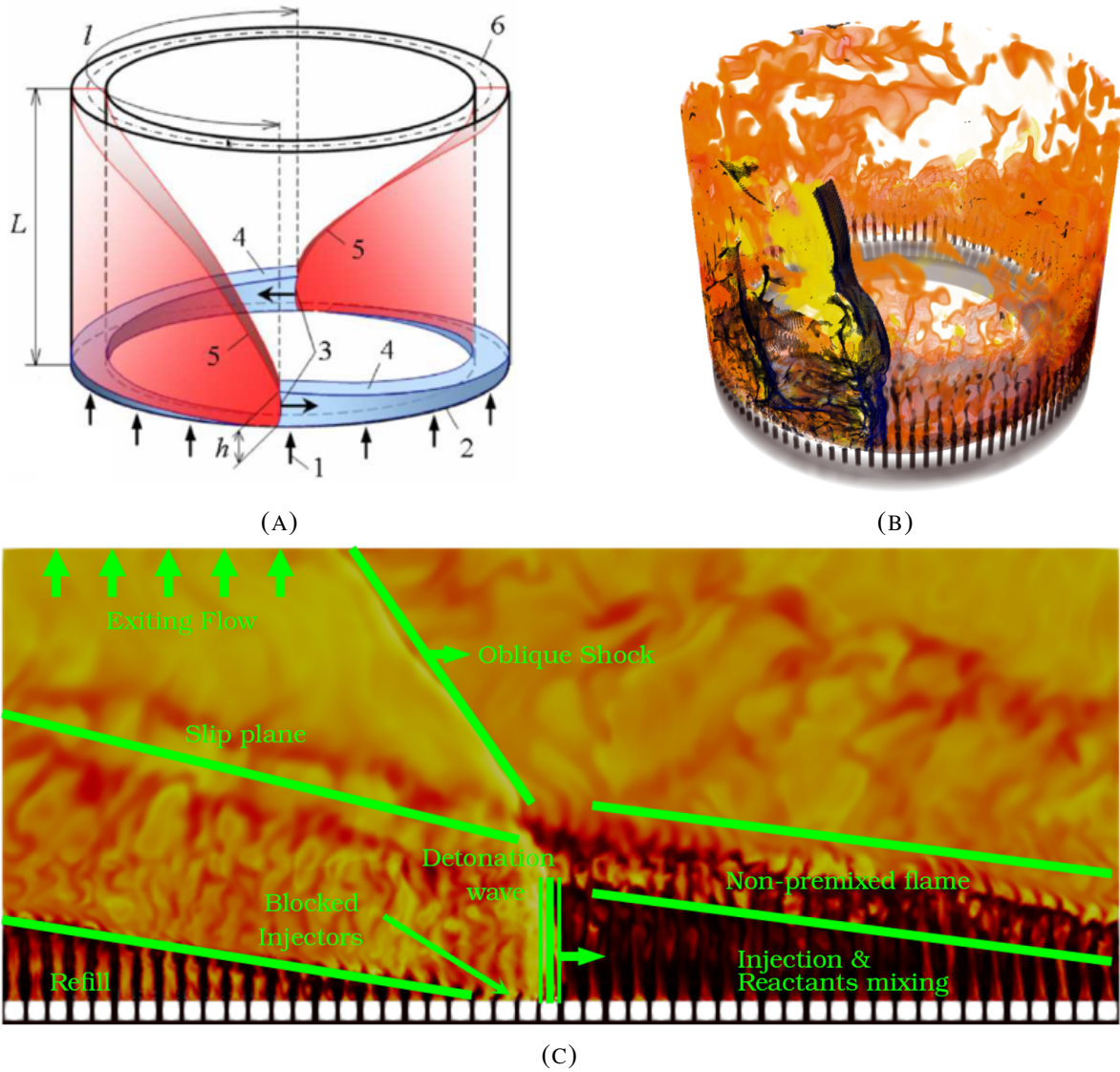


FIGURE 1.2. Rotating detonation engine (RDE) illustrations. (A) Shows a schematic of an RDE annular combustion chamber with air (1) and fuel (2) injections, detonation fronts (3), fresh mixture (4), and oblique shocks (5). Injected air and fuel are highlighted in blue, and the detonated mixture in red [17]. (B) 3D temperature volume render and (C) 2D slice of temperature contours around the circumference of the annular chamber from Implicit Large Eddy Simulations (ILES) results published in [18]. Regions both ahead and behind the detonation wave are outlined, showcasing the importance of the fuel-oxidiser shear-induced mixing that occurs ahead of the detonation wave.

As the detonation wave travels, it is followed by a rarefaction as the gas expands, allowing new fuel and oxidizer to enter the chamber for the next cycle. Optimum efficiency results from rapid and perfect fuel/air mixing downstream of the injection ports and containment of all the heat release to a nearly constant-volume process over the detonation wave [19], [20]. The added sharp pressure rise provided by RDEs due to the isochoric rapid compression and ignition of the air-fuel mixture is advantageous over classical isobaric gas turbines and scramjets, potentially leading up to 50% increased efficiency [20]. However, efforts to advance and adopt RDE technology are afflicted by the same challenges posed to scramjets, as discussed, particularly pertaining to transitional mixing and flame stability.

Even outside of combustion, the resolution of initial transitional layers has been highlighted as a key weakness for high-frequency noise prediction in jet nozzle flows [21]. With transition as a common factor stymieing practical progress in high-speed propulsion, many recent efforts have focused on enhancing turbulence transition and its control in these applications [15], [22], [23]. However, most of these studies are application-based rather than fundamental and do not directly help inform the much-needed subgrid model development for transitional reacting flows, which can then help enable more accurate full-scale application-based simulations that can support practical progress.

The focus is drawn back to the fuel-oxidiser mixing in an RDE, as shown in Figure 1.2 (C), to appreciate the underlying transitional regime in these applications. The initially laminar and sharp interface between fuel and coflowing air is wrinkled substantially by primary instabilities – mainly Kelvin-Helmholtz (KHI, shear driven), but also Rayleigh-Taylor (RTI, buoyancy/acceleration driven) and Richtmyer-Meshkov (RMI, shock driven) – leading to turbulent transition. The strong deformation of the transitional interface between fuel and air by KHI, RTI and RMI, determines mixing rates and detonation viability. It is these fundamental instabilities and their interactions that trigger the transition to turbulence [24].

This thesis focuses on the shear effects due to KHIs, which dominate the mixing process in these flow regimes. Among the three primary instability types, the modes that govern KHIs are inherently unstable and grow exponentially, rendering KHI a dominant turbulence-generating phenomenon. For instance, conversely, the modes that govern RMIs tend to reduce Reynolds

number with time and impede turbulence growth [25], [26]. Moreover, KHIs are prevalent in all interfacial (shear) and stratified flows, regardless of the Mach number [27], [28]. With combustion and propulsion aside, the shear-induced rapid molecular mixing following the stretching and contortion of an interface between two fluids is central to many problems in geophysics, oceanography, meteorology, astrophysics, engineering, and fusion science. KHIs are also inherently incompressible physical phenomena [27], [28], which allows the study of the ensuing transitional mixing effects in isolation of compressibility and buoyancy. Since it can be studied in incompressible flows, a thorough parameter sweep of the instability is feasible under current computational amenities as undertaken in this thesis.

1.2 Research Objectives and Gap Addressed

This thesis aims to thoroughly investigate and provide detailed knowledge on the underlying shear-related fundamental physics of turbulence development and mixing in reacting and non-reacting flows. This is done through systematically varying elements of the fundamental seeding shear perturbations to improve the understanding of the isolated effects of these changes on each of the flow, turbulence, and mixing developments, along with the wider implications on flame stability. The experimental investigation of these instabilities in transitional reacting flows is difficult and prohibitive, particularly if the physics needs to be simplified to isolate individual effects in these complex flow regimes. Additionally, the design of facilities able to repeatably generate transitional mixing layers at a range of initial conditions and Reynolds numbers whilst accurately measuring the quantities necessary to derive and validate models is challenging and impractical.

Previous computational work on this topic has been conducted through Large Eddy Simulations (LES) that capture the largest scales but model the smaller ones. However, with the physics of transition not well understood, turbulence models were often used in these studies, which is inaccurate and doesn't serve the current purpose and research needs [17], [29]–[35]. This motivates the use of high-resolution direct numerical simulations (DNS), which resolve all the scales of the flow and allow comprehensive insight into the full array

of flow and chemistry parameters. This work, therefore, aims to collate a comprehensive and self-consistent high-fidelity dataset on shear-induced mixing in developing flows in both reacting and inert conditions. Such a dataset did not previously exist globally; however, with the reacting DNS framework developed in this study and the significant utilization of HPC resources, this study aims to supply and analyze such a dataset to inform on the physics in question.

Ultimately, this thesis aims to address three main holistic points. To date, there has been limited work that informs on the temporal transition to turbulence and mixing. Most studies induce established turbulence directly either from random noise [11], [31], [36] or from a spectral function already derived to conform to the asymptotic profile of established turbulence as per Kolmogorov hypotheses (highlighted in Chapter 2) [37], [38]. Instead, in this study, turbulence is driven by tractable perturbations and modes derived from linear theory and confined within a narrowband range to model turbulence development more naturally.

Firstly, this thesis aims to investigate the statistics of shear-triggered time-dependent transition to turbulence through fully resolved, validated computations and provide insights to support the development of a model for transitional scalar mixing. This is first done without the influence of chemistry in inert flows in Chapter 4 in isolation of any flow chemistry coupling to simplify and track the flow and turbulence behaviour. Then, it is extended to reacting flows in Chapter 5, with a focus on the mixing evolution.

Secondly, there has to be a clear consensus on how to characterize the onset of turbulence in the context of shear-induced instabilities, which this thesis aims to provide, given that current literature on the topic is divided. This is needed to support closure and accurate modelling of subgrid terms in the conservation equations of transitional flow regimes that are approaching a fully established turbulent state.

Thirdly, this study aims to assess the flame-structure evolution in non-premixed combustion of developing rather than fully turbulent flows to inform on the wider implications of the flow and mixing dependence on the seeding instability parameters.

Using DNS to study full-scale applications is impossible due to the significant computational overhead required, particularly in high-speed propulsion applications that involve compressible effects (which both reduce the simulation time steps and impede the growth of mixing layers [14]) and complex fuels (that require transporting hundreds of gas species for their reaction mechanisms). Therefore, this study aims to provide insights into the statistics of non-premixed combustion in developing flows so that future efforts can assess how more accurate LES approaches and models can be developed for accurate closure of flow and chemical terms and drive practical progress.

Overall, throughout this study, the following fundamental questions are investigated:

- (1) How would varying the initial instability wavenumber range affect the flow development, the asymptotic state, and the flame profile? Traditionally, the expectation is that the effects of the initial instability are diluted once the flow is developed, but this view is tested in this study
- (2) How to characterize the onset of self-similar evolution in reacting and non-reacting flows, also commonly referred to as the mixing transition? The onset of turbulence in inert flows is well characterized in the literature. Do reacting flows ever exhibit such asymptotic behaviour in tractable quantities or does the presence of chemical reactions perpetuates statistical variations?
- (3) Do the initial conditions still manifest effects at a late time, past the mixing transition, particularly ones that affect the flame profile? Literature is divided on this subject, and this study aims to identify parameters that can help explain the division.

1.3 Thesis Structure

This thesis is structured as follows. Chapter 2 provides an overview of the fundamentals of turbulence and transition. A detailed outline of the physics and formulation of KHIs is presented, and many of the parameters and analysis frameworks that will be used in later chapters are introduced. In Chapter 3, the governing equations and simulation setup are thoroughly outlined. A thorough formulation of how the KHIs are incorporated to produce novel and physical divergence-free initial conditions that trigger the onset of turbulence

is provided. Additionally, a meticulous and systematic assessment is conducted on the simulation quality to ensure the resolution of both the large and small scales of motion and the chemistry. A full breakdown of the DNS dataset that is exhaustively analyzed in the subsequent chapters is also provided.

In Chapter 4, the focus is brought to the results of the inert DNS cases to investigate the effects of the initial perturbation on the flow development, growth rates, and the onset of turbulence, followed by a focus on the Reynolds number dependence. In the absence of chemical reactions, this investigation isolates the dependence of the turbulence development on the seeding perturbation and sets a reference against which subsequent chapters that consider chemical reactions can compare. Both spectral and temporal analyses are conducted. Characterization of the mixing transition and the onset of turbulence is conducted, initially based on approaches outlined in the literature, followed by extended approaches refined in this study. Key quantities that exhibit asymptotic profiles towards the mixing transition are highlighted. Important flow and instability time and length scales are also outlined and analyzed.

In Chapter 5, the focus is switched towards the mixing development in reacting cases. With a direct focus on mixing characterization rather than general flow or turbulence evolution and consideration of reacting cases, this chapter enables a direct correlation between the mixing evolution and flame structure characterisation to be developed in the subsequent chapter. The distinction between mixing effects and general flow/turbulence development is emphasised, and a range of different large-scale and fine-scale mixing parameters are explored in their dependence on the initial KHIs.

Furthermore, discrepancies between the resulting flame structures of the different cases are highlighted in Chapter 6. This chapter presents a comprehensive analysis framework of the flame structure that assesses the wider implications of the initial instability variations on the unfolding combustion regimes. It also provides a wide range of insights and analyses that can help inform and validate future modelling efforts of combustion in developing flows.

Chapter 7 concludes the thesis with a summary of the key results and recommendations for future work.

Fundamentals of Turbulence and Transition

2.1 Overview

This chapter overviews the relevant theoretical frameworks for this study. The fundamentals of turbulence, including its equilibrium state and relevant statistics, scales, and characterizations, are presented. The notation convention for all the statistics produced in this thesis is also outlined in a single section, 2.2.1.2, that the reader is advised to consult to follow the analyses presented in the following chapters. Fundamentals of shear-triggered transition to turbulence through Kelvin-Helmholtz instabilities are also presented along with linear theory analysis of the instability, which is used to inform on the initial condition implementation in Chapter 3. A summary of how turbulence is usually generated in computational studies is also provided to clarify the research gap investigated in this thesis. Highlighting the challenges and gaps in accurately extending conventional turbulence and combustion modelling approaches for developing flows is a common theme brought up throughout the different sections, which sets the stage for a key outcome of this work: to track and characterize turbulence development from fundamental shear instabilities and relate the asymptotic mixing parameters to the seeding instabilities.

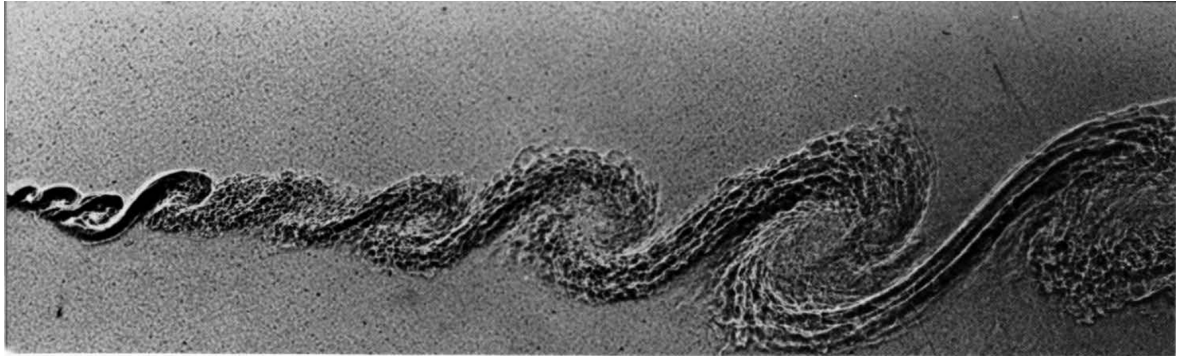
2.2 Turbulent Flows

Turbulence induces an array of mechanisms that significantly enhance mixing. The mixing process in incompressible flows can be divided into 3 stages: entrainment, dispersion, and diffusion [39]. An intrinsic complexity in turbulent flows is that these three stages occur

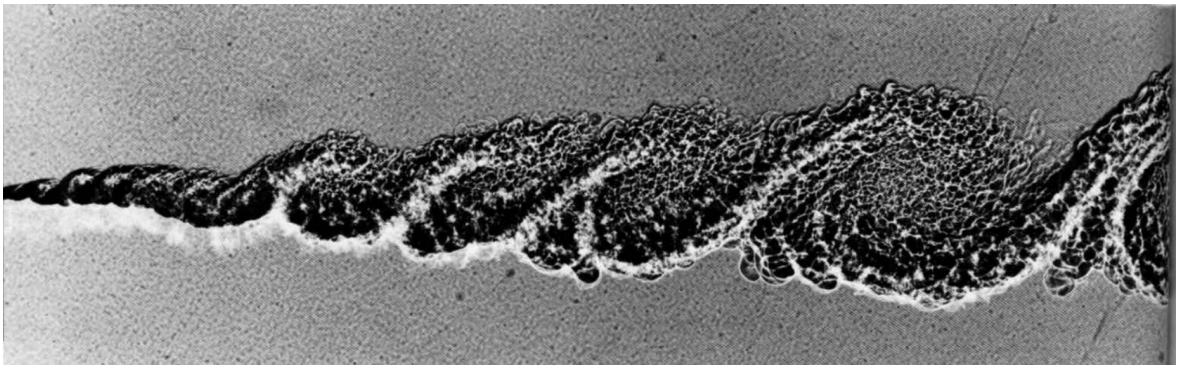
concurrently across a wide range of spatial and temporal scales. This aggravates the challenge of numerically solving the underlying non-linear flow governing equations as it exerts tremendous pressure on the computational requirements to fully resolve and visualise the required scales. Dimotakis [3] categorized turbulent mixing into three main groups in order of increasing complexity: passive scalar mixing (Level 1), mixing that's coupled to dynamics (Level 2), mixing that produces changes in the fluid (Level 3). Relative to levels 1 and 2, very limited studies have focused on level 3 flows. Since this study considers developing reacting flows, the highest level of complexity of turbulent mixing, as per Dimotakis's convention, is of relevance.

Most turbulent studies have focused on high Reynolds number applications where the turbulence is fully developed [3]. These self-similar flow conditions are relevant to many practical applications and are predominant in natural flows. But what exactly is turbulence? And how is it characterized? As briefly discussed in Chapter 1, in most practical applications, the predominant approach engineers and scientists take to classify flow regimes is binary and dependent on a single non-dimensional parameter: the Reynolds number. Threshold values have been empirically determined and collated for well-defined Reynolds numbers at different flow configurations and are used to delineate between laminar and turbulent flow regimes. This distinction, although quite powerful and practically useful, is simplistic. Flows that behave orderly, with parallel non-interacting fluid parcels that flow smoothly in a layered arrangement, can usually have their flow parameters analytically defined and are, as a result, highly predictable. These flows are called laminar and exhibit poor mixing characteristics. All other flows with some chaotic behaviour are usually lumped up as turbulent.

The problem is that beyond laminar flows, there are varying degrees of this chaotic behaviour, and although this may not significantly matter from an applied fluid mechanics perspective, like for pipe flows, aerodynamics, or open channel flows, it carries significant ramifications for mixing flow applications. Differing degrees of turbulence induce differing mixing rates. To illustrate this, consider the shear flow visualisations of a mixing layer experiment as outlined in Figure 2.1. In (A), Nitrogen flows on top with a velocity of 10 m/s, while a helium-argon mixture is set to flow at the bottom in the same direction but at 3.8 m/s. The



(A)



(B)

FIGURE 2.1. Spark shadow photography of a turbulent mixing layer experiment between two co-flows with a velocity gradient across [40]. Nitrogen is at the top, and a helium-argon mixture is at the bottom. Both (B) and (A) have the same flow configurations and gaseous composition, but the Reynolds number is doubled for (B) by doubling the pressure.

velocity difference between the coflows induces shear forces against the interface between the two gaseous streams that produce rotational effects and perturbs it. This shear instability leads to turbulence and is called Kelvin-Helmholtz Instability (KHI). This instability is focused on in this thesis and is explained in more detail in the following sections.

In the reference text [40], both flows are referred to as turbulent, although they exhibit drastic differences in the scales of their motion and the ensuing mixing behaviour. The lower figure in (B) has twice the Reynolds number of (A) and, as a result, attains a much higher level of turbulence. As the figures show, this leads to a more chaotic flow in (B), characterized by a larger degree of small-scale motions and eddy structures superimposed onto the larger eddies that also appear in (A). This leads to enhanced mixing in (B). The lack of explicit distinction

between the levels of flow turbulence is particularly problematic from a modelling perspective for a turbulent flow mixing problem, as when all varying degrees of turbulence are lumped together in the same flow regime, it can imply the universality of model closure constants, which is misleading and inaccurate [32].

Therefore, a more rigorous depiction of fully developed turbulence has been developed and refined over the years. The most significant development of this definition was Kolmogorov's hypotheses for fully turbulent flows. Graphically, the universal characteristics of fully developed turbulence and its energy cascade are commonly represented in a spectral schematic as shown in Figure 2.2, but theoretically, these are summarized below:

- (1) All small-scale turbulent motions are statistically isotropic, and this is problem-independent. So, the motions are isotropic for any fully turbulent flow if you are sufficiently away from the boundaries or any flow discontinuities.
- (2) The motions of scales smaller than the energy-containing ranges, or more precisely smaller than the integral length scales, can be universally characterised by turbulent kinetic energy dissipation, ε , and kinematic viscosity, ν . This hypothesis is commonly referred to as the first similarity hypothesis and spans both the inertial and dissipation subranges.
- (3) An inertial subrange exists at an intermediate range of scales, larger than the dissipation range where the motions are overwhelmed by viscous dissipation forces but smaller than the energy-containing range. Within this range, the functional dependence from the first hypothesis reduces to only ε . The upper and lower limits to this range can sometimes be approximated as the integral and Taylor length scales, respectively, as will be discussed later in this chapter and with the simulation results in the following chapters. This is commonly referred to as the second similarity hypothesis.
- (4) The inertial subrange maintains a universal energy spectrum function that follows a power law with a $-\frac{5}{3}$ slope in wavenumber space. This is not explicitly a similarity hypothesis but is emphasized here since it is a widely held depiction of full turbulence behaviour.

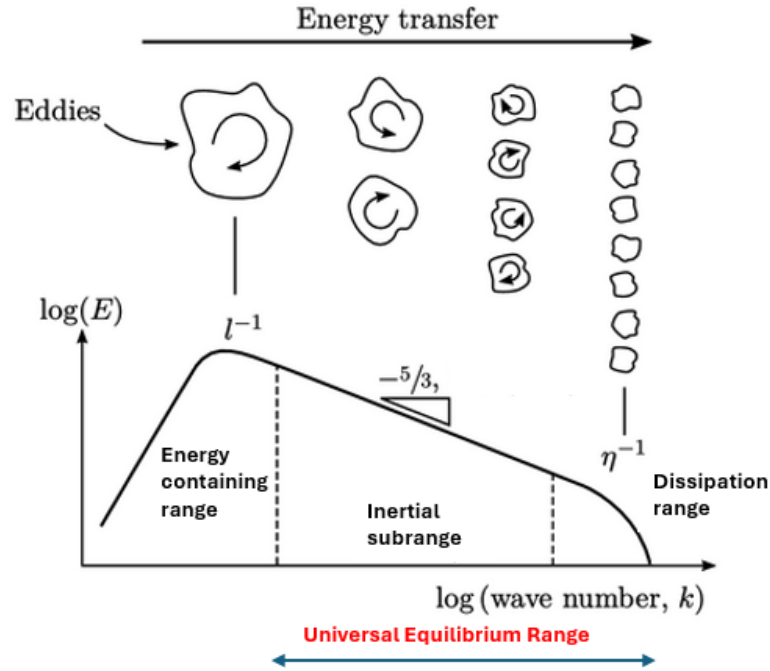


FIGURE 2.2. The energy cascade and scales of fully developed turbulence on a spectral diagram, adapted from [41]

It is important to re-iterate that these hypotheses mostly hold at the equilibrium state of fully developed turbulence, which exists at very high Reynolds numbers. A direct consequence of these hypotheses is the well-known energy cascade phenomenon of turbulent eddies and the widely held concept of scale separation. In this context, ε can be thought of as the rate of energy transfer from the energy-containing scales to the inertial subrange. The inertial and dissipation subranges are parts of the equilibrium range as highlighted in Figure 2.2, owing to their universal behaviour in fully established turbulence, regardless of the problem or flow configuration. It is within this universal equilibrium range where the local isotropy hypothesis is realised. The term separation of scales refers to this behaviour: within the equilibrium range, the inertial subrange is strictly dependent on ε , whereas the dissipation range is on ν , which distinctively separates the two scale ranges.

It is important to appreciate that applying the above hypotheses for fully turbulent flows is statistical and not absolute. In other words, the characteristics of fully established turbulence are mostly useful in defining the statistics of the flow parameters and not their absolute values,

as turbulent flows remain chaotic and random in nature. The Reynolds number is used to assess whether flows attain this universal statistical behaviour. The original formulation of the above hypotheses stipulated the requirement of an adequately high Reynolds number while keeping the explicit values ambiguous.

Research work over the last number of decades has attempted to consolidate explicit thresholds for the Reynolds number needed for fully developed turbulence. Dimotakis's work [3], [9] is the most notable, where he consolidated a large number of experimental and numerical studies of developing flows and reported a transitional outer-scale Reynolds number with an order of magnitude of 10^4 . Beyond this Reynolds number, the flow behaviour is qualitatively different as it conforms to an asymptotic mixing state. The terminology "outer scale", sometimes also called visual thickness scale, was used since it refers to the scale of the largest eddies, which varies between different flow configurations and is easily measured and recognized. For instance, in a jet flow, the transverse width of the jet can be regarded as the outer-scale, and in free shear flows, as studied in this work, it can be a measure of the mixing layer width [9]. However, the outer-scale definition can be difficult to apply to a universal definition as it can be difficult to define in some flow configurations. Instead, defining the transitional Reynolds number in terms of the Taylor microscale is also common. The Taylor microscale is related to the autocorrelation function and is more rigorously defined in later sections. For now, it can be considered the smallest eddy scale related to the outer-scale dynamics and in the vicinity of the lower end of the length scales where the second similarity hypothesis applies and viscous effects do not yet overwhelm inertial effects (inertial subrange). It is not, however, representative of the smallest eddies as this is the Kolmogorov scale that will be defined further on. Based on the Taylor scale, the threshold Taylor Reynolds number, Re_λ , is defined by Dimotakis to be of order 10^2 (between 100-140) [9].

However, in literature, it hasn't always been the case that these threshold values consistently well-predicted developed turbulence. For instance, in their study of shock-induced mixing via Richtmyer-Meshkov Instability (RMI), Tritschler et al. [42] characterized fully developed turbulence with Taylor Reynolds number of less than 80. Zhou et al. [13], [43] later contested this, explaining that the 10^4 outer-scale Reynolds threshold only applies to stationary flows,

whereas for time-varying flows, the introduction of an additional diffusive scale in the inertial range may amplify this threshold Reynolds number by an order magnitude, i.e. up to 10^5 . Regarding scalar mixing, similar conflicting evidence is presented in the literature when characterizing fully developed turbulence even in inert flows [44]. For instance, in terms of characterizing probability density function (PDF) behaviour of passive scalar mixing, both experimental and numerical investigations spanning outer-scale Reynolds numbers between $2.3 \times 10^4 - 2 \times 10^5$, presented conflicting results [11], [45]–[51].

The discrepancy between these study results demonstrates that in addition to the Reynolds number, other factors must play a role in attaining a fully developed turbulence state. A potential factor that appears to influence the development of turbulence is the nature of the seeding perturbation, as multiple studies demonstrated flow sensitivities to initial perturbations at high Reynolds numbers [11], [52]–[55]. Another one is the flow domain dimensions relative to the seeding perturbation which can impede turbulence development and preserve two-dimensional coherent structures [31], [51], [56]. This thesis, therefore, aims to methodically investigate the influence of the initial perturbation on turbulence and mixing development, particularly the dimensions and amplitudes of the initial perturbation relative to the domain size quantified through the wavenumbers and convective velocity magnitudes, respectively, as explained in further sections. But firstly, it is important to demonstrate the statistical attributes of turbulence and the relevant scales of fluid motion that need to be considered.

2.2.1 Statistical Quantities and Definitions

2.2.1.1 General Definitions

Turbulence is a random phenomenon such that instantaneous flow field values are almost entirely unpredictable; the statistics of established turbulence, however, can be, under certain conditions, tractable, i.e. it is possible to establish the likelihood of a turbulent flow field taking certain values. When analyzing turbulent flows, it is common to make simplifications based on how the statistics behave. Stationary flows are ones where the statistics stay constant with time. It is also very common to find the term homogeneous turbulence in literature. A

statistically homogeneous flow is one where the statistics are invariant under a shift in position as long as that shift is along the same spatial direction (i.e. a translation). Homogeneous turbulence specifically refers to the homogeneity of the velocity fluctuations' statistics in each respective direction. When this statistical invariance extends to rotations and reflections in physical space, the turbulence is referred to as isotropic, i.e. the turbulence statistics are uniform in every spatial direction, and any N-point PDF that depicts the turbulence statistics is only dependent on a single spatial coordinate (and time if the flow isn't stationary). To link back to the previous section, it is this isotropy that Kolmogorov hypothesised at the local scale in fully developed turbulence, i.e. even if the bulk flow is not isotropic, at the local level, below an adequately small scale, the turbulent statistics are always isotropic for all fully established turbulent flows.

There is also the term self-similarity, which is commonly used to refer to the statistics of turbulent flows and sometimes in conjunction with statically stationary or homogeneous descriptions of the flows. This can sometimes cause confusion about what self-similarity exactly implies, so it is important to highlight the distinction. Self-similarity is when a statistic of a flow variable under appropriate normalisation becomes strictly a function of non-dimensional parameters and loses some of its variable dependencies, even if it is over a limited range of these variable values. For instance, returning to the hypotheses of fully developed turbulence, the fluid behaves self-similarly under a spectral lens at high enough Reynolds numbers (the limited range of variable values) as demonstrated later with the energy spectrum in Figure 2.4. In fully developed turbulence, the Reynolds number dependence is lost, and under appropriate normalisation of the wavenumber and the energy spectrum (defined in the following section), a collapse is observed regardless of the original flow configuration or experimental setup. This collapse has been observed to conform to Kolmogorov's hypotheses. Checking for self-similarity is a powerful analytical approach that is commonly used in fluid mechanics and has significant practical benefits for engineers and in setting up standards and codes. The choice of normalisation is usually based on both empirical evidence and dimensional analyses.

To analyze turbulent flows, a suite of statistical tools and quantities must be appropriately defined to allow for deriving meaningful insights into the flow state [2]. The most fundamental of these are the first and second-order moments, i.e. the mean and variance. Let u_i be a component of the random turbulent velocity field and $f(V)$ the probability density function (PDF) value of u taking a value of V , then the mean is given by:

$$\overline{u_i} = \int_{-\infty}^{\infty} V f(V) dV \quad (2.1)$$

and the variance given by:

$$\overline{u_i'^2} = \int_{-\infty}^{\infty} (V - \overline{u_i})^2 f(V) dV \quad (2.2)$$

Here u_i' denotes the Reynolds fluctuation such that $u_i' = u_i - \overline{u_i}$. In this thesis, $\overline{(\cdot)}$ hereafter denotes Reynolds averaged quantities where the averages are computed in the homogeneous plane (in the context of this thesis, these are along the y and z directions as per the domain setup in Chapter 3). Computing Favre averaged quantities in combustion studies where flow composition and densities vary is particularly pertinent. For an arbitrary field, Ψ , the symbol $\widetilde{(\cdot)}$ denotes a Favre average such that the Favre average and fluctuation in the homogeneous plane are calculated by $\widetilde{\Psi} = \frac{\overline{\rho\Psi}}{\overline{\rho}}$ and $\Psi'' = \Psi - \widetilde{\Psi}$. Higher order moments can also be obtained by adapting Equation 2.2 and raising the fluctuation to a higher power than 2. The moment calculations are all linear, so the moments of the functions of random variables can be similarly defined.

When working with turbulence, it is rare when the analysis is strictly concerned with a single flow variable. More commonly, joint statistics are of interest as they help characterize interactions and valuable flow physics. For instance, if the evolution of turbulent structures is of interest, then joint statistics between different spatial points in the domain are needed. The joint PDF of two velocity field components, u_1 and u_2 , taking up values of V_1 and V_2 respectively, is denoted by $f_{12}(V_1, V_2)$. The joint cumulative density function (CDF) is then defined by:

$$\mathbb{P}(V_{A1} \leq u_1 \leq V_{B1}, V_{A2} \leq u_2 \leq V_{B2}) = \int_{V_{A1}}^{V_{B1}} \int_{V_{A2}}^{V_{B2}} f_{12}(V_1, V_2) dV_2 dV_1 \quad (2.3)$$

When analyzing both combustion and turbulence, in many situations, it is desirable to look at the joint PDFs of vector or scalar fields conditioned on a field taking certain values. An example could be when analyzing the flame quality or ignition modes by looking at flame-marking radicals conditioned on mixture fraction values. Taking the same random turbulent velocity field components introduced earlier (u_1 and u_2), the PDF of u_2 taking a value of V_2 conditional on $u_1 = V_1$ is:

$$f_{2|1}(V_2|V_1) = \frac{f_{12}(V_1, V_2)}{f_1(V_1)} \quad (2.4)$$

Mixed second moments can also be considered from the definition of the joint PDFs. An important one is the covariance, defined by:

$$\overline{u'_1 u'_2} = \int_{-\infty}^{\infty} (V_1 - \overline{u_1})(V_2 - \overline{u_2}) f_{12}(V_1, V_2) dV_2 dV_1 \quad (2.5)$$

The covariance is extensively used to define important turbulence statistics, such as in Reynolds stresses. It is an invaluable statistical tool to help highlight correlations between flow variables. Appropriate normalization of the covariance defines a correlation coefficient, which can be an auto-correlation if the variable is correlated with itself, albeit at a temporal or spatial offset. For the same flow variables defined earlier, a generic correlation coefficient can be defined by:

$$\rho_{ij} = \frac{\overline{u'_i u'_j}}{\sqrt{(\overline{u'^2_i})(\overline{u'^2_j})}} \quad (2.6)$$

Similarly, if the two variables in the covariance calculation are taken at two different spatial locations, then the covariance is called a two-point correlation as it compares the variables at two separate spatial points. As will be seen in the next section, the two-point correlation is quite fundamental to turbulence analysis and modelling as it is the simplest statistic to convey information on spatial structures and can be used to relate the turbulence physical and empirical hypotheses to the numerical governing equations as was done by Taylor [57] and then von Karman and Howarth [58].

Since the realization of flow parameters at different temporal or spatial increments is not characterized by the same instantaneous and local PDF, the auto-correlation can be quite a useful tool to help estimate and supplement PDF behaviour. Local isotropy is an important

characterization of established turbulence, besides the independence from further Reynolds number increases. With the turbulent flow fields varying randomly in space and time, at any one instant, small spatial increments will span correlated turbulent structures, but as the separation in space between the reference points increases, the auto-correlation should tend to zero.

The statistical frameworks presented in this section are pivotal to analysing and studying turbulence and its development. However, it is important to remember that due to the random nature of turbulence, its statistics aren't necessarily fully characterized by n-point one-time PDFs and covariances. Technically, the joint PDF of all points in space and time is needed to characterize a random field, which isn't practically feasible. Only in the limiting case when the random variable is Gaussian is it fully characterized by one-time PDF and covariances without this extensive joint PDF requirement [2]. Although turbulence generally isn't Gaussian, some of its statistics may approach Gaussian or joint-normal behaviour in certain flow conditions. This simplification has supported the development of some turbulent mixing models [59] but is not a widely held premise. For stationary flows, where the turbulence statistics are constant with time, the statistical characterization of turbulence becomes less onerous. The main purpose of the statistical representation of turbulence here is to connect the physics observed with turbulent flows, like the Kolmogorov hypotheses, for instance, to the Navier-Stokes or other underlying governing equations.

2.2.1.2 Notation Convention

This thesis leverages a range of statistical analyses in its results chapters, and to help guide the reader through these, this section provides the convention used to denote different statistical quantities, which is consistently maintained throughout the thesis. The reader is, therefore, advised to return to this section when in doubt to follow any presented analyses.

Firstly, the analyses and discussions presented in this thesis are three-dimensional, and to help orient the reader and provide clarity on the convention used, Figure 2.3 summarizes the terms and subscripts used throughout this thesis to refer to the different directions in the computational configuration considered.

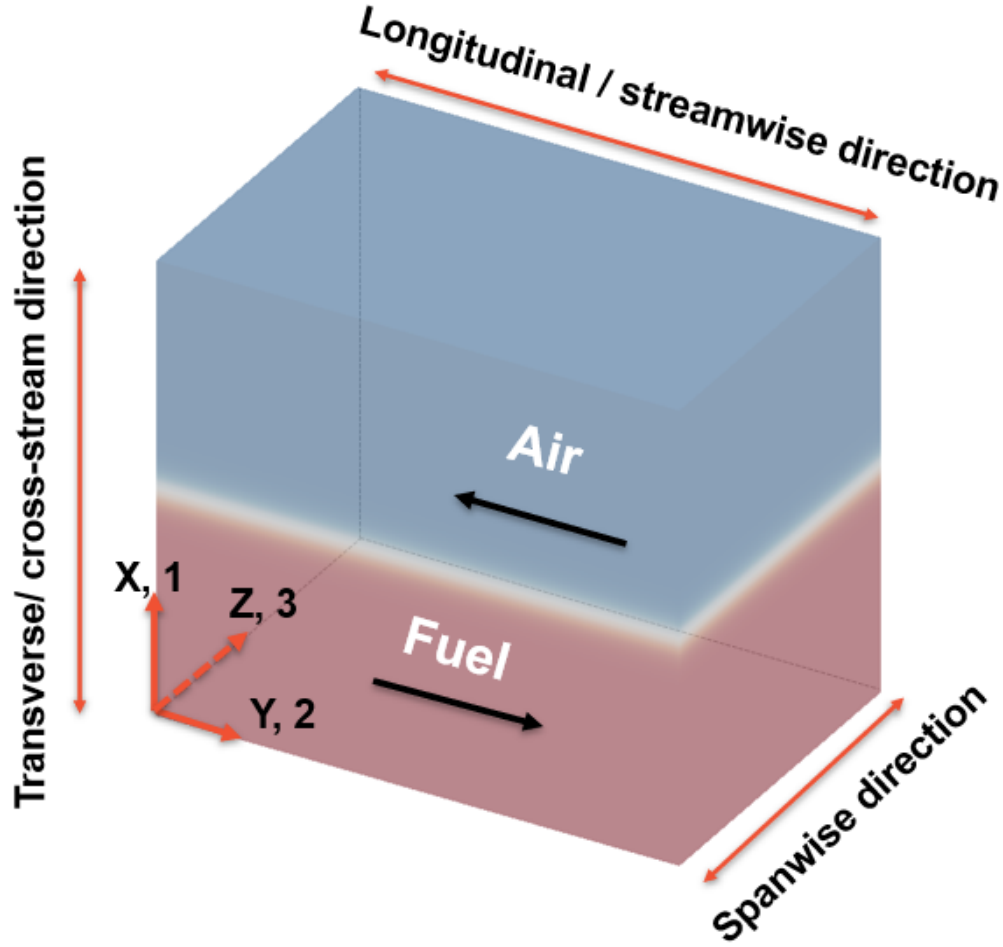


FIGURE 2.3. The domain configuration and the orientation conventions used to refer to different directions in this thesis. The notations around the coordinate axes denote the directional subscripts used to denote the different component directions.

Planar averages are computed along the homogeneous directions for every point in time, which, as described in Chapter 3, are the y and z directions throughout this thesis. These statistics can either be directly computed without any weightings, in which case they correspond to Reynolds averages denoted by $\overline{(\cdot)}$, or they can be density-weighted and correspond to Favre averages denoted by $\widetilde{(\cdot)}$. These were defined earlier in this section. Here, ψ is still used to denote an arbitrary field. Note that this is only in this section; in other sections/chapters, ψ can denote specific field variables as explained in the accompanying text. Planar Reynolds variances can then be computed from either Reynolds or Favre fluctuations. From Reynolds fluctuations, planar Reynolds variances are denoted by $\overline{\psi'^2}$. From Favre fluctuations, these are

denoted by $\overline{\psi'^2}$. Sometimes in literature, the latter are referred to as Favre variances, but here, Favre variances include density weighting when averaging the square of the Favre fluctuations and are denoted by $\widetilde{\psi'^2}$.

To obtain representative statistics for the entire mixing layer, it can be useful to further average these planar averages across the span of the mixing layer (along the cross-stream direction) for every point in time. These averages are computed directly and without any further density weighting (i.e. similar to Reynolds earlier) and are denoted by $\langle \psi \rangle_{\delta_\phi}$, where δ_ϕ is an arbitrary measure used to define the time-dependent mixing layer width.

Instead of computing planar averages, sometimes it is more insightful to condition the averaging on specific variables. These are also calculated for every instant in time (i.e. time-dependent). The following notation is used to describe the generalised expressions for the Favre averaged conditional mean of an arbitrary variable, ψ , conditioned on an arbitrary parameter space, Ξ , taking a specific value Ξ^* . Since these are numerically computed in the results chapters, they are presented here in the discretized version:

$$\langle \psi \mid \Xi = \Xi^* \rangle = \frac{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} (\rho(x_i, y_j, z_k) \psi(x_i, y_j, z_k) \mid \Xi = \Xi^*)}{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} (\rho(x_i, y_j, z_k) \mid \Xi = \Xi^*)} \quad (2.7)$$

The variance, σ^2 , of these conditional statistics is then given by:

$$\langle \sigma_\psi^2 \mid \Xi = \Xi^* \rangle = \frac{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} (\rho(x_i, y_j, z_k) (\psi(x_i, y_j, z_k) - \langle \psi \mid \Xi = \Xi^* \rangle)^2 \mid \Xi = \Xi^*)}{\sum_{i=1}^{N_x} \sum_{j=1}^{N_y} \sum_{k=1}^{N_z} (\rho(x_i, y_j, z_k) \mid \Xi = \Xi^*)} \quad (2.8)$$

While joint PDFs are the ultimate statistical tools to highlight correlations and patterns between different field variables, sometimes computing them is nonfeasible owing to computational or storage limitations. In these cases, observing trends in weighted PDFs can be advantageous, providing some valuable insights at the integral level, for instance, as was used in [60], [61]. The weighting is done by the conditional means that were shown in Equation 2.7. Therefore, while considering the density weighting of the Favre averaged conditional means, the general

equation of the weighted PDFs is given by:

$$P_\phi(\Xi) = \frac{\langle \rho\phi \mid \Xi \rangle P(\Xi)}{\overline{\rho\phi}} \quad (2.9)$$

An intuitive appreciation of this definition would reveal that this formulation measures the fraction of quantity ϕ instilled within the bounds of a Ξ bin.

Instead of weighting the PDFs by conditional means, they can also be weighted by the conditional variance. These are formulated as:

$$P_{\phi'^2}(\Xi) = \frac{\langle \rho\sigma_\phi^2 \mid \Xi \rangle P(\Xi)}{\overline{\rho\sigma_\phi^2}} \quad (2.10)$$

These weighted PDFs are extensively utilised in the combustion analysis presented in Chapter 6 as they can help concentrate the statistics towards interesting elements of the analysis.

2.2.2 The Energy Spectrum

To connect the statistical turbulence characterizations and Kolmogorov hypothesis to the Navier-Stokes equation, it is common to resort to the statistics of the two-point correlation. This is formally the covariance of velocity fluctuation components at two separate points in space, usually at the same point in time. Hence:

$$A_{ij}(r_1, r_2, r_3, t) = \overline{u'_i(x, y, z, t) u'_j(x + r_1, y + r_2, z + r_3, t)} \quad (2.11)$$

At zero spatial offsets (i.e. $\mathbf{r} = 0$), the two-point correlation reduces to the Reynolds stresses $\overline{u'_i u'_j}$, which constitutes a second-order tensor with normal and deviatoric components. Here, the Reynolds stress tensor is Reynolds averaged, but it is also possible to compute and analyze Favre averaged (or density-weighted) Reynolds stress tensor, as shown in Chapter 4. For all turbulent flows, the two-point correlation is the simplest statistic to provide some appreciation of the underlying flow structures and, hence, some (although limited) quantitative measure of large-scale characteristics of the flow turbulence. Therefore, it is no surprise that significant advances in understanding the physics of turbulence were achieved through studying two-point correlations as they provide a relatively simple means of connecting Kolmogorov

hypotheses and turbulence theory to the Navier-Stokes equations. The development of the Karman-Howarth equation, extensively utilized in turbulence studies, was motivated by a desire to fully elucidate the dynamics of the two-point correlation.

Further insights can be derived from the two-point correlation by observing it in spectral space. The three-dimensional velocity spectrum tensor φ_{ij} is defined to be the Fourier transform of the two-point correlation such that:

$$\varphi_{ij}(\omega_x, \omega_y, \omega_z, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-i(\omega_x r_1 + \omega_y r_2 + \omega_z r_3)} A_{ij}(r_1, r_2, r_3, t) dr_1 dr_2 dr_3 \quad (2.12)$$

and since they form a Fourier transform pair, then:

$$A_{ij}(r_1, r_2, r_3, t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i(\omega_x r_1 + \omega_y r_2 + \omega_z r_3)} \varphi_{ij}(\omega_x, \omega_y, \omega_z, t) d\omega_x d\omega_y d\omega_z \quad (2.13)$$

In the above equations, if discrete Fourier transforms were applied, then the $(\frac{1}{2\pi})^3$ factor is superseded with $\frac{1}{N_x \times N_y \times N_z}$. The $\omega_x, \omega_y, \omega_z$ refer to the wavenumbers in the x,y, and z directions respectively e.g $\omega_x = \frac{2\pi}{x}$.

The total aggregate of the three-dimensional contributions from the range of modes in the isotropic components of the velocity spectrum tensor, defined over the three-dimensional radial wave number ($\kappa = \sqrt{\omega_x^2 + \omega_y^2 + \omega_z^2}$), gives the three-dimensional energy spectrum:

$$E(\kappa, t) = \frac{1}{2} \int_{-\infty}^{\infty} \varphi_{ii}(\boldsymbol{\omega}, t) \delta(|\boldsymbol{\omega}| - \kappa) d\boldsymbol{\omega} \quad (2.14)$$

where bold symbols were used to denote vector fields for more compact expressions.

However, computing $\varphi_{ii}(\boldsymbol{\omega}, t)$ this way is inefficient and computationally expensive. It is more convenient to realise that the two-point correlation is a covariance, which is an integral itself from Equation 2.5. Thus, the convolution theorem (also called Weiner-Kinchin Theorem) can be invoked on Equation 2.12 such that the trace of the velocity spectrum tensor may be alternatively defined by:

$$\varphi_{ii}(\boldsymbol{\omega}, t) = |\mathcal{F}\{u'_i(\mathbf{x}, t)\}|^2 = \widehat{u'_i}(\boldsymbol{\omega}, t) \widehat{u'_i}^*(\boldsymbol{\omega}, t) \quad (2.15)$$

Here the $\mathcal{F}$ operator denotes a three-dimensional Fourier transform, the $\widehat{(\cdot)}$ symbol denotes the Fourier transform of a vector field, and $\widehat{(\cdot)}^*$ denotes the conjugate of the Fourier transformed vector field. This definition of the energy spectrum is such that the sum of all modal contributions (i.e. incremental vicinity about individual wavenumber modes: $\kappa - 0.5\Delta\kappa < \kappa < \kappa + 0.5\Delta\kappa$) across all radial wave numbers leads back to the mean turbulent kinetic energy ($\mathcal{K}$) (from Equation 2.13:

$$\mathcal{K} = \frac{1}{2}\overline{u'_i u'_i} = \frac{1}{2}A_{ii}(0, 0, 0, t) = \int_0^\infty E(\kappa, t)d\kappa = \frac{1}{2}\int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty \varphi_{ii}(\boldsymbol{\omega}, t)d\boldsymbol{\omega} \quad (2.16)$$

Note how the mean turbulent kinetic energy $\mathcal{K} = \frac{1}{2}\overline{u'_i u'_i}$ is the trace of the Reynolds stress tensor whose components can be defined by $A_{ii}(0, 0, 0, t)$ in Equation 2.11.

The energy spectrum is used to provide a scalar measure of the energy distribution across the various scales of turbulence but lacks any directional information due to the nature of the integration in Equation 2.14. It measures the proportion of kinetic energy contained within incremental bounds about a wavenumber of magnitude κ , i.e. $|\boldsymbol{\omega}| = \kappa$. Observing the energy spectrum for fully developed turbulent flows confirms the energy cascade and Kolmogorov hypothesis. This is only true at sufficiently high Reynolds numbers when there is adequate separation of scales and a clearly defined inertial sub-range. Figure 2.4 shows the normalised longitudinal energy spectrum from several studies at various Reynolds numbers, highlighting the self-similar nature of fully developed turbulence in the equilibrium range of scales. While the formulation above has been presented for a three-dimensional energy spectrum, the longitudinal energy spectrum, E_{22} , can be similarly calculated by considering the integration over the longitudinal wavenumber. Similarly can the transverse energy spectra (E_{11} or E_{33}) be calculated. In experimental investigations, it is common to see this one-dimensional spectrum of stream-wise (longitudinal) components as it is conveniently measured using a hot-wire anemometer.

In certain case setups, presenting one or two-dimensional energy spectra is desirable. For instance, when analyzing free shear flows or turbulent jets, the flow is statistically one-dimensional [2], [63]. It is, therefore, sensible to compute the two-dimensional energy spectrum in the homogeneous plane at key locations, for instance, at the centre of the mixing

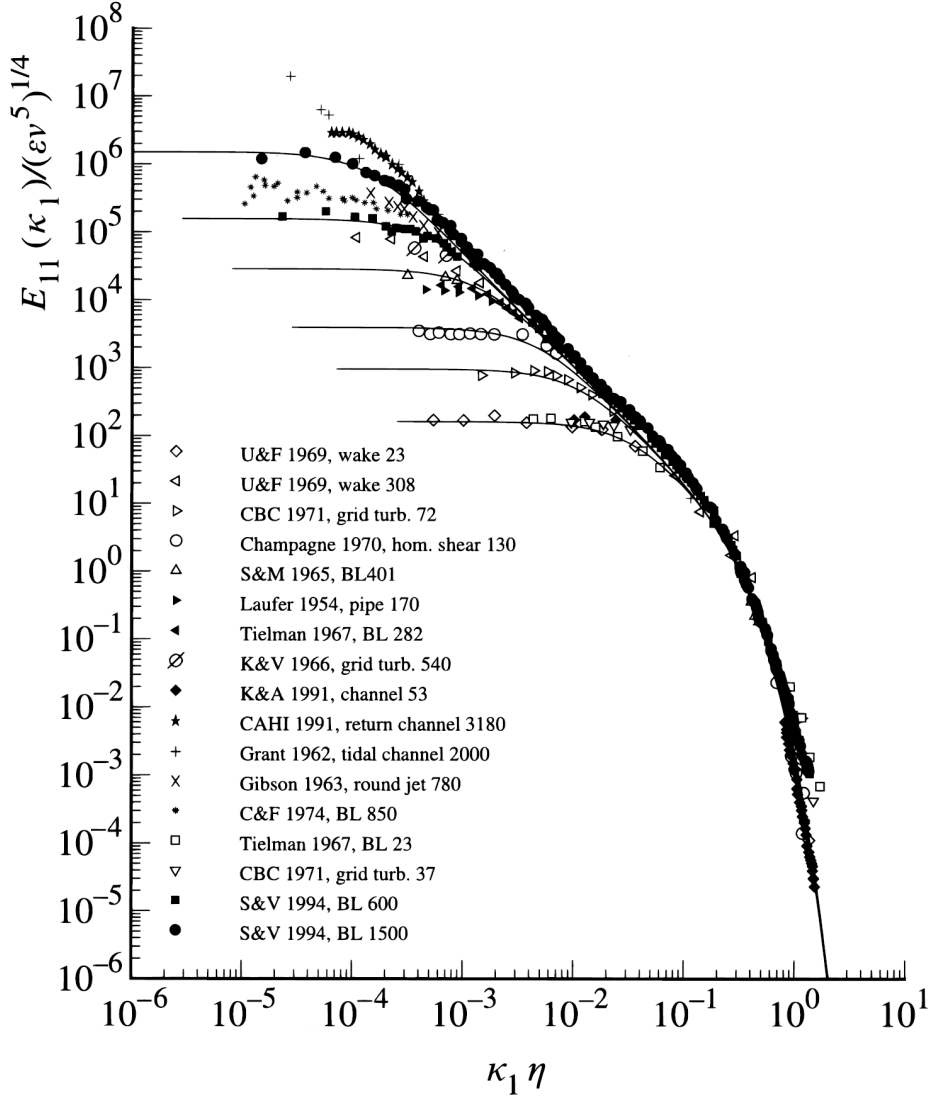


FIGURE 2.4. Experimentally determined scaled one-dimensional energy spectrum at varying Reynolds numbers reproduced from [2] that adapted the figure from the experiments and reporting in [62]. The number at the end of each entry corresponds to the Taylor-based Reynolds number, Re_λ (defined in 2.2.3). The inertial sub-range becomes increasingly better defined with a more obvious separation of scales as the Reynolds number is increased. The scaled spectra exhibit a universal $-5/3$ power law with the longitudinal wavenumber

layer. Moreover, for shear-dominated flows (prevalent KHIs), as demonstrated later in Section 2.3.2, the seeding amplitude fluctuation of the instability spans and varies within this homogeneous plane. Therefore, analyzing the two-dimensional energy spectrum in such

a configuration is more advantageous, as is extensively done in Chapter 4. Here, the two-dimensional energy spectrum is also computed as per the definition in Equations 2.15, 2.14 but with only the streamwise (y) and spanwise (z) homogeneous directions considered (domain convention used in this study is presented in Chapter 3). Therefore, the two-dimensional energy spectrum is defined on a two-dimensional radial wavenumber, $\underline{k}$, space as consistent with Section 2.3.2 and the initial perturbation derivations in 3.4.

The $-\frac{5}{3}$ slope of the inertial subrange and the universality of the spectrum for all the experimental results in Figure 2.4 are both a direct consequence of the Kolmogorov hypothesis outlined at the start of this Chapter, as can be verified through dimensional analyses [2]. The higher the Reynolds number of the experiments, the more extensive, across wavenumber space, this universal behaviour is. The $-\frac{5}{3}$ slope in the inertial range, based on the Kolmogorov hypotheses, should apply to all fully developed turbulent flows in the total energy spectrum function (Equation 2.14) and also in omnidirectional components (longitudinal and transverse). Furthermore, using these hypotheses on isotropic turbulence can show that within the inertial range, the magnitude of the transverse energy spectrum (E_{22} or E_{33}) is $\frac{4}{3}$ times the magnitude of the longitudinal energy spectrum, E_{11} . However, if the Reynolds number is sufficiently high and turbulence is fully developed, this can extend to anisotropic turbulence if the entirety of the inertial range is itself isotropic, provided the local isotropy hypothesis applies. This was observed experimentally in anisotropic boundary layer experiments at a Taylor Reynolds number exceeding 1000 [62].

An important attribute of the first and second similarity hypotheses is the dependence of the inertial range on the net rate of energy transfer from energy-containing scales, which is captured by the kinetic energy dissipation rate, ε . This appears as a separate term in the conservation equation of mean turbulent kinetic energy and can be formulated as follows:

$$\varepsilon = \overline{\frac{1}{\rho} \tau'_{ij} \frac{\partial u'_i}{\partial x_j}} = 2\nu \overline{\left(s'_{ij} s'_{ij} - \frac{1}{3} \theta'^2 \right)} \quad (2.17)$$

Here s'_{ij} is the fluctuating rate-of-strain tensor ($s'_{ij} = \frac{1}{2}(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i})$), and θ is the divergence of the velocity fluctuation vector field i.e. $\theta' = \frac{\partial u'_k}{\partial x_k}$. In incompressible formulation, θ goes to zero but is retained here as the compressible form of the Navier Stokes equation is solved

(Chapter 3). τ'_{ij} is the fluctuating viscous stress tensor, which is assumed Newtonian as shown in the governing equations solved in the following Chapter. Note that this formulation also assumes zero bulk viscosity (Stoke's hypothesis) as common with shear flow formulations [14], [37]. ρ and ν are the density and kinematic viscosity, respectively. Here, both the turbulent kinetic energy and its dissipation have been formulated using Reynolds fluctuations and averaging, but corresponding formulations can be derived using Favre fluctuations as used, for example, in Chapter 4.

The dissipation as defined in Equation 3.15 takes on units of J/(kg s) and directly measures the rate of turbulent kinetic energy dissipating into heat due to viscous effects. This dissipation can be related back to the velocity spectrum tensor while taking advantage of simpler spatial differentiation in wavenumber space:

$$\varepsilon = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} 2\nu\kappa^2 \varphi_{ij}(\boldsymbol{\omega}) d\boldsymbol{\omega} + \int_0^{\infty} \frac{4}{3} \nu \kappa^2 E(\kappa) d\kappa \quad (2.18)$$

For isotropic turbulence, this can be expressed strictly in terms of the energy spectrum function:

$$\varepsilon = \int_0^{\infty} 2\nu\kappa^2 E(\kappa) d\kappa \quad (2.19)$$

The above equations can be used to define the dissipation spectrum, and a comparison of the energy and dissipation spectra can help draw insights into the extent of scale separation and, hence, the extent of turbulence development and application of Kolmogorov hypotheses (i.e. energy cascade). Through invoking these hypotheses and applying dimensional and asymptotic analyses of developed turbulence spectral statistics, Pope [2] derived a model energy spectrum to represent fully developed turbulence and, through that, demonstrated the dependence of the overlap between the dissipation and energy spectra on Reynolds number. It was shown that to maintain less than 10% overlap and hence a high extent of separation of scales, Taylor-based Reynolds number of order 10^3 are required, once more an order of magnitude larger than Dimotakis's[9] estimate but consistent with Zhou's prediction [13].

Lastly, it is important to note that some formulations of the energy spectrum can also account for shear effects. As mentioned, normally, one-dimensional longitudinal or transverse spectra are measured in experiments and, therefore, constitute most spectra results in the literature.

However, it is also possible to measure one-dimensional shear spectra and, in numerical studies, remove the one-dimensionality requirement altogether. The $\frac{-5}{3}$ wavenumber power scaling of the universal inertial range in fully developed turbulence holds for the total spectrum function or the one-dimensional longitudinal and transverse components. However, for shear spectra, i.e. ones that consider velocity fluctuation contributions in both the longitudinal and a transverse direction, the spectra have been shown to exhibit more aggressive decay in the equilibrium range, with a wavenumber power scaling of $\frac{-7}{3}$. The shear spectra are particularly prominent in shear flows like the ones considered in this study, where there is a high degree of anisotropy.

2.2.3 Scales

An important element of turbulence is the range of scales it spans since some scales have universal characterization at the fully developed turbulence limit, whereas others hold most of the flow kinetic energy, as hypothesized by the energy cascade, but are flow configuration dependent. This section introduces the various scales of turbulence. Appreciating the different scales and their contribution to turbulent mixing and flow development is an important topic when studying turbulent combustion, as is utilised in Chapter 6.

Starting off with the largest eddies, their length scale, $\mathcal{L}$ can be approximated by the ratio of turbulent kinetic energy and its dissipation:

$$\mathcal{L} = \frac{\mathcal{K}^{\frac{3}{2}}}{\varepsilon} \quad (2.20)$$

Characterizing these largest eddies is important as they hold most of the turbulent energy and so is, therefore, defining a Reynolds number based on the largest eddies:

$$Re_t = \frac{\sqrt{\mathcal{K}} \mathcal{L}}{\nu} = \frac{\mathcal{K}^2}{\varepsilon \nu} \quad (2.21)$$

This turbulence Reynolds number is usually an order of magnitude smaller than the large flow Reynolds number, Re , that is setup dependent (for instance, for a jet, it would take the convective velocity as the velocity scale and the jet width as the length scale, or for a pipe,

it would take the average velocity as the velocity scale and the pipe diameter as the length scale...etc.).

Meanwhile, at the other end of the spectrum, the smallest eddies are of the Kolmogorov scale, where dissipative forces dominate inertial ones:

$$\eta = \left(\frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} \quad (2.22)$$

In isotropic fully developed turbulence, the smallest and the largest eddies can be related by the turbulent Reynolds number:

$$\frac{\eta}{\mathcal{L}} = Re_t^{-\frac{3}{4}} \quad (2.23)$$

This shows how the dependence of the energy spectrum on Reynolds number as the higher its value, the greater the separation of scales, i.e. the smaller η is and the larger $\mathcal{L}$ is.

With the limits of the relevant scales defined, focus is diverted towards the inner scales. Since as discussed in the previous sections, a lot of the progress in turbulence characterization was undertaken through examination of the two-point correlations, similarly the inner scales defined here are derived from this statistic. The first scale is within the energy-containing range but smaller than $\mathcal{L}$. It is obtained by integrating the normalised auto-correlations over any entire domain dimension and is called the integral scale. The integration should converge to a constant that defines the largest span of turbulent spatial scales present in that dimension. Hence, it can be defined for any of the three dimensions of Cartesian coordinate systems. For example, the integral length scale in the streamwise direction is therefore defined as:

$$I_y(t) = \int_0^\infty \frac{\overline{u'_y(x, y, z, t)u'_y(x, y + r, z, t)}}{\overline{u'_i(x, y, z)^2}} dr \quad (2.24)$$

The integral length scale, therefore, measures the average length of correlated turbulent eddies within the energy-containing scales as per Kolmogorov's hypotheses. These scales are defined by the flow configuration and are significantly affected by the turbulence-inducing instabilities and the specific case-underlying mechanics.

It is also possible to relate the energy spectrum back to the integral length scale, taking into account that the auto-correlation is an even function, and from Equations 2.24, 2.12, 2.14:

$$I_i(t) = \frac{\int_0^\infty A_{ii}(\mathbf{r}, t) d\mathbf{r}}{8\overline{u_i'^2}} = \frac{(2\pi)^3 \varphi_{ii}(0, t)}{8\overline{u_i'^2}} = \frac{2E(0, t)\pi^3}{\overline{u_i'^2}} \quad (2.25)$$

It is sometimes useful to assume that the end of the energy-containing scale can be approximated by scales of the order $\approx \frac{1}{6}I$. Given that the integral scale also lies within the energy-containing range, it should be related to the scale of the largest eddies. Pope [2] demonstrates through asymptotic analysis of model spectrum function for developed turbulence that:

$$\frac{I_2}{\mathcal{L}} \approx 0.43 \quad (2.26)$$

and that this ratio stays constant for fully established turbulence to guarantee a constant rate of energy transfer from the largest eddies to the smaller ones and enforce the energy cascade, which makes the smallest eddies in the energy-containing range 7% the size of the largest ones.

With the integral length scale tending towards the upper end of the large flow scales where velocity components remain correlated, it is advantageous to also define a scale that marks the lower end of the flow scales' correlation. Once more, this is based on the cornerstone of our statistical characterization of turbulence, i.e. the two-point correlation. It is obvious from the auto-correlation definition (ρ_{ii} from Equation 2.6) that at the smallest separation, i.e. $\mathbf{r} \approx 0$, the flow scales are entirely correlated and ρ_{ii} takes a maximum value of unity and hence has an initial gradient of 0. As the separation increases, the flow correlation should decrease, so the auto-correlation should decay with increasing $\mathbf{r}$. Since the focus here is on defining a small scale that relates to the flow correlation and the first derivative at the smallest separation is zero, relating this small length scale definition to the initial curvature of the auto-correlation function, i.e. the second derivative of ρ_{ii} at $\mathbf{r} = 0$, is the first other meaningful alternative. This is exactly the basis of the Taylor scale definition [57].:

$$\lambda_i = \left[-\frac{1}{2} \frac{\partial^2 \rho_{ii}(0, t)}{\partial r_i^2} \right]^{-\frac{1}{2}} = \sqrt{\frac{\overline{u_i'^2}}{\left(\frac{\partial u_i'}{\partial x_i} \right)^2}} \quad (2.27)$$

The reader is referred to [2], [57] for the full mathematical derivation of this. The Taylor micro-scale represents eddies at the lower end of the inertial subrange. It is however, not representative of the smallest eddies, these are instead better characterized by the Kolmogorov scale as defined earlier. However, the advantage of the definitions of the Taylor and Integral scales provided in Equations 2.24 and 2.27, is that they convey directional information which helps account for flow anisotropy. Therefore, using these scales is quite versatile in characterizing the turbulent transition regardless of whether the considered flows are isotropic. This ties back to how it is sensible to define the turbulent transition Reynolds numbers in terms of the Taylor scale, as this definition is more easily adapted to different flow configurations. The Taylor Reynolds number is therefore defined as:

$$Re_{\lambda_i} = \frac{q_i \lambda_i}{\nu} \quad (2.28)$$

q_i is the velocity r.m.s. in the i th direction. Without isotropy, the Taylor scale conventionally used in this Reynolds number is oriented along the defined mean flow, which for shear layers is the stream-wise (longitudinal) direction.

The Taylor length scale can be related to the Kolmogorov and large eddy length scales by:

$$\lambda = C_1 Re_t^{-\frac{1}{2}} \mathcal{L} = C_1 \eta^{\frac{2}{3}} \mathcal{L}^{\frac{1}{3}} \quad (2.29)$$

where C_1 is a constant that is equal to $\sqrt{20}$ in isotropic turbulence. Furthermore, the length and velocity scales of the Taylor-Reynolds number well characterize the time scale of the smallest eddies such that:

$$\frac{\lambda_i}{q_i} = C_2 \tau_\eta \quad (2.30)$$

where $\tau_\eta = \left(\frac{\nu}{\epsilon}\right)^{\frac{1}{2}}$ is the Kolmogorov time scale and C_2 is a constant equal to $\sqrt{30}$ in isotropic turbulence.

Furthermore, if isotropy applies, $q = \sqrt{\frac{2\mathcal{K}}{3}}$ becomes the turbulence rms, then the following relationship between the dissipation rate and the Taylor scale can be derived [2], [64]:

$$\epsilon = 15 \frac{\nu q^2}{\lambda_t^2} \quad (2.31)$$

where λ_t is the transverse Taylor scale, which in isotropy can be related to the streamwise (longitudinal) Taylor scale with $\lambda_t = \frac{\lambda_l}{\sqrt{2}}$. Therefore, the isotropic Reynolds Taylor number can be defined by:

$$Re_\lambda = q^2 \sqrt{\frac{30}{\epsilon \nu}} = \mathcal{K} \sqrt{\frac{40}{3\epsilon \nu}} \quad (2.32)$$

It is also meaningful to similarly define a Reynolds number for the integral length scale:

$$Re_I = \frac{q I_{ii}}{\nu} \quad (2.33)$$

This is once more a definition that accounts for directional effects, but it can be shown that in isotropic conditions $Re_I = \left(\frac{1}{C_1} Re_\lambda\right)^2$. Moreover, all the aforementioned Reynolds numbers can be related as follows:

$$Re \approx 10 Re_I \approx 4.3 \frac{C_1}{C_2} Re_t \approx 4.3 \frac{3}{C_1 C_2} Re_\lambda^2 \quad (2.34)$$

Consolidating the different scales together in terms of magnitude:

$$\eta < \lambda < I < \mathcal{L} < \delta \quad (2.35)$$

where δ is an outer length scale used to define the outer Reynolds number Re and can, for instance, correspond to jet width in jet flows, pipe diameter in pipe flows, distance downstream of a flat plate in flow over a flat plate, or a measure of mixing layer width like momentum thickness in shear flows. This can be commonly assumed to be of the order of $2\mathcal{L}$.

Dimotakis [9] produced a further refinement of this turbulent scale distinction on which he relied to derive the turbulent transition Reynolds number threshold. Since developed turbulence is characterized by a well-defined inertial subrange, it is sensible to undertake the scale refinement within that range, particularly around the Taylor length scale. A lower-bound Taylor length scale marks the end of the inertial subrange and the beginning of the dissipation range. This is called the inner-viscous scale, λ_ν , and Dimotakis hypothesised that at the start of the turbulent transition $\lambda_\nu = 50\eta$ whereas Pope [2] maintained through his asymptotic analyses that the demarcation between the inertial and dissipative range for fully developed turbulence occurs at 60η . On the larger end of the Taylor length scales, the Liepmann-Taylor scale, λ_{LT} is derived as a scale in the inertial range that represents the upper limit of the

inner eddies while still adequately disjoint from the outer scale, i.e. lies outside of the energy-containing range. Dimotakis quantified this scale's dependence with/on Re based on the outer laminar thickness of the boundary layer by invoking Blasius conditions [65]. Therefore, the span of turbulent length scales becomes:

$$\eta < \lambda_\nu < \lambda < \lambda_{LT} < I < \mathcal{L} < \delta \quad (2.36)$$

Dimensional analyses of Equations 2.29 and 2.34, reveal that λ_{LT} can be between 1.2-2 times larger than the Taylor micorscale, λ . Through this Taylor scale refinement, Dimotakis stipulated that the transition to fully developed turbulence requires adequate formation of an inertial subrange with enough separation of scales such that $\frac{\lambda_{LT}}{\lambda_\nu} > 1$, and from this result along with application of the Reynolds number dependencies, the requirement of a transition outer-scale Reynolds number of order 10^4 is achieved. Dimotakis then used the $Re_\lambda = \sqrt{Re}$ to convert this into a Taylor-based Reynolds number criteria of 100. However, this omits the constant coefficients above in equation 2.34, and inclusion of these would require $Re_\lambda \geq 500$ for fully developed turbulence and adequate separation of scales.

For completeness, the diffusive scales still remain to be defined. In gaseous flows, however, the ratio of inertial to molecular diffusion measured by Schmidt number $Sc = \frac{\nu}{D}$ is ≤ 1 . This renders the Batchelor [66] and Obukhov–Corrsin [67] scales of similar magnitudes to their viscous counterparts, namely the inner-viscous, λ_ν , and Kolmogorov, η , scales respectively.

To summarize, for stationary flows, modification of Dimotakis analyses to include the coefficients in Equation 2.34 along with Pope's asymptotic analyses and the plentiful experimental results on the topic ([3]), support that fully established turbulence occurs for $500 \leq Re_\lambda \leq 1000$.

However, it is important to remember that this is based on the separation of scales element of developed turbulence, which has to do with the smaller isotropic-tending scales of turbulent motion (within the Universal equilibrium range as in Figure 2.2). What about the larger eddies in the energy-containing range? These are not universal as they are influenced by the flow geometry, but do they evolve self-similarly and demonstrate some elements of turbulent transition other than the separation of scales even at a lower Reynolds number

than the threshold quoted? Does their self-similar or asymptotic evolution depend on other (non-dimensional) parameters besides the Reynolds number?

These scales contain the most turbulent energy, so understanding and predicting their evolution has significant practical implications for mixing (which impacts combustion). The larger scales also maintain a long memory owing to their large time scales, and therefore, their evolution is influenced by the initial instabilities that triggered the turbulence development. This explains why linear stability analysis can sometimes well-predict these scales' behaviour [24]. Furthermore, once the transition to turbulence begins and the net energy cascade starts forming, it is the attributes of these large scales that affect the rate of energy transfer to the smaller scales and, consequently, the formation of the inertial range. Therefore, it is expected that the initial perturbation not only influences the asymptotic state of the large scales but also the rate of turbulence development and subsequent separation of scales, and understanding this dependence can equip engineers and scientists with the knowledge to carefully design flow geometries and system residence times to control and manage turbulence development and hence mixing and its dependent applications like combustion or nuclear fusion.

Studies that explore the dependence of turbulence development on the initial perturbations in reacting flows are very limited. But even in inert flows, the choice of initial conditions is often arbitrary, utilising random noise signals, and the analyses are usually limited to constant density flows without systematically looking at turbulence development in its varying scales and Kolmogorov hypotheses framework. Here, an attempt is made to advance these investigations with tractable initial perturbations derived from linear theory that are methodically varied between the different cases explored. Further different to previous studies, the initial perturbations leading to turbulence development are analyzed as elements of a dynamic system with well-defined eigenvalues and eigenfunctions as described in the next section (2.3.2) and their implementation into the code used more rigorously formulated in 3.4.

2.3 Transition to Turbulence

Fully established turbulence has well-characterized and predictable statistics that have informed the development of accurate turbulent combustion models [68]–[72]. Reacting transitional flows, however, have proven more elusive to study. Similar to fully turbulent combustion, directly resolving all the relevant chemical and flow scales is still computationally prohibitive for practical configurations and is therefore reserved for canonical simplified geometries as in this study, but then, even on the modelling side, there is a lack of accurate and versatile flow and chemical models to well predict the evolution of transitional statistics before fully developed turbulence. This is due to the absence of the universal behaviour of developed turbulence, as explained in previous sections, which usually forms the basis of conventional turbulence modelling. It is, therefore, inaccurate and non-physically representative to approximate transitional flow regimes as turbulent. Since this study focuses on the flow evolution leading up to turbulence, it is important to first explain the primary relevant phenomena that eventually lead up to turbulence and how these can be modelled.

2.3.1 Primary Instabilities

The transition of a laminar flow into a turbulent one can be fundamentally triggered by three types of instabilities:

- (1) Shear-driven instabilities known as Kelvin-Helmholtz Instabilities (KHI)
- (2) Acceleration (due to buoyant forces) driven instabilities known as Rayleigh-Taylor Instabilities (RTI)
- (3) Shock-driven instabilities known as Richtmyer-Meshkov Instabilities (RMI).

KHIs are due to the velocity and density differences between two adjacent fluids. The discontinuity at the fluids interface induces shear effects that develop vortices due to the lifting of the denser fluid and pushing down of the lighter one (this distinction is only significant in buoyant flows; otherwise, it doesn't matter if it is the denser or the lighter fluid that is lifted). The hydrodynamically formed spirals disrupt the initially uniform flows in each fluid and

drain some of their mean kinetic energies as they form. These rolling structures then undergo mechanisms such as pairings and amalgamations [36], [73] that culminate with 3-dimensional instabilities from what once was a 2-dimensional shear instability. As a result, the mixing layer grows, and turbulence starts developing.

RTIs are also due to the interactions between adjacent fluids at different densities, but the driving factor, in this case, is the pressure gradient between the two fluids that can cause the less dense fluid to accelerate the denser one and even support it against gravity. This causes a perturbed interface that grows in an inhomogeneous, 3-dimensional fashion. As the perturbations grow, the lighter fluid tends to entrain the heavier, forming bubbles, and the heavier flow penetrates the lighter one as spikes. This contributes an additional primary mechanism for mixing layer growth. A detailed account of multimode RTIs, their modelling, and how initial conditions influence them can be found in [74], [75].

RMIs are similar to RTIs but with the involvement of shockwaves. As the shockwave passes between the different density fluids, small perturbations on the interface or non-uniform impulses imposed on either fluid induce an impulsive acceleration owing to the deposition of baroclinic vorticity. Unlike with RTIs, this acceleration can occur in both directions, i.e., fluids tend to accelerate one another instead of only the lighter fluid accelerating the heavier one. This causes the interface perturbation to grow, first linearly, then non-linearly, demonstrating mushroom-shaped bubbles and spikes as mixing builds up and turbulence develops. A comprehensive account of the influence of initial conditions on RMIs and their contribution to turbulence can be found in [76]–[78].

These three instabilities are outlined in Figure 2.5, demonstrating how they affect the flow upstream and downstream of the detonation wave in a Rotating Detonation Engine (RDE). Obviously, these instabilities play a vital role in the mixing process in non-premixed combustion, making them a very important aspect of turbulence development. It is, therefore, paramount to carefully and realistically capture these instabilities when studying the transitional flow. Numerous studies [11], [31], [44], [53], [55] have demonstrated the importance of the initial perturbations on influencing the effects of the primary instabilities. The choice of initial turbulent-triggering-perturbations is pivotal when studying the transition to turbulence.



FIGURE 2.5. Simulated flow in Rotating Detonation Engine combustion chamber as the detonation wave progresses through the injected fuel and the consequential disruption to the shock due to the lag in fuel and oxidiser mixing [19].

2.3.2 Linear Stability Analysis of KHI

Since KHI is a focus of this study, this section aims to derive how the instability arises from fundamental principals to showcase its dominance over the other instabilities as a turbulence-inducing agent and help guide the rationale for how the initial conditions are implemented in this study. Understanding the linear analysis of the small initial perturbation is important as that perturbation creates instability that grows non-linearly, eventually leading to large flow features and turbulence development.

KHI is a prevalent instability with important implications in various fields besides engineering design, such as geophysics and meteorology. The occurrence of KHI even extends to a range of extra-terrestrial phenomena, such as in the motion of interstellar clouds [79], [80], amalgamations in supernova remnants [81], and quantum fluids involving quantized vortices. It is difficult to think of any mixing or flow problem where KHIs don't play a key role. Naturally, this extends to any shear layer problem where KHIs are the dominant vortex-inducing instability, whether it is in engineered engines/turbines (low or high-speed flows) involving classical fluids or in more advanced laser applications involving high energy density plasmas [82], [83].

Although it is prevalent in a wide range of applications including both continuously and discontinuously stratified flows [28], in its classical form, KHI was analyzed in incompressible, inviscid shear layers between two fluid layers, each of uniform velocity and density profiles

and a discontinuity at the interface between them [84], [85]. The fluids could be in either co-flowing or counter-flowing configurations. The following linear analysis concerns KHI in this classical sense and is, in a counter-flowing configuration, most relevant to this study. The term linear analysis here is commonly used to refer to the linearization of the underlying governing equations, validated by the small size of the perturbations, to derive expressions and formulations for the perturbation growth. Now, through this process, the resulting formulations may be non-linear (e.g. exponential), but they remain derived from linear theory.

Looking at a two-dimensional, infinitesimally small perturbation (relative to the flow geometry) in a counter-flowing shear layer in Figure 2.6, we consider the bulk of the two fluids mostly unperturbed and irrotational. An irrotational velocity field implies $\mathbf{u} = \nabla \Phi$, where Φ is a velocity potential. Since the fluid considered is incompressible, then through continuity, $\nabla \cdot \mathbf{u} = 0$. Therefore, combining these two conditions gives the Laplace equations for both the top and bottom fluid layers: $\nabla^2 \Phi = 0$. Furthermore, for the sake of also highlighting Rayleigh-Taylor effects and comparing them with KHI, let's include buoyant forces, such that the pressure is given by $p_2 = p_0 - g\rho_2 x$ and $p_1 = p_0 - g\rho_1 x$ in the top and bottom fluids respectively. Let ζ denote the x-direction displacement of the interface surface due to the small initial disturbance. Although the flow in both fluids is irrotational (under the previous assumptions), the counter-flow setup induces rotation of the vortex sheet at the interface, as shown in 2.6.

Considering the conditions on the vortex sheet, a formulation of the instability can be established. The full details of the derivation have been omitted here for brevity and focus, and only the main stages are listed as these inform on the initialisation implementation in 3.4 and results analyses. For the full derivation [24], [28].

The following conditions need to apply to the vortex sheet:

- (1) Through continuity, at a particular plane in the vertical direction (i.e. $x = \zeta$), the movement of the vortex sheet is entirely dictated by the movement of the surrounding fluid. This sets the following kinematic condition from each fluid's side:

$$\frac{\partial \Phi}{\partial x} = \frac{\partial \zeta}{\partial t} + \mathbf{u} \cdot \nabla \Phi$$

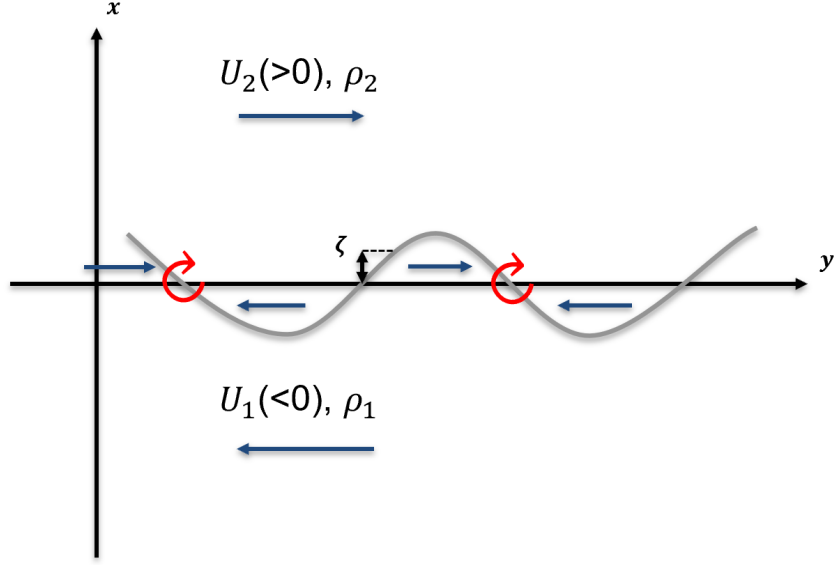


FIGURE 2.6. Schematic of a two-dimensional infinitesimal (relative to the bulk-flow dimensions) Kelvin-Helmholtz instability across a discontinuous shear layer [24]

- (2) Through applying the Navier Stokes, invoking the irrotational flow condition and integrating, we arrive at the unsteady Bernoulli's equation, which dictates the dynamic condition:

$$\rho_1(C_a - \frac{1}{2}(\nabla\Phi_1)^2 - \frac{\partial\Phi_1}{\partial t} - gx) = \rho_2(C_b - \frac{1}{2}(\nabla\Phi_2)^2 - \frac{\partial\Phi_2}{\partial t} - gx)$$

, where C_A and C_B are the constants of integration, can be found by applying the derived Bernoulli's equation to the free streams of the two fluids.

Applying linear analysis and simplifying this system of equations, the perturbation and vector potential fields can both be solved using normal mode analysis, such that

$$\zeta = \zeta^* e^{i(\omega_y y + \omega_z z) + st} \quad (2.37)$$

$$\Phi = \Phi^* e^{i(\omega_y y + \omega_z z) + st} \quad (2.38)$$

where ζ^* and Φ^* are the initial perturbation amplitude and vector potential respectively and ω_y and ω_z are the streamwise and spanwise wavenumbers respectively. Using the Laplacian

condition on the vector potential, a general form for Φ^* can be defined:

$$\Phi_2^* = A_2 e^{-\kappa x}, \Phi_1^* = A_1 e^{-\kappa x} \quad (2.39)$$

This is then substituted in the linearized kinematic and dynamics conditions of the vortex sheet (defined above) to get the eigenvalue of:

$$s = i\omega_y \frac{\rho_1 U_1 + \rho_2 U_2}{\rho_1 + \rho_2} \pm \left[\frac{\omega_y^2 \rho_1 \rho_2 (U_1 - U_2)^2}{(\rho_1 + \rho_2)^2} - \frac{\kappa g (\rho_1 - \rho_2)}{\rho_1 + \rho_2} \right]^{\frac{1}{2}} \quad (2.40)$$

and the eigenfunctions of:

$$A_2 = \frac{-(s + i\omega_y U_2)\zeta^*}{\kappa}, A_1 = \frac{(s + i\omega_y U_2)\zeta^*}{\kappa} \quad (2.41)$$

κ is the radial wavenumber, given by $\sqrt{\omega_y^2 + \omega_z^2}$. From the eigenvalue and the expressions for Φ and ζ , it is clear that both KHIs and RTIs grow exponentially. However, with both buoyant forces and density differences, some of the possible modes of RTI can be neutrally or marginally stable. This is different for KHIs alone, as the KHI modes are unconditionally unstable for either non-buoyant or constant density conditions. Furthermore, it can be seen through inspection of the first real term in equation 2.40 that the KHI modes that grow the most rapidly and dominate the flow are the ones oriented along the main flow (the y-direction), i.e. the streamwise modes. This supports the notion in this study regarding focusing on KHI, as not only is it widely prevalent and synonymous with most mixing applications, but it is a major turbulence-inducing mechanism, and it retains a lot of its initial characteristics (at least at the large energy-containing scales), which can possibly extend and help define the final self-similar state of the flow affecting mixing and combustion. Figure 2.7 shows the occurrence of KHI in the atmosphere.

Primary instabilities would naturally manifest as a combination of different perturbation wavelengths. However, some wavelengths influence the initial growth of the instabilities more heavily than others. Linear stability theory is concerned with monitoring the most unstable wavelength. Identification of the most unstable wavelength involves consideration of both the initial energy spectrum of the instability and the individual growth rates of the wavelengths. If the instability is initialised by a constant power spectrum (as undertaken in this study),



FIGURE 2.7. Kelvin-Helmholtz instability forming surf-like billows of clouds captured by pilot in Missouri, USA [86]. It is rumoured that such phenomena inspired Van Gogh's famous *Starry Night*.

and the instability is a KHI, then based on the above equations, it is clear that the instability with the highest wavenumber (smallest wavelength) would possess the largest eigenvalue and hence the fastest growth rate in time. Therefore, in this study of KHIs with a constant power spectrum, the smallest wavelength of the initial instability is the most unstable wavelength.

Looking at KHI in isolation under the physical lens and assuming an inviscid, non-buoyant ($g = 0$), homogeneous ($\rho_1 = \rho_2$), and incompressible fluids in a two-dimensional problem, Batchelor [87] explains the exponential growth of KHI by looking at the transport of vorticity along the perturbed interface. Without viscous or buoyant forces and variable density effects, vorticity accumulates in areas on the perturbed interface, which not only serves to exponentially grow the perturbation but also retains its structural shape until the perturbation grows large enough that it affects the surrounding flow dynamics and the linear approximation ceases to remain pertinent. It is, therefore, natural for KHI to be the first point of focus amongst the instability when developing turbulence and combustion models that extend into

the transitional flow-development regimes rather than the well-characterized, self-similar states.

2.4 Direct Numerical Simulations

2.4.1 DNS vs. RANS vs. LES

Numerically studying developing and reacting flows can be undertaken by adopting one of three main approaches. The first and most straightforward is to numerically solve the governing equations by considering all the spatial and temporal scales in the flow. This can be considered a brute-force approach where enough points are considered in the domain to fully resolve the turbulence to its smallest scales (Kolmogorov), and the time increments are kept small to capture unsteady effects and perform accurate numerical integrations. The approach requires considerable computational resources and is restricted to fundamental studies. As a result, such studies of reacting flows only started in the early 2000s due to parallel computing advances. This approach is known as Direct Numerical Simulation (DNS) and is utilised in this study.

The second is a practical approach commonly used in commercial codes and involves ensemble averaging the governing equations. The idea is that the process drastically cuts down its computational expense by observing ensemble averages instead of tracking and storing the information of a considerably much larger number of individual points. This is known as Reynolds-Averaged-Navier-Stokes (RANS) modelling. The problem, however, is that this averaging introduces unclosed terms in the equation that require modelling. Many validated models have been developed to fulfil this purpose, and RANS is deemed acceptable for many applications and commercial packages. Nevertheless, when studying the transition to turbulence, the inherent inaccuracy in some of the modelled terms in the RANS approach (which are formulated for developed turbulence), in addition to the lack of transparency to the fine details of the flow, makes this approach unsatisfactory to inform on the physics studied. Within these limitations, however, there are some successful RANS models that well

approximate large-scale quantities based on simple empirical relations that attempt to factor in some intermittency between the laminar and the turbulent regimes [88]. These approaches, however, have very significant limitations and are restricted to a small range of practical applications outside of which they are inaccurate.

The third approach to modelling turbulence combines the other two and is known as the Large Eddy Simulation (LES) approach. This recognises the statistical pattern of turbulence known as the energy cascade, where in fully developed turbulence, large eddies break down into smaller ones that break down further until all the energy is dissipated by viscous forces. The larger structures hold most of the turbulent kinetic energy and undergo the mechanisms that dictate the energy transfer to the smaller eddies and, eventually, the formation of an equilibrium state. The LES approach involves filtering the Navier-Stokes equations (governing equations) such that the larger eddies are fully resolved (as with DNS), whereas the smaller structures are modelled using a subgrid model. A wide range of subgrid models and LES approaches have been developed over the years, making LES very robust. At the current stage of this study, LES has not been very relevant, but it is crucial for future work where an appropriate subgrid model is developed and validated, as studying practical systems with DNS can be computationally prohibitive. Dynamic SGS LES models, specifically the stretched-vortex SGS model, has shown some promise when used to model transitional flows [44], [89], although that has only been examined for inert flows.

DNS requires the resolution of the finest turbulent scales (Kolmogorov), which is a considerable computational expense. This is exacerbated further when studying the transition to turbulence due to the fine scales and conditions involved when considering the primary instabilities, which require a low CFL number and appropriately formulated discretized governing equations to prevent excessive numerical dissipation. This dissipation is not just due to truncation errors in the interpolation and gradient or integration schemes utilised but also due to the discretization of the governing equations that may lead to undesirable source and sink terms that reduce the conservation of second-order scalars (or higher), such as turbulent kinetic energy, enstrophy, or helicity [90], [91]. When studying non-premixed combustion, DNS must provide resolution to capture the flow properties and the flame structure, including

the reaction zone [92]. This implies that the procedure needs to fully resolve all scales of chemical reaction, viscous dissipation, and diffusion.

2.4.2 Initial Perturbations

When conducting a DNS study, the initial conditions are key to its reliability and accuracy. This is of extra significance when the focus is on the transitional stage, so the seeding perturbations and flow fields must be designed carefully to try and represent realistic scenarios and boost the practicality and versatility of the study. Most literature studies focus on turbulent regimes and so it is sensible to start the discussion with these. There are two main techniques used to generate the turbulent flow field initial conditions:

- (1) Synthesizing initial turbulent conditions
- (2) Running precursor simulations and using their information as input with re-scaling as necessary

The second technique can sometimes be impractical as it incurs additional computational and storage expenses and the burden of rescaling and processing to generate the required conditions. For the latter technique to be reliable, adequate domain geometries and run times are required for the flow to establish turbulent structures for the inlet conditions. Moreover, when complex inhomogeneous turbulent inflow conditions are required, they will be difficult to generate using the second technique, which usually leads to homogeneous grid-like turbulence fields. This limits its versatility.

Methods to synthesize initial turbulent conditions usually involve prescribing a velocity field conforming to a spectral function or profile representative of established turbulence. The specified profile depends on the studied case and may be obtained from experimental data (for instance, a turbulent boundary layer profile as used in [11]), previous simulation studies (like [93]), or spectral functions derived from asymptotic turbulence theories [14], [37]. Most commonly, turbulent combustion studies aim to abruptly initiate turbulence by prescribing an initial simplified broadband turbulent velocity profile and superimposing that

on the mean velocity profile [36], [61], [93], [94]. This, however, generally tends to produce fully developed homogenous turbulence with scant transitional phenomena.

Another common and simple approach to synthesising an initial turbulent field is to use random noise to represent the turbulent fluctuating quantities. The problem with this method is that it can struggle to sustain turbulence [95], [96] as a Gaussian signal has a constant energy spectrum, and therefore, after some distance in the domain (if it is spatially developing) or time (if it is temporally developing), the energy of the attempted turbulence can more readily divert to the high wave number fluctuations. However, due to this approach's intrinsic simplicity, it can't be used to target specific turbulent-triggering-instabilities, which is useful when studying transitional phenomena.

Comparatively, limited work in literature looked at initialising flow fields with fundamental perturbations that organically lead to turbulence development. Even more limited is studying the dependence of turbulence development on specific attributes of the seeding perturbation, as most studies were interested in triggering turbulence most rapidly to save computational cost. The main element of the initial perturbation commonly studied in the literature for its effect on turbulence has been the convective Mach number and compressibility effects [14].

Pantano [14], [38] utilised a temporal shear layer configuration to comprehensively study a range of different Mach number shear layers spanning subsonic and compressible regimes, extending to reacting cases but of a single fluid (constant density) with constant viscosity and without varying the initial perturbation nor considering ones directly attributable to a fundamental instability. Both methane and hydrogen reactions were considered but only under fast chemistry conditions, which removes any chemistry-flow coupling (or vice-versa) and effects such as extinction and re-ignitions. The results of Pantano's work were consistent with previous investigations that concluded a significant reduction in mixing layer growth rate with increasing Mach number and describing the physical processes responsible for that reduction. These findings reaffirm the importance of divergence-free initial conditions commonly emphasized in literature (e.g. [97]), as compressibility effects can significantly impede mixing.

Pantano's work set the stage for many of the following temporal shear layer studies. The results of that investigation are quite conclusive (see Figure 2.8) in how increased Mach number and compressibility reduce mixing layer growth and attenuate turbulence development due to a reduction of the normalised pressure-strain tensor with increased Mach number, which leads to less energy transfer from the bulk streamwise flow to the cross-stream and spanwise eddies. This reduction clearly inhibits turbulence development. For this reason, although the implications of this study are of direct relevance to high-speed propulsion applications, the simulations undertaken in this present study are restricted to low-mach flow regimes as compressibility increases computational cost twofold, firstly by requiring higher resolutions to resolve the smaller scales, and secondly by impeding mixing layer growth and slowing down turbulence development. It would, therefore, be impractical to computationally run a range of DNS for a thorough parametric study of high-Mach flows. The present study focuses on the effect of the seeding KHI perturbation on the mixing evolution and turbulence development, in addition to the interplay between chemistry and flow development. This alone is missing from the literature and needs to be adequately understood before compressibility effects are included. Nevertheless, as explained in the next Chapter, the solver used solves the compressible Navier-Stokes equations to reduce the turbulence debilitating numerical dissipation characteristic of conventional pressure-based solvers like Open-Foam that significantly adversely affect studying developing flows.

Initial perturbation attributes, like wavenumber range (relative to domain geometry dimensions) or amplitude, have not been adequately studied or maturely understood in terms of how they affect turbulence or mixing evolution. Attili [53] observed a more natural turbulence development in mixing layers but perturbed the flow with broadband white noise initial velocity fluctuations spanning two orders of magnitude. However, this prevents studying the influence of specific perturbation dimensions (relative to the domain size) on the developing flows and is less natural as perturbations are likely to be initially rooted from a narrowband range like, for instance, with a vortex sheet from a nozzle or blade tip or surface roughness dimensions. In 1992, Roger and Moser [99] looked at a handful of Kelvin-Helmholtz modes in the initialisation, which was quite insightful but provided limited results on mixing and resolving a realistic configuration owing to the computational limitations at the time. It is also

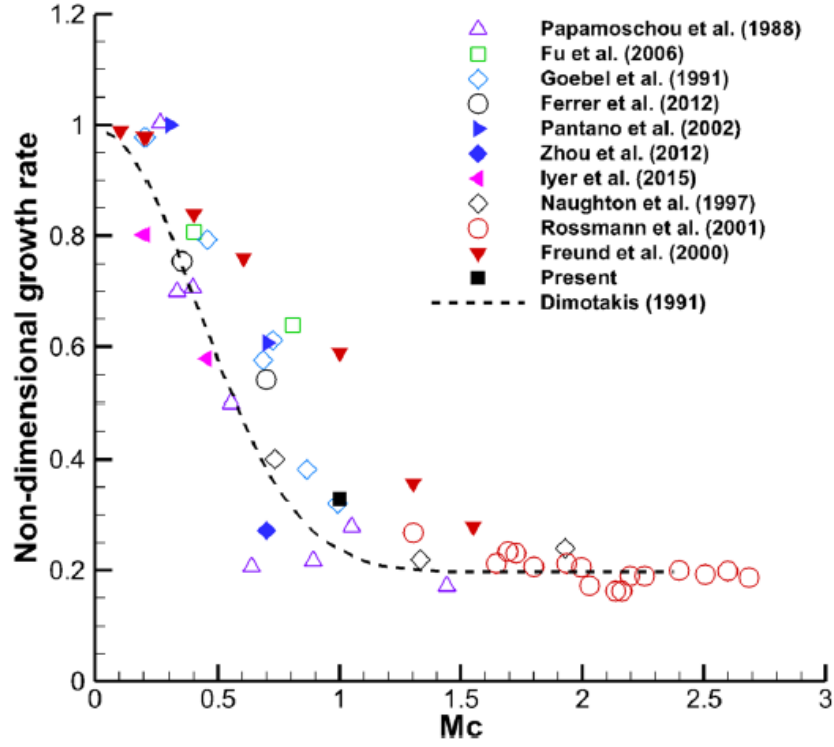


FIGURE 2.8. Consolidated experimental and simulation results of shear layers to demonstrate the dependence of the shear layer growth rate on the convective Mach number. The figure is reproduced from [98].

more likely that realistic flow perturbations manifest within a narrow range of modes rather than individual perturbations. Therefore, in this thesis, the perturbation initialisation avoids these two extremes, i.e. either broadband or a handful of individual modes, and relies on a narrowband range perturbation initialization as formulated in Chapter 3. Groom's recent work [12], [100] looked at narrowband range perturbation initialisation but in shock-induced (RMI) mixing of an inert flow configuration. However, RMI mixing doesn't sustain high Reynolds numbers (i.e., it doesn't readily lead to developed turbulence alone) and has different mixing attributes from vortex-based (KHI) mixing.

A recent study [44] attempted to look at this gap with a focus on scalar mixing attributes, but it provided conflicting results with earlier work of [11], [53] and without resolving all the relevant scales of fluid motion since it relied on Large-Eddy Simulations. Although this study varied the perturbation dimensions between the cases, it also relied on random fluctuations

similar to [53] rather than tractable perturbations consistent with linear theory. Moreover, neither of these studies investigated variable density flows, which are important for combustion applications. The ones that looked at density attributes, like [37], [55], lacked focus on the initial perturbations or the developing nature of the mixing layer. This, therefore, presents a research gap that can be addressed by an appropriate parametric study even in inert flows, although this thesis extends the investigation to reacting flows. Such investigation requires running repeatable and controlled setups, which are difficult and impractical experimentally.

Simulation Setup and Numerical Implementation

3.1 Overview

This chapter formulates the governing equations and the numerical implementation of the initial conditions used in the simulations conducted for this study. The numerical methods and simplifying assumptions/models used in the solver code are only briefly but completely listed. Full derivation and assessment of these are omitted from this thesis as they are not the focus of this work, and a complete list of references that outline the intricate details of the numerical frameworks utilised are enclosed in the relevant sections throughout this chapter for the reader's benefit. However, since it is unique to this work and an important element of this thesis's investigation, the formulation of the initial perturbation implemented in the simulations is outlined in detail in 3.4 with a clear definition of what constitutes the perturbation eigenvalues and eigenfunctions to relate back to the linear theory presented in 2.3.2 and help guide the discussions in the following chapters.

An important output of this work is to produce a comprehensive library of high-quality, fully resolved simulation data on shear-triggered developing flows, both inert and reacting. To this purpose, the directory of different cases run with their defining variables is outlined in 3.5. Most but not all the cases in this directory are analysed and discussed in this thesis. Cases with double shear layers and varying fuel compositions are reserved for future work. Finally, the quality of the simulation setup is evaluated through a systemic and comprehensive mesh convergence assessment for the base case and the rationale for the resolution used for all other cases is explained. The chapter ends with an outline of the large and small-scale resolutions of the cases analysed in this thesis.

3.2 Governing Equations, Transport Models and Numerical Techniques

The DNS code used for the reacting shear layer simulations is `Flamenco` [101], a Godunov-type finite volume compressible solver. The compressible reacting Navier-Stokes equations solved are highlighted below, starting with continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (3.1)$$

where ρ is density and u_i is velocity. The compressible momentum equation is formulated as:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} + \frac{\partial p}{\partial x_i} - \frac{\partial \tau_{i,j}}{\partial x_i} = 0 \quad (3.2)$$

where p is the pressure and $\tau_{i,j}$ is the viscous stress tensor which is assumed Newtonian and computed as

$$\tau_{i,j} = -\frac{2}{3}\mu \frac{\partial u_k}{\partial x_k} \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.3)$$

Sutherland's law calculates the temperature-dependent viscosities for each species considered. The mixture's average viscosity, μ , is computed using Wilke's mixing rule and is the one that appears in the equations above as the governing equations solve for the mixture averages.

Since variable density and combustion with finite-chemistry effects are considered in this study with a multi-species chemical reaction mechanism, a species transport equation is also solved:

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} + \frac{\partial \rho Y_k V_{k,i}}{\partial x_i} = \dot{\omega}_k \quad (3.4)$$

where $\dot{\omega}_k$ is the net rate of k th species production from all the chemical mechanism reactions. $V_{k,i}$ is the species diffusion velocity in the i th direction and is evaluated using Fick's law, such that $V_{k,i} = -D \frac{1}{Y_k} \frac{\partial Y_k}{\partial x_i}$. D is the mixture averaged molecular diffusivity computed from the thermal diffusivity and unity Lewis number assumption. This non-differential diffusion simplification is acceptable for the scope of this study, as both fuel and oxidizer streams are heavily diluted with passive N_2 for all the cases considered, and the focus here is on the effect of the initial perturbations on the overall flame and mixing profiles. Additionally, [94] observed small influences of differential diffusion for similar shear flow configurations to

those studied here. Due to the unity Lewis number enforcement, the resulting Schmidt (Sc) and Prandtl (Pr) numbers are equal across the domain. They are not explicitly defined (they are just a function of the constituent mixture averaged transport properties), but the average Sc and Pr were observed to be approximately 0.7 at initial conditions, consistent with the common values in fuel-air mixture studies.

For energy balance, the specific total non-chemical (sensible and kinetic) energy, E , transport equation is solved:

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u_i E)}{\partial x_i} + \frac{\partial q_i}{\partial x_i} + \frac{\partial u_i p}{\partial x_i} = \frac{\partial \tau_{i,j}}{\partial x_i} - \frac{\partial}{\partial x_i} \left(\rho \sum_{k=1}^N h_{s,k} Y_k V_{k,i} \right) + \dot{\omega}_T \quad (3.5)$$

where q_i is the heat diffusion term that is evaluated by Fourier's Law, such that $q_i = -\lambda \frac{\partial T}{\partial x_i}$; λ is the mixture-averaged thermal conductivity, which also uses Wilke's mixing rule to average the individual species thermal conductivities that are each computed from kinetic theory as a function of the chemical species corresponding dynamic viscosity (the ones computed from Sutherland's law).

The second term on the right side constitutes the enthalpy diffusion flux term, which has been shown to play an important role in maintaining the stability and accuracy of non-premixed combustion simulations [102]. The last term on the right side is the reaction source term corresponding to the aggregate heat release rate from all reactions involved in the chemical mechanism considered, such that $\dot{\omega}_T = -\sum_{k=1}^N \Delta h_{f,k}^0 \dot{\omega}_k$, with $\Delta h_{f,k}^0$ is the standard enthalpy of formation for the k th species, and N is the total number of species considered in the reaction mechanism. The energies and enthalpies are computed using a thermodynamic database of JANAF polynomials linked to the state variables with the ideal gas law.

Flamenco employs a fifth-order MUSCL scheme for the spatial reconstruction of inviscid terms [103]. Pressure and density variations are scaled using a low Mach correction to enhance the resolution of low Mach features and reduce numerical dissipation. The Harten, Lax, and Leer Contact (HLLC) Riemann solver is used for inviscid flux components [104], and second-order central differences are applied for viscous and diffusive terms. Temporal

integration is through a second-order total variation diminishing (TVD) Runge–Kutta scheme [105].

3.3 Simulation Setup

The computational domain is 3D Cartesian, with x, y , and z denoting the cross-stream, stream-wise, and spanwise directions, respectively, with a counter-flowing temporally developing shear layer flow configuration as shown in 3.1. When vector component notation is used in future chapters, the 1, 2 and 3 subscripts correspond to the x , y , and z directions, respectively, e.g. U_1, U_2 , and U_3 . The dimensions of the domain in each respective direction are denoted by L_x, L_y , and L_z , which vary between the different cases, as highlighted in 3.5. The choice of temporal rather than spatially developing mixing layers is to maintain computational efficiency as previous work involving stationary mixing layers demonstrated strong qualitative and quantitative similarities with both approaches [11], [37], [106], [107]. For instance, Attili [53] confirmed quantitative agreement of turbulent statistics between their spatially developing shear layer simulations and the temporally developing ones by Rogers & Moser [11] during the self-similar turbulent regimes.

Some cases use a double shear layer configuration where the domain is extended in the x direction and the fuel slab is sandwiched between two counterflowing air flows similar to [61], [93]. Unlike similar configurations in the literature, the fuel jet is not turbulent, and the KHI perturbations are localised within the upper and lower shear layers. The idea of the double-shear layer setup is to investigate the interactions between different shear layers, which is a research gap in published studies on the subject, but the analysis in this thesis is restricted to single-shear layers, and that of double-shear layers is reserved for future work.

The initial stream-wise mean velocity profile is defined as a hyperbolic tangent as is common in a wide range of mixing layer simulations [14], [37], [55], [108]–[110]. The mean profile in terms of the cross-stream coordinate is given by:

$$\overline{U}_2(x) = \frac{\Delta U}{2} \left(1 - \tanh \left(\frac{x - x_0}{2\delta_{m,0}} \right) \right) \quad (3.6)$$

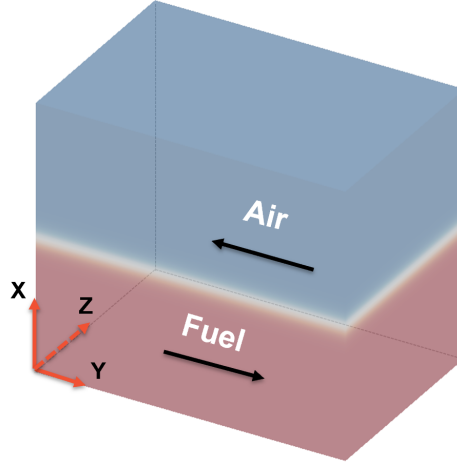


FIGURE 3.1. Single shear layer simulation domain setup and coordinate system

where $\delta_{m,0}$ is the initial momentum thickness used to define the domain dimensions for the different cases as shown in 3.5. This thickness is chosen to ensure an adequate number of cells across the shear layer to capture the growth of the instability without it being excessively thick that it damps some of the instability modes. The position of the mixing layer centre plane upon which the initial velocity perturbations are set is denoted by x_0 . The initial mean span-wise and cross-stream velocities are zero, with their initial fields strictly comprised of instability-seeding velocity fluctuations. The fuel and oxidiser free-streams flow in opposite directions with an equal velocity magnitude of $\frac{\Delta U}{2}$, where ΔU is the difference between the fuel and oxidiser free-stream velocities, i.e. twice the magnitude of the fuel or oxidizer free-stream initial streamwise velocity.

The initial convective Mach number as defined in [14], [111], [112] is

$$Ma = \frac{\Delta U}{c_{fuel} + c_{oxidiser}} \quad (3.7)$$

where c is the speed of sound in each of the respective streams. Since all cases (whether inert or reacting) analysed in this thesis have the same initial chemical composition and temperature profiles, the initial convective Mach number is varied by changing ΔU as shown in 3.5. The Mach numbers considered are either lower ($Ma = 0.08$), intermediate ($Ma = 0.16$), or higher ($Ma = 0.32$) such that all cases considered are effectively incompressible, by design,

to avoid the addition of sizeable compressibility effects that interfere with the mixing evolution (as highlighted in 2.4.2) and may skew the comparison between the cases. Here, the focus remains on the effects of the initial perturbation in isolation of compressibility effects.

Periodic boundary conditions are enforced in the stream-wise and span-wise directions, and a subsonic outflow boundary condition is used in the cross-stream direction with a constant atmospheric static pressure and extrapolated velocity and scalar boundary values (from the ghost cells to enforce the constant pressure condition). This cross-stream boundary condition is placed far away from the initial flame and works to reduce spurious pressure fluctuations from outgoing waves, particularly during ignition events [113].

Both inert and reacting cases considered here utilize the same fuel and oxidizer stream chemical composition and have the same initial density distribution across the shear layer. Syngas (CO/H₂) combustion was chosen for this study since it is both a subset of larger hydrocarbons utilised in relevant applications and the fact that it also has hydrogen as one of the reactants, which is a directly relevant fuel to propulsion. The same skeletal Syngas chemical mechanism in [93] is used here since it conserves computational expense while maintaining adequate fidelity. The mechanism encompasses 11 species and 21 reactions.

The chemical kinetics are modelled using the empirical Arrhenius law and consider a range of relevant third-body reactions. The chemical mechanism was fully integrated with `Flamenco`'s code to compute the net reaction rates for each of the chemical species and close the reaction source terms in Equations 3.4 and 3.5. Direct temporal integration is used to solve these terms. Normally, this incurs additional computational expense to ensure a small enough time step for the chemical solver's stability and accuracy. However, since `Flamenco` utilizes an explicit compressible formulation and a maximum Courant–Friedrichs–Lewy (CFL) number of 0.3 to accurately capture the flow transition, then the time steps are already small enough that no additional computational cost is incurred for the direct chemical integration.

Combustion is initialised by a flamelet condition at 75% of the extinction scalar dissipation rate, χ_q , which is determined by solving the steady laminar flamelet equations. The flamelet

equations were solved in Chemkin at this value of scalar dissipation and the chemical composition tabulated along with mixture fraction. The initial mixture fraction profile is defined in the heterogeneous direction as a hyperbolic tangent, similar to the streamwise mean velocity:

$$\bar{\xi}(x) = \frac{1}{2} \left(1 - \tanh \left(\frac{x - x_0}{2\delta_{z,0}} \right) \right) \quad (3.8)$$

The characteristic thickness of the mean mixture fraction profile, $\delta_{z,0}$, is chosen to be larger than the equivalent velocity profile characteristic thickness, $\delta_{m,0}$. This is firstly done to maintain the same number of cells across the initial flame surface as in [93] for a more consistent chemical resolution of the flame structure that is adequate for the fuel-air mixture to continue burning throughout the simulation. Secondly, it is common for simulations of reacting cases to have a thicker mixture fraction thickness than a velocity profile thickness, as the initial slight misalignment of the flame surface and the mixing layer centre is necessary to prevent excessive dissipation of the growing instabilities at the flame centre where the temperature and hence the viscosity are both high. Using this mixture fraction profile, the transverse profile for every chemical species is obtained from the generated flamelet solution which initialises the one-dimensional chemical composition field in the entire domain. This creates an initial flame with strong flow-chemistry interactions having prominent regions of extinction and re-ignition throughout the temporal simulation but also reduces the extent of the laminarizing effect of combustion, which allows for the initial instabilities to grow and for adequately high Reynolds numbers to be attained.

The syngas stream is diluted with Nitrogen to provide a thick (in mixture fraction space), easily resolved flame surface, with an H_2 to CO to N_2 volume ratio of 1:5:4 and a stoichiometric mixture fraction, ξ_{st} of 0.42. The oxidiser stream is a 1:4 by-volume mixture of O_2 and N_2 . Both free streams have an initial temperature of 500 K.

All DNS cases were run on 8064 CPU cores, consuming in excess of 6 million CPU hours in total. Simulations were all conducted on the Australian National Computational Infrastructure (NCI) high-performance computing (HPC) facility, Gadi, while using up to 39 TB of RAM during runtime. OpenMPI version 4.1.4 was used for the parallelization, and `Flamenco`

was compiled to double precision in grid (mesh) and solver code on Gadi with Intel compiler version 2021.

Rather than starting with an originally turbulent field as used in [93], the KHI is induced via a narrowband range of two-dimensional multimode velocity perturbations at the fuel-oxidiser interface in the streamwise and spanwise directions [114]. Since the definition and setup of the initial condition are crucial in this study to allow for reasonably accurate modelling of the physical Kelvin-Helmholtz instability and the ensuing transition to turbulence, a full account of the instability initialisation is provided in the following section.

3.4 The Kelvin-Helmholtz Instability Initialisation

KHI velocity perturbations are superimposed on the mean velocity field at $t = 0$ to trigger turbulent transition. KHIs physically manifest as amplitude perturbations at the fuel-oxidiser interface as defined by linear theory [24]. These are converted to equivalent velocity perturbations through a vector potential approach to satisfy the continuity equation [114]. The seeding multi-modal amplitude perturbations are defined over a narrowband range of wavenumber while conforming to a constant power spectrum defined to be $\propto \sigma^2$. The modal amplitudes of the perturbations are selected from a random seed Mersenne Twister algorithm, which allows repeatability. The algorithm picks the coefficients from a Gaussian function. The total standard deviation of the amplitude perturbation is scaled to equal σ , which is set to $0.1\lambda_{min}$ where λ_{min} is the smallest wavelength in the assigned narrowband range. The final form constitutes an eigenvalue:

$$\Phi_0 = \frac{\omega_y \sqrt{\rho_1 \rho_2} |U_1 - U_2|}{\underline{\kappa}(\rho_1 + \rho_2)} \quad (3.9)$$

that follows directly from linear theory [24], and an eigenfunction that complies with the general form derived from linear theory, whilst satisfying all the aforementioned requirements. ω_y is the streamwise wavenumber, $\underline{\kappa} = \sqrt{\omega_y^2 + \omega_z^2}$ which is the radial wavenumber with ω_z the spanwise wavenumber. ρ_1, ρ_2 and U_1, U_2 are the fuel and oxidizer free-stream initial densities and velocities, respectively. The vector potential components in the stream and

spanwise directions are then defined as:

$$\begin{aligned}\phi_j = & \Phi_0 \frac{\omega_z}{\underline{\kappa}} [b_{jk} \cos(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & - a_{jk} \cos(\omega_y(y - y_0)) \sin(\omega_z(z - z_0)) \\ & + d_{jk} \sin(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & - c_{jk} \sin(\omega_y(y - y_0)) \sin(\omega_z(z - z_0))] e^{-\underline{\kappa}|x - x_0|}\end{aligned}\quad (3.10)$$

$$\begin{aligned}\phi_k = & \Phi_0 \frac{\omega_y}{\underline{\kappa}} [-c_{jk} \cos(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & - d_{jk} \cos(\omega_y(y - y_0)) \sin(\omega_z(z - z_0)) \\ & + a_{jk} \sin(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & + b_{jk} \sin(\omega_y(y - y_0)) \sin(\omega_z(z - z_0))] e^{-\underline{\kappa}|x - x_0|}\end{aligned}\quad (3.11)$$

Denoting partial derivatives such that i,j,k are the cross-stream(x), streamwise(y), and spanwise (z) directions, the velocity fluctuations are then defined by:

$$u'_i = \frac{\partial \phi_k}{\partial x_j} - \frac{\partial \phi_j}{\partial x_k}, \quad u'_j = -\frac{\partial \phi_k}{\partial x_i}, \quad u'_k = \frac{\partial \phi_j}{\partial x_i} \quad (3.12)$$

A damping function is added to ensure the magnitude of the perturbations is greatest at x_0 , and decays in the positive and negative cross-stream directions towards the boundaries. The full details of the derivation and implementation of the KHI initialisation are presented in Appendix A.

3.5 Cases Directory

3.5.1 Cases Included in Thesis Analysis

This thesis is concerned with studying the dependence of the mixing and turbulence evolution on the seeding instability- specifically KHI. The aim is to observe: 1) if tractable changes in the fundamental instabilities affect the transition process, 2) whether the ensuing developed state retains information about the seeding instability, and 3) ultimately if variations in perturbations can be impressed on the flow by design, whether that would lead to mixing and

combustion control in propulsion systems. As highlighted, the focus in the present study is on KHIs, and the variations explored are all related to the linear stability theory formulation of the instability. The idea is that since linear theory is effective at capturing the perturbation evolution during the initial linear stages, then commencing the DNS from this instance should provide a physically representative framework.

The variations between the cases analysed in this thesis are based on four factors that effectively vary the seeding perturbations and the mixing/turbulence evolution in different ways. These are the initial perturbation narrowband range, domain size, convective Mach number (effectively ΔU variations), and chemistry (on/off). Starting from the base case, BC-R-SS:4-8 (Table 3.1), the setup is varied along these parameters, and these parametric variations are analysed in the following chapters of this thesis.

The case names provide a complete account of the initial setup. The naming convention for each of the cases starts with one of the following identifiers to distinguish between the initial case setups:

- (1) BC= Base Case (reference)
- (2) HRe = High Reynolds Number (at initial conditions relative to reference)
- (3) LRe = Low Reynolds Number (at initial conditions relative to reference)
- (4) HMa = High Mach Number (at initial conditions relative to reference)
- (5) LD = Large Domain

These identifiers are then followed by a designation (R/NR) for whether the case is reacting or non-reacting, a further designation (SS/DS) for whether the case is single or double shear (only SS cases are analysed in this thesis), and finally, the normalised wavenumber range of the initial KHI perturbation. Normalisation of the perturbation wavenumber range is such that the lower bound corresponds to $\frac{\kappa_{min}}{\kappa_0}$ and the upper bound to $\frac{\kappa_{max}}{\kappa_0}$ of the initial perturbation such that $\kappa_0 = \frac{2\pi}{L_y}$ relating the initial perturbation to the domain dimensions through the streamwise length. Note that the Reynolds number here is not an independent parametric variation between the cases. The parametric variations are strictly in ΔU and the wavenumber range of the initial KHI, but incidentally in some cases, this leads to a different initial Reynolds

number than the base case, which is reflected in the naming. Further, these initial Reynolds number variations differ depending on the definition of the Reynolds number used which is another reason why it is omitted from Table 3.1 (in addition to being a dependent variable). The differing Reynolds number characteristics between the cases are further analysed and discussed in Chapter 4 for the inert cases and in Chapter 5 for the reacting ones.

Case	Ma_c	$\frac{\kappa_{min}}{\kappa_0} \leq \underline{n} \leq \frac{\kappa_{max}}{\kappa_0}$	$\frac{L_x}{\delta_{m,0}} \times \frac{L_y}{\delta_{m,0}} \times \frac{L_z}{\delta_{m,0}}$	$N_x \times N_y \times N_z$
BC-R-SS:4-8	0.16	$4 \leq \underline{n} \leq 8$	$524.2 \times 600 \times 400$	$504 \times 576 \times 384$
HRe-R-SS:4-8	0.32	$4 \leq \underline{n} \leq 8$	$699 \times 600 \times 400$	$1344 \times 1152 \times 768$
BC-NR-SS:4-8	0.16	$4 \leq \underline{n} \leq 8$	$524.2 \times 600 \times 400$	$756 \times 864 \times 576$
HMa-R-SS:8-16	0.32	$8 \leq \underline{n} \leq 16$	$524.2 \times 600 \times 400$	$1008 \times 1152 \times 768$
HMa-NR-SS:8-16	0.32	$8 \leq \underline{n} \leq 16$	$524.2 \times 600 \times 400$	$1008 \times 1152 \times 768$
LD-R-SS:4-8	0.08	$4 \leq \underline{n} \leq 8$	$699 \times 1200 \times 800$	$336 \times 576 \times 384$
LD-NR-SS:4-8	0.08	$4 \leq \underline{n} \leq 8$	$699 \times 1200 \times 800$	$504 \times 864 \times 576$

TABLE 3.1. Simulation parameters. The domain sizes are expressed as multiples of the initial incompressible domain thickness, $\delta_{m,0}$, which is defined in the mean velocity profile thickness in Equation 3.6 and is fixed to be the same for all cases. N_x, N_y, N_z are the number of cells in the computational domain for each case in the x,y and z directions, respectively. The base wavenumber is $\kappa_0 = \frac{2\pi}{L_y}$, and the radial mode numbers for the narrow band range defined for each case are denoted by $\underline{n}$.

There are two reasons why the domain dimensions varied in some cases. Firstly, in temporal simulations, it has been repeatedly brought up how the domain size can saturate the flow development and impede turbulence from fully developing [11], [31], [56]. Here, the investigation aims to link this domain limitation to the seeding perturbation as effectively it is the variation of the seeding perturbation relative to the domain size that is investigated since the initial perturbation wavenumbers are a function of the domain dimensions as shown in the previous section. Secondly, varying the initial perturbations can lead to different mixing layer growth rates and attain a later non-dimensional time with different cases, which is desirable for the following analyses; the domain dimensions are extended in the cross-stream direction to prevent the boundaries from interfering with the shear layer. The domain dimensions and other setup parameters for each case are shown in Table 3.1. The dimensions are given in terms of the initial interface thickness, $\delta_{m,0}$ (Equation 3.6) that is kept the same for all cases (to maintain the same initial mean strain rates).

Some cases are designed such that certain flow/chemistry parameters are varied in isolation from others to study the independent effects of the variations. For example, the HMa cases reduce the flow length scales due to enforcing a higher wavenumber perturbation but increasing the initial Mach number by the same ratio to maintain the same outer-scale initial Reynolds number. It is important to understand that these variations attempt to control the initial condition alone, as larger wavenumber perturbations tend to grow more rapidly with time as predicted from linear theory (outlined in Section 2.3.2) and therefore controlling parameters throughout the flow evolution is difficult. The analysis of all cases listed in Table 3.1 is the subject of the remainder of this thesis. Inert cases are studied in Chapter 4 to report on flow and mixing evolution in isolation of chemical reactions. Reacting cases are analysed in Chapter 5 in the context of mixing and in Chapter 6 for their flame structure.

3.5.2 Cases Reserved for Future Analysis

Further simulations were conducted to investigate three other elements of mixing layer physics. These simulations are not analysed in the following chapters and are prepared for future analysis, so they are outlined separately in Table 3.2. They are presented and discussed here for completeness since an important output of this thesis is to provide a library of DNS data on mixing layers.

Case	Ma_c	$\frac{L_x}{\delta_{m,0}} \times \frac{L_y}{\delta_{m,0}} \times \frac{L_z}{\delta_{m,0}}$	$N_x \times N_y \times N_z$
LRe-R-SS:4-8	0.08	$349.5 \times 600 \times 400$	$336 \times 576 \times 384$
BC-R-DS:4-8	0.16	$699 \times 600 \times 400$	$672 \times 576 \times 384$
BC-NR-DS:4-8	0.16	$699 \times 600 \times 400$	$672 \times 576 \times 384$
BC-R-SS-CV:4-8	0.16	$524.2 \times 600 \times 400$	$504 \times 576 \times 384$
HMa-R-SS-CV:8-16	0.32	$524.2 \times 600 \times 400$	$1008 \times 1152 \times 768$
BC-R-SS-CVHDa:4-8	0.16	$524.2 \times 600 \times 400$	$1008 \times 1152 \times 768$

TABLE 3.2. Simulation parameters for the other cases conducted in this study but not analysed in this thesis. The naming convention follows that introduced earlier, with CV denoting cases where Sutherland's law was removed and viscosity fixed. HDa in the last row refers to the case where the initial Damkohler number is increased by reducing the N_2 dilution of Syngas fuel in the fuel stream.

The first element is the impact of multiple shear layer interactions on mixing, turbulence evolution, and chemistry, which is investigated through a double shear layer extension of the base case in both reacting and inert configurations while varying the random seed of the velocity perturbation in each shear layer. This looks similar to conventional jet configurations studied in literature [61], [115], but the difference is instead of a turbulent fuel jet, the initialisation here is based on fundamental KHI perturbations in both layers.

The second element is the effect of viscosity on the mixing and chemical evolution investigated by removing Sutherland's law and fixing the mixture dynamic viscosity (effectively also the kinematic as the cases have the same initial flow compositions and hence densities) to the initial average of the viscosity field in the base case. The mixture's thermal conductivity is then evaluated by fixing the Prandtl number to the initial average in the base case.

The third element explores the effects of varying the chemical time scales on the mixing and chemical evolution through varying the chemical composition of the fuel and oxidizer streams. While the parametric variations analyzed in this thesis (Table 3.1) effectively change the Damkohler number, they do so by varying the mixing scales, whereas the chemical scales stay fixed. Varying the initial fuel composition varies on these chemical scales. It can provide valuable insight into the effects of chemistry on flow development (a commonly overlooked element of the flow-chemistry interactions in modelling). These variable composition simulations run without Sutherland's law but now fix kinematic viscosity (instead of dynamic) as the densities differ.

3.6 Grid Convergence and Simulation Quality

3.6.1 Base Case Convergence and Assessment of Simulation Quality

3.6.1.1 Overview

To help the reader with a visual image of the evolving shear layer in preparation for the upcoming analyses, Figure 3.2 shows the mixing layer at the final simulation time for both the

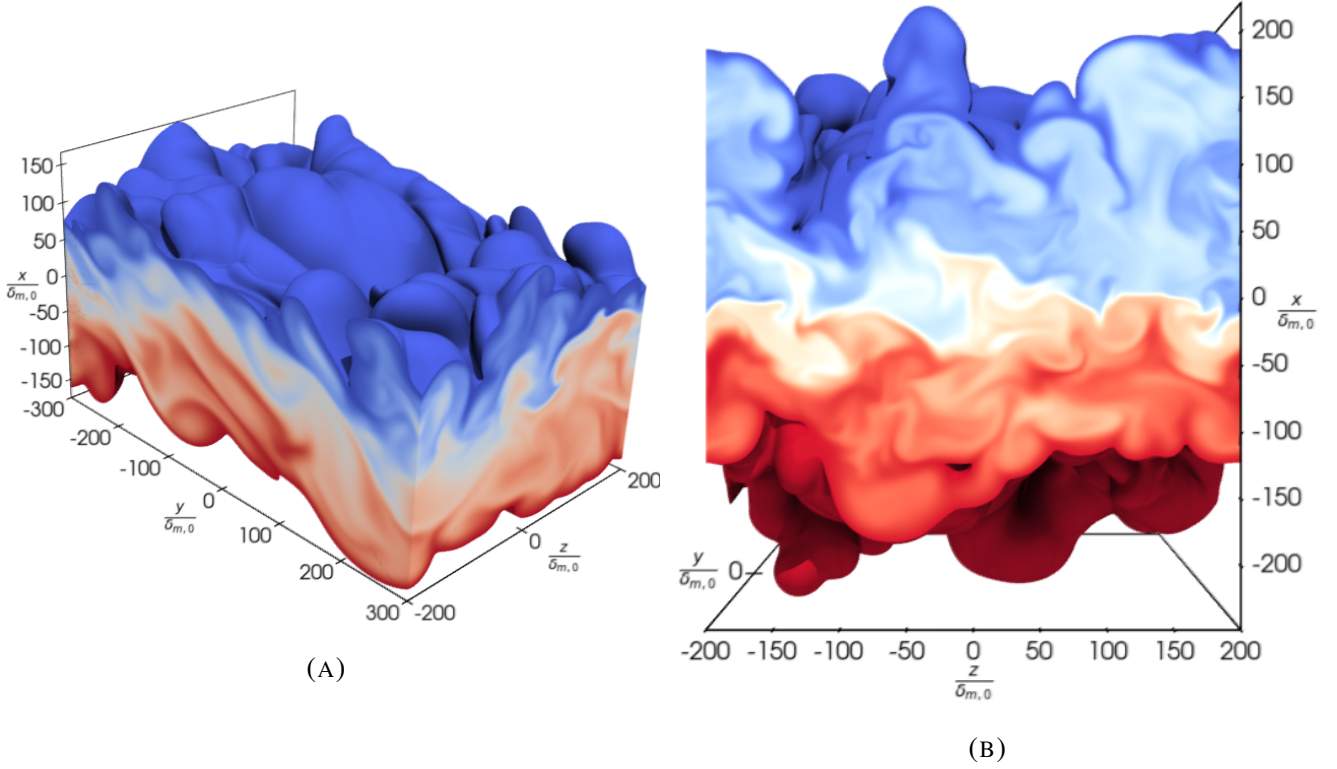


FIGURE 3.2. Isosurfaces of mixture fraction with a cutoff at $\xi = 0.01$ and $\xi = 0.99$ at the latest runtime for BC-R-SS:4-8 (left), and HRe-R-SS:4-8 (right).

base case and the higher Reynolds number variant of the base case. The figures only go up to the extent of the iso-contours in the transverse direction rather than the entire domain to focus on the mixing zone. Both cases show a highly chaotic profile with extensive three-dimensional variations, although the higher Reynolds number case shows a greater range of resolved eddies in the spanwise direction.

The DNS simulation results generated in this study inform the physics of developing flows and their parametric dependence on the initial conditions. It is, therefore, important to guarantee a reasonable accuracy of the simulation data, at least to the same order of the parameters investigated [2]. Firstly, showing consistency in the results and determining the resolution that captures all the relevant chemical and flow scales is important. Secondly, since the goal here is to observe and understand the factors that affect full turbulence development, the domain dimensions must be large enough to accommodate growing modes. This section investigates these elements by inspecting the results of three different mesh resolutions of

the base case (BC-R-SS:4-8 in Table 3.1). The resolutions assessed, corresponding with $N_x \times N_y \times N_z$ order are coarse: $252 \times 288 \times 192$, intermediate: $504 \times 576 \times 384$, and fine: $1008 \times 1152 \times 768$.

Using the base case for this investigation involved a compromise for feasibility. The idea is that this convergence assessment of the base case can be used to gauge the minimal required resolution for each of the other cases without requiring an independent mesh convergence, which would be computationally nonfeasible. The LD cases would have been a computationally cheaper but less conservative choice for the mesh convergence assessment. Similarly, the HRe or the HMa cases would have been more conservative but impractical, as running three sets of mesh resolutions for these cases with a doubling factor between each set is nonfeasible. Therefore, using the base case in this assessment strikes the right balance between conservative and practical. Discussion of how the converged resolution results are extended to the other cases, particularly the non-reacting ones, are outlined in Section 3.6.2 and the resulting different simulation qualities are illustrated.

3.6.1.2 Domain Size Constraints and Temporal vs Spatial Setups

The domain sizes and resolution choices for the simulation had to be well-considered. As in [55], if turbulence transition is to be realised, then the domain sizes need to be large enough in the cross-stream (x) direction to allow the mixing layer to grow to adequate lateral extents. This allows the flow to achieve self-similar statistics for a sufficient duration for the analysis. The stream-wise to span-wise lengths ratio is maintained as in [93] to be 1.5, ensuring that the modes oriented in the stream-wise directions are longer- a characteristic of physical shear flows. Consistently, in the KHI perturbation initialisation, the number of modes initialised in the span, and stream-wise direction maintains the same ratio as the domain lengths in the respective direction.

Mesh convergence depends on adequate resolutions of the flow's smallest and largest scales. In traditional DNS studies, most of the focus in mesh convergence has been devoted to adequate resolution of the smallest scales [56], [116], [117] with simulations repeated with the same domain size but finer grid resolutions to ensure convergence. The rationale is that,

in such studies, the small scales evolve independently of the large scales as the flow exhibits the scale separation characteristic of fully developed turbulence as discussed in Chapter 2. The majority of classical DNS studies either focus on elucidating small-scale flow physics to support subgrid-scale model development or focus on the physics of local phenomena that occur at the smallest scales such as with combustion [118]–[120].

However, this asymptotic scale separation behaviour does not exist in developing flows. Without a sufficiently large domain size, the growth of the largest flow scales is impeded by the domain restriction. As a result, these flow scales could become saturated and not realise the larger growth potential needed for their subsequent breakdown and further turbulence development. These saturation effects result in persistent two-dimensional coherent structures that impede progress towards the asymptotic state where Kolmogorov hypotheses apply [11], [31]. Moreover, since these are energy-containing scales, they drive the mixing layer growth and the onset of turbulence and are of primary importance to engineering design. Therefore, their restriction diminishes turbulence development and can impede the goal of this study in observing the full span of mixing evolution.

Additionally, as these scales grow with time, not capturing their full-extent results in a deficient sample space, which distorts statistical calculations and prevents statistical convergence at late times.

Larger mode saturation is not a numerical artefact. Even in experiments or spatially developing configurations, if the spanwise dimensions are not large enough, then turbulence evolution and mixing Reynolds number growth would be restricted as mixing scales (like turbulent scales) are three-dimensional, and so, for instance, unlike flow past a flat plate (as discussed in Chapter 1), the mixing Reynolds number wouldn't just be reliant on a one-dimensional distance, like down-stream distance, so observing the flow evolution at significant distances downstream in experiments may still manifest coherent two-dimensional structures if the spanwise and cross-stream directions saturate the large scales and impede the flow evolution towards an asymptotic fully developed turbulent state where the energy cascade and scale separation is observed. This distinction here is important. With sufficient downstream distance (or time in temporal simulations) and without any further impedance or forcing of

the flow downstream, all flows will reach an asymptotic self-similar state. Still, unless that state exhibits scale separation and the energy cascade, it is not the fully developed turbulent asymptotic state where Kolmogorov hypotheses and conventional turbulence modelling have been validated.

In temporal simulation, the restriction of the streamwise direction becomes an added limitation and a possible source of numerical inaccuracy relative to experiments and spatially developing flows. Temporal simulations of developing flows may also have extra sensitivities to the initial perturbations than spatially developing ones or experiments, and due to this, along with the limitation of Taylor's hypothesis in non-stationary flows, introduces some inaccuracies in the results [121], [122]. Nevertheless, temporally evolving mixing layer simulations have been extensively used to draw valuable physical insights regarding mixing in a range of different flow conditions [11], [12], [14], [32], [37], [55], [61], [115], [123], [124]. Therefore, since a spatially evolving configuration is computationally prohibitive for exploring a wide parameter space as in this study, temporal configurations are used here to help advance the understanding of the mixing evolution until exascale high-performance computing (HPC) and GPU solver adoption are more accessible to refine and extend this study's findings in future work. Moreover, according to Rogers & Moser [11], the correspondence between spatially and temporally evolving shear layer simulations approaches an exact limit if the velocity ratio between the two streams is close to one- which is the setup used for all simulations in the present study and further validates the choice of a temporal configuration.

In temporal simulations of mixing layers induced by fundamental KHIs, the domain constraint is mostly in the homogeneous directions (stream-wise (y) and span-wise (z)) since these are aligned with the main flow and the shear instability and are set with periodic boundary conditions for the temporal configuration. Ample length is given in the heterogeneous cross-stream (x) direction since that is needed to allow the mixing layer to grow without reaching the boundaries, which makes this direction less constricted.

Furthermore, another separate consideration is that together the domain size and the number of mesh elements considered provide an adequate statistical sample for statistical convergence. This is particularly important during the later stages of flow development and towards the

onset of the turbulent transition when the modes are saturating and the largest self-similar structures have developed.

Thornber [56] has shown that the most rapid growth of integral scales occurs during the transition for homogeneous decaying turbulence. Therefore, it's important to ensure that the domain is not restrictive to further growth at the end of the transition (i.e., the start of turbulence). Hence, the convergence assessment in this section has been completed until late into the transition stage.

3.6.1.3 Convergence of the Large Flow Scales

Studies [14], [56] have shown that to avoid these finite-domain length effects and ensure adequate resolution of the largest scales, integral length scales of the flow should not exceed 10% of the corresponding domain length. This conservative requirement prevents the onset of undesirable saturation of the largest scales in the flow and satisfies the resolution requirement for the large scales. As explained, the two most critical integral length scales are the ones that correspond to the homogeneous directions, namely I_y and I_z as computed by Equation 2.24.

The integral length scales are calculated at the centre plane of the domain (i.e. at $x = \frac{L_x}{2}$). This plane has been shown to well-approximate the centre of the mixing layer for the single shear layer cases setup since both the flame surface and the flow stream-wise velocity inflection points are in its vicinity. Calculations computed at adjacent planes (within the momentum thickness) produced integral scales within 5% of the centre plane value. Therefore, the integral scale calculated from the centre plane flow field adequately represents the mixing layer. The same applies to the Taylor and Kolmogorov scale calculations, and therefore, the results here are all computed in this centre plane. From Figure 3.3, the integral scales are converged without exceeding 10% of the respective domain lengths, and the normalised auto-correlations, calculated by Equation 2.6, decay to zero within half the domain length in Figure 3.4. These two results satisfy the large-scale convergence criteria. The satisfaction of this requirement by BC-R-SS:4-8 is a good preliminary indicator for the other cases since BC-R-SS:4-8 utilises the larger narrowband range in its initialisation (relative to the domain lengths).

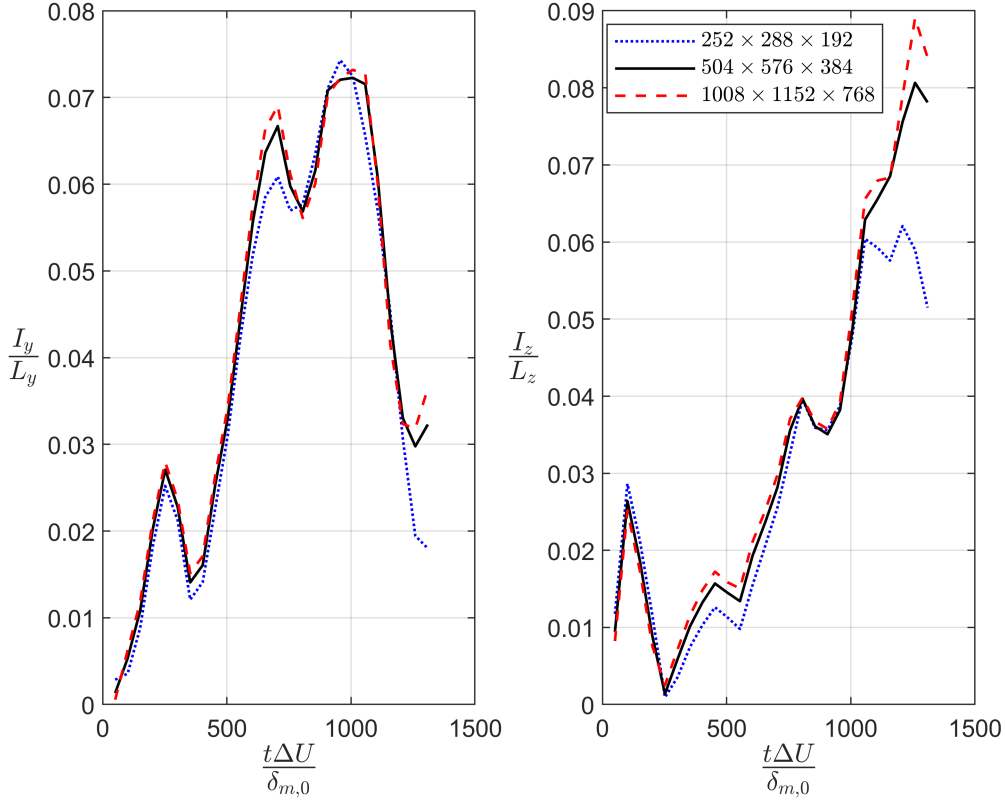


FIGURE 3.3. Grid convergence of the stream-wise (left) and span-wise (right) integral scales for three mesh resolutions of BC-R-SS:4-8. Time was normalised by the free-stream velocity differences and the initial momentum thickness, which are commonly done to facilitate comparisons between different studies.

3.6.1.4 Consideration of the Seeding Perturbation Dimensions Relative to the Domain Size

Aside from resolving the largest eddies and preventing their premature saturation, the domain size also plays another important role in determining whether turbulence eventually develops in temporal configurations. This may seem straightforward initially as flows attain turbulence at sufficiently high Reynolds numbers, increasing with length. However, more fundamentally, there appears to be a direct relation between the most unstable wavelength, λ_p , in the turbulence-inducing perturbation at the flow initialisation and the onset of turbulence. λ_p is the wavelength corresponding to the wave number with the peak energy in the initial flow

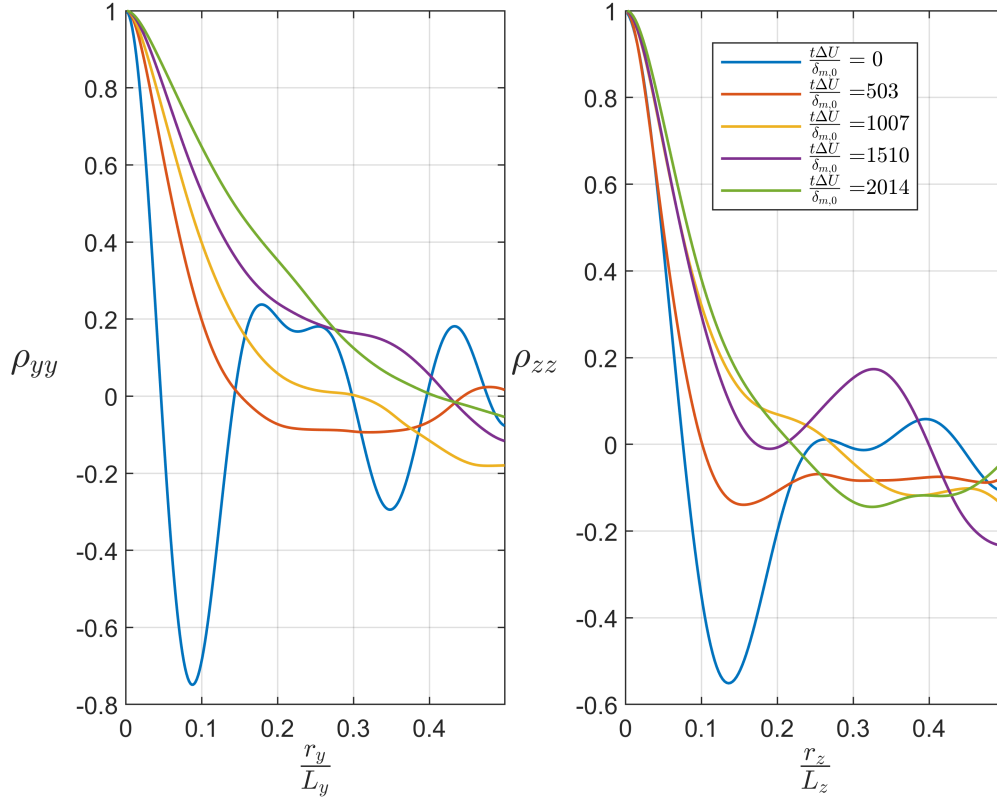


FIGURE 3.4. Decay of the stream-wise (left) and span-wise(right) auto-correlation coefficient of the intermediate resolution of BC-R-SS:4-8 at different times

energy spectrum. It can, therefore, be expressed as a fraction of the domain size for a given flow initialisation spectrum.

Thornber [56] concluded that in Homogeneous Decaying Turbulence, for full turbulence to be realized, the domain length needs to be more than $256\lambda_p$. On the other hand, in shear flows, the turbulence development is accelerated by vortex pairing events [99], which relaxes the domain size requirement. Consequently, the domain size requirement can be re-expressed in terms of the number of vortex-pairing events it accommodates. Vreman [32] and Baltzer [37] have shown that the domain size in temporal shear layer simulations needs to be at least $8\lambda_p$. This implies 3 vortex pairing events. Baltzer [37] used a domain size of $64\lambda_p$ in their simulations, which is almost double the minimum required number of pairing events needed to allow for the onset of turbulence to ensure the most rapid development.

For the case setups employed in this study, since the initial flow field has a constant power spectrum over a prescribed narrow-band range, as explained in Section 3.4, all initial wavelengths hold the same energy. From the linear theory of KHIs as outlined in Section 2.3.2, provided all initial wavelengths hold the same energy, the most unstable mode is the one corresponding to the highest wavenumber aligned in the stream-wise direction as outlined in the eigenvalue expression in Equation 2.40 with the exponential growth scaling with ω_y . This is also, by design, consistent with the initialisation implemented as evident from the magnitude of Φ_0 in Equations A.11, A.13, A.14. From the case directory outlined in Table 3.1, all cases considered in this study ensure a presence of initial perturbation wavelengths that are 1/8th of the streamwise dimension, consistent with the minimum requirement outlined by [32] and [37].

3.6.1.5 Convergence of the Initial Perturbation

It is also important to ensure convergence of the flow initialization by adequately capturing the sharp velocity gradients used in the initial velocity field definition as outlined in Section 3.4. It was determined through numerical tests that fully capturing the initial perturbations and achieving grid independence at the initial flow time required a minimum of 16 cells across the smallest initial wavelength in the perturbation. Table 3.1 shows that the resolutions are well above that. A uniform grid size was used with the same resolution in all three directions since turbulence is isotropic at the smallest scales, as outlined by Kolmogorov hypothesis [2] and mixing layer geometry considered is simple and cartesian.

3.6.1.6 Convergence of the Medium to Small Flow Scales

When it comes to the small scales, it is common practice in DNS studies to use an adequately high resolution such that the Kolmogorov scale is resolved as scales smaller than this only hold relatively minuscule amounts of energy and for minute durations as they quickly dissipate with viscous forces [125]. The grid size, therefore, had to be carefully considered to ensure adequate resolution of the small scales and mitigate the non-physical effects of numerical dissipation. For DNS studies, the framework for the resolution requirements has been designed

around turbulent flows, where the Reynolds number is high enough that the Kolmogorov hypotheses apply (Chapter 2), and an adequate separation of scales exists with net energy cascade from the largest to the smallest scales of the turbulent eddies. In such cases, the grid size needs to be fine enough to resolve the viscous scales adequately, i.e. Kolmogorov scales η [126]–[128]. The rationale behind this is that any further smaller scales are overwhelmed by physical viscous forces. Therefore, the arising numerical dissipation from the numerics employed reasonably emulates the physical viscous dissipation at these scales. However, in [126], Moin & Mahesh suggest that resolving the Kolmogorov scale might be overly stringent when the analysis presented revolves around first and second-order statistics. Looking at the grid resolution of established DNS studies, Pantano [14], Almagro [55], and Baltzer [37] reported grid resolutions of $3-4\eta$, less than 1.8η , and 1η , respectively during self-similar flow regimes. In summary, for classical DNS, the aim is to resolve the scales up to the ones where the energy transfer from larger turbulent structures is entirely balanced by the dissipative effects of viscosity [127] i.e. the inertial forces experienced by these smaller structures are entirely balanced by viscous forces.

In developing and non-stationary flows as simulated here during early times, the resolution requirements for DNS are less well defined in literature as self-similarity has not been established. Therefore, the calculation and resolution of the Kolmogorov scales is more arbitrary. Convergence studies conducted by Groom [129] of RMI before the onset of turbulence show that the most stringent resolution requirement for mesh convergence is during the early transitional period regarding the ability of the mesh to resolve smaller scales. Baltzer [37] reported that resolution quality reduces during the early-time transition to 1.8η . Here, the convergence of directional Taylor scales, Taylor-based Reynolds numbers, Kolmogorov scales, and turbulent kinetic energy dissipation rate are shown in Figures 3.5-3.7. The plane averaged directional Taylor length scales and Reynolds number are calculated respectively as:

$$\lambda_i = \sqrt{\frac{\overline{u_i'^2}}{\left(\frac{\partial u_i'}{\partial x_i}\right)^2}} \quad (3.13)$$

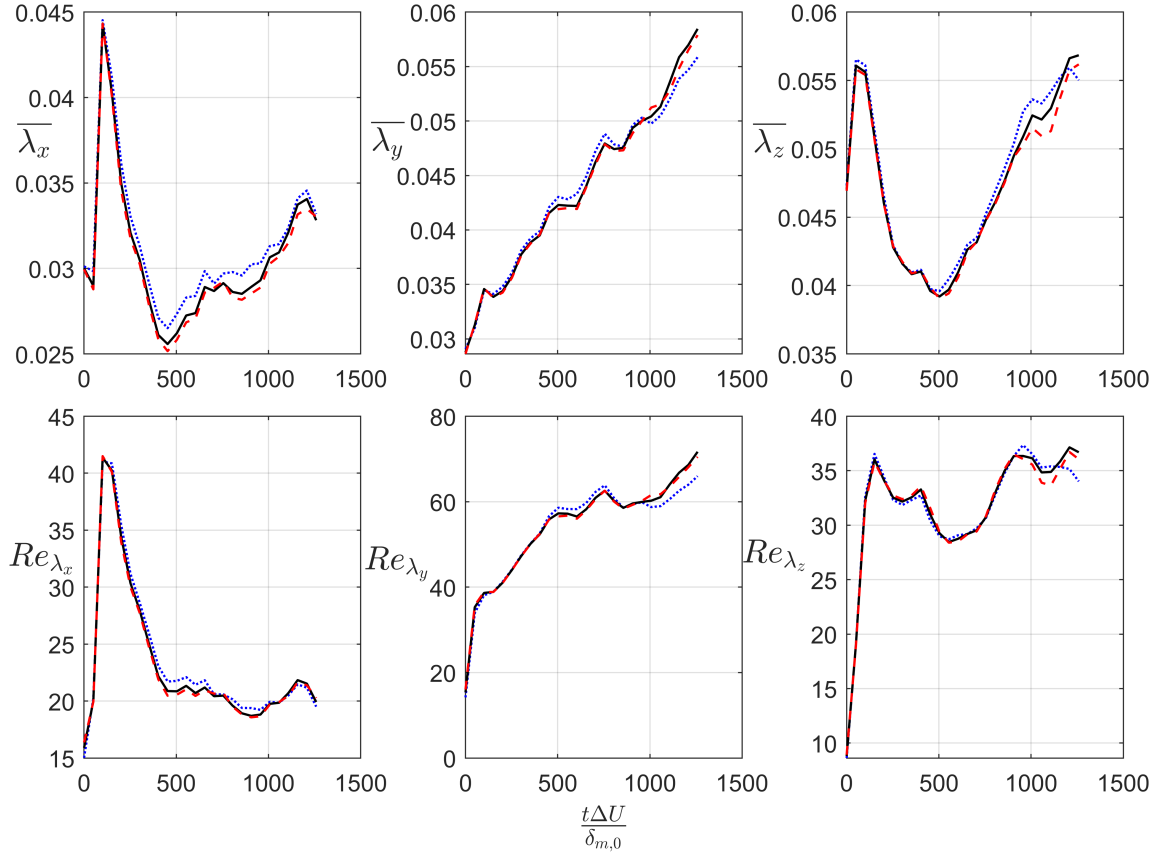


FIGURE 3.5. Grid convergence of the directional Taylor length scales and corresponding Reynolds numbers for three mesh resolutions of BC-R-SS:4-8 in Table 3.1. The plots' colour schemes are consistent with those in Figure 3.3.

$$Re_{\lambda_i} = \frac{\lambda_i \sqrt{u_i'^2}}{\bar{\nu}} \quad (3.14)$$

This is consistent with the previous general formulation in Equation 2.28 while taking into consideration the averaging to explicitly evaluate the RMS as $q_i = \sqrt{u_i'^2}$. Note that the plane averaging notation convention is consistent with Section 2.2.1.2. An interesting observation for all Re_{λ_i} in Figure 3.5, is that after a short duration with rapid variations, the directional Taylor Reynolds numbers stabilize with relatively much smaller variations afterwards. This is despite the increase in the corresponding Taylor length scales observed after $\frac{t\Delta U}{\delta_{m,0}} = 500$. Such observation implies that at later times, the increase of both the corresponding Taylor length scales and RMS is well balanced by the increase in viscosity due to the rise in temperature from

combustion, which somewhat stabilises the Taylor-Reynolds number. Initially, however, the flame is highly strained and endures a short period of intermittency that fuels the initial rapid Reynolds number growth. This result demonstrates the strong influence of combustion on the turbulence development of non-stationary flows. The turbulent kinetic energy dissipation

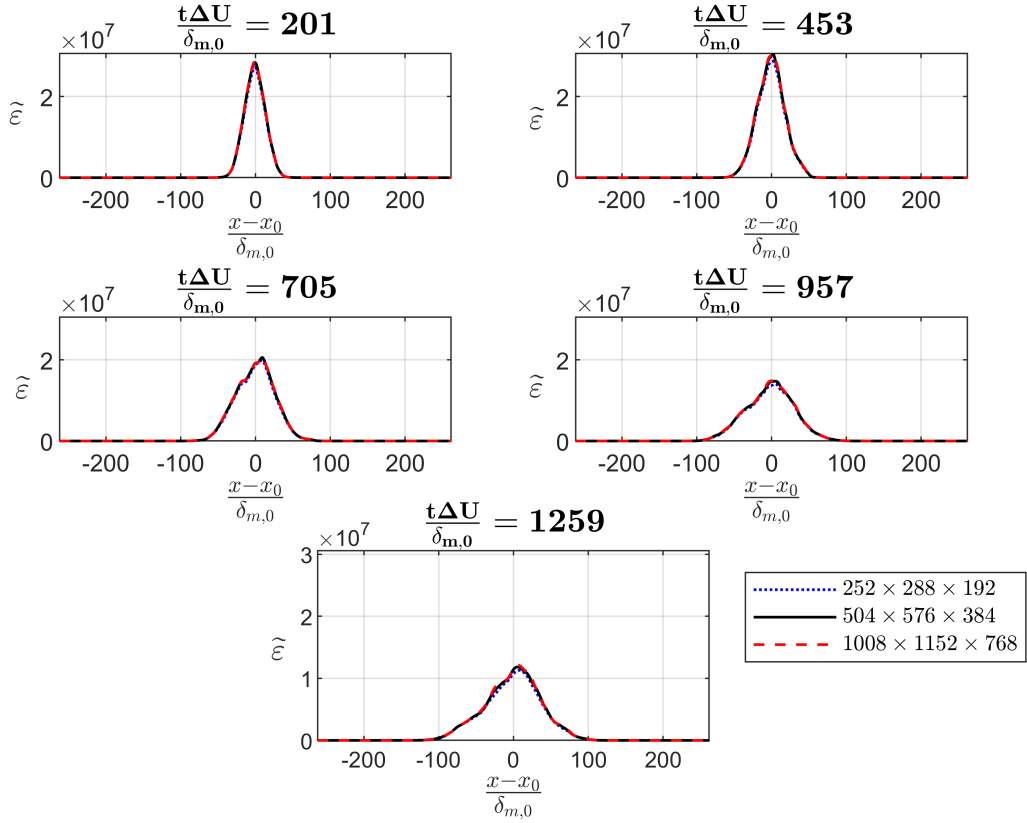


FIGURE 3.6. Mesh convergence of turbulent kinetic energy dissipation across the non-dimensional heterogeneous x-direction for five normalised times and three resolutions of BC-R-SS:4-8 (the base case).

rate is calculated following the definition in Equation 3.15 but taking into consideration the averaging as in [37];

$$\bar{\varepsilon} = 2\mu \overline{\left(s'_{ij} s'_{ij} - \frac{1}{3} \theta'^2 \right)} \quad (3.15)$$

and

$$\tilde{\varepsilon} = \frac{\bar{\varepsilon}}{\rho} \quad (3.16)$$

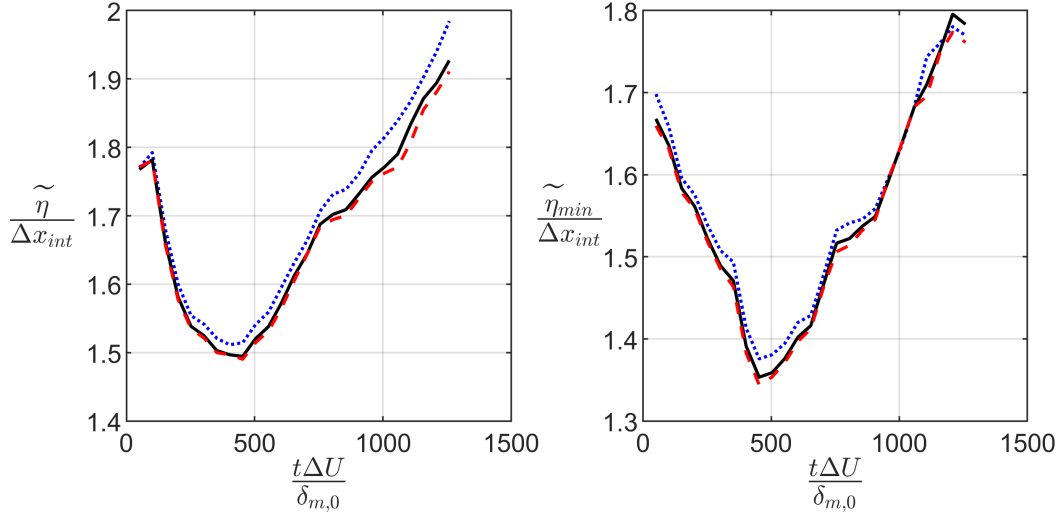


FIGURE 3.7. Grid convergence of planar averaged Kolmogorov length scales with normalised time at three mesh resolutions of BC-R-SS:4-8. The y-axis is normalised by the uniform grid size of the intermediate resolution, Δx_{int} to provide a sense of scale. The normalisation was kept the same for all resolutions to prevent the separation of the different plots. The left plot calculates the Kolmogorov planar averages in the domain central plane, and the right one plots the minimum heterogeneous planar value against normalised time. The plots' colour schemes are consistent with those in Figure 3.3.

Note how this results in only the units of $\tilde{\varepsilon}$ and not $\bar{\varepsilon}$ to correctly correspond to the specific rate of energy transfer, i.e. power per unit mass. The plane averaged Kolmogorov number is then calculated as:

$$\tilde{\eta} = \left(\frac{\bar{\nu}^3}{\tilde{\varepsilon}} \right)^{\frac{1}{4}} \quad (3.17)$$

For transitional flow regimes, i.e. before the onset of turbulence, there is no well-established resolution requirement for DNS. During such regimes, the characteristic energy cascade profile is not in effect, and the flow dynamics can involve significant backscatter as the smaller scales grow rapidly, as predicted by linear theory calculations. This continues until modes saturate and non-linear mixing layer growth mechanisms, like pairings and entrainment, take over and dominate the process. It is therefore important for the resolution at an early time to adequately resolve the sharp gradients that induce the initial growth mechanisms, and reliance on the resolution of Taylor and Kolmogorov scales at these early times is an insufficient measure. Instead, mesh convergence of key quantities must be demonstrated with time. Since

many statistical quantities of interest are of second order, choosing equal or higher order statistics as the parameters to test for mesh convergence [130] is important. Combining the two aforementioned requirements of both conserving second-order scalars and also resolving sharp gradients, Figure 3.8 shows the convergence of key integral second-order quantities at three different mesh resolutions of the base case (BC-R-SS:4-8). These are integrated across the entire domain and all three flow directions. Enstrophy is a second-order gradient-based

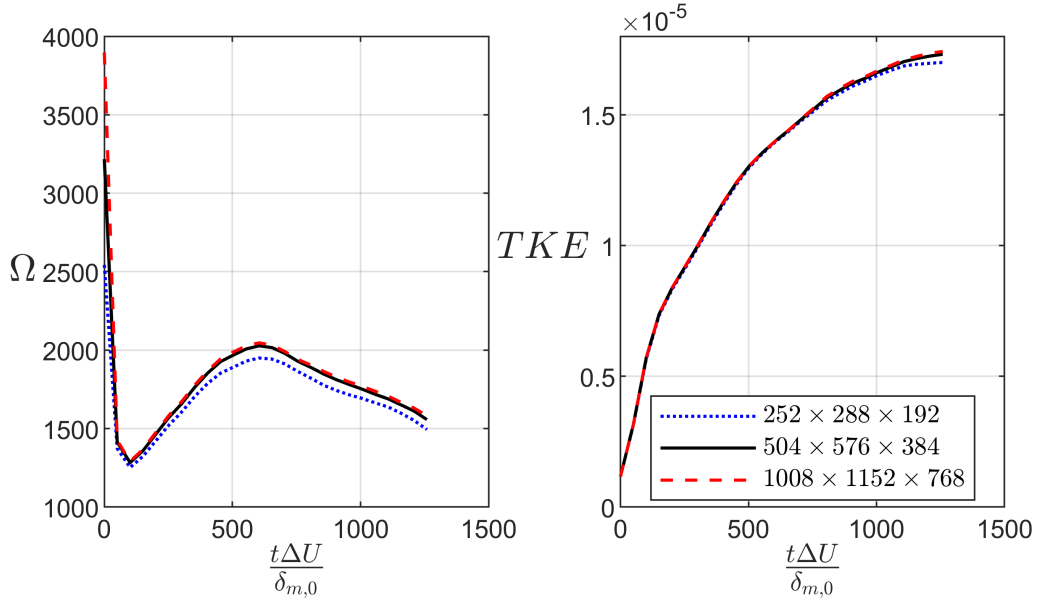


FIGURE 3.8. Mesh convergence of total domain integrated flow second order flow gradient quantities against non-dimensional time for three mesh-resolutions for the base case BC-R-SS:4-8 in Table 3.1.

quantity, and its integrated value, Ω , is calculated by:

$$\Omega(t) = \sum_{i=1}^3 \int \rho \omega_i \omega_i \partial V \quad (3.18)$$

where ω_i is the vorticity in the i th direction such that, for example, ω_1 is:

$$\omega_1 = \frac{\partial u_3}{\partial x_2} - \frac{\partial u_2}{\partial x_3} \quad (3.19)$$

While total kinetic energy is expected to decrease with time due to viscous dissipation taking away the energy, total integrated turbulent kinetic energy in developing shear layers should increase as the velocity fluctuation and turbulence increase until the flow becomes

stationary. It is, therefore, key to check TKE for dissipation when observing transitional flows, which impedes physical flow development. Dissipation of TKE can either be due to excessive numerical dissipation from low-order schemes employed or from the implied discretized transport and conservation equation of TKE that arises from the choice of numerical discretization of the Navier Stokes. For instance, it is common for incompressible collocated solvers to suffer from excessive dissipation of second-order scalars due to the de-coupling of the momentum and pressure equations [90], [131]. TKE is calculated by:

$$TKE(t) = \sum_{i=1}^3 \int \frac{1}{2} \rho u_i'' u_i'' \partial V \quad (3.20)$$

The plots in Figure 3.8 confirm the convergence of these second-order quantities and gradients and satisfy the resolution requirement of the developing flow while ensuring no excessive energy dissipation as the flow develops until it reaches a stationary state.

3.6.1.7 Convergence of the Chemical Scales

The previous sections discussed the convergence criteria of the flow scales, but since reacting cases are also considered in this investigation, the convergence of the chemical scales also needs to be tested. Firstly, the Syngas chemical mechanism from [93] was manually implemented and integrated with FLAMENCO, and so that needed to be verified. This was done by running a 0D case where the governing equations were solved over time under isobaric conditions, and the results were compared against those obtained from CHEMKIN simulations using the same reaction mechanism and kinetics files. The results of this comparison are shown in Figure 3.9, which shows agreement between the two codes and confirms the correct implementation and integration of the mechanism in FLAMENCO.

There has to be an adequate resolution across the flame thickness to resolve the chemical gradients and sustain combustion. From Hawkes [93], which investigated the same chemical mechanism and flame used here, it was determined that a minimum of 10 cells are required across the initial mixture fraction profile thickness, $\delta_{z,0}$ (3.8), to fully resolve the initial flame surface and the steep gradient of the critical flame-marking OH radical. Numerical tests in this study confirmed that any lower resolution of the flame thickness extinguishes the flame.

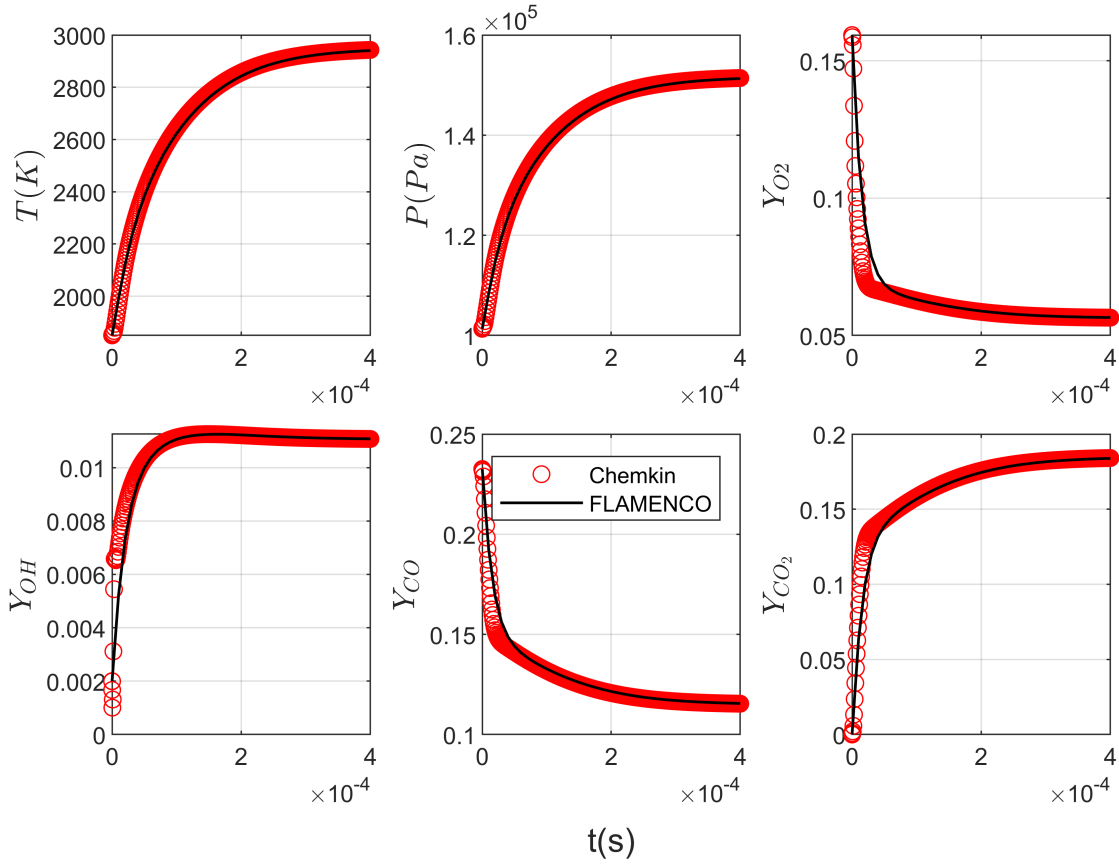


FIGURE 3.9. Comparison of a zero-dimensional case in FLAMENCO with CHEMKIN to test the implementation of the chemical mechanism and whether it leads to the right equilibrium conditions in a stoichiometric mixture.

It is important to note that combustion is a molecular phenomenon. Therefore, chemistry-flow coupling effects start at small scales, which must be resolved to encompass the underlying chemistry-flow interactions. Combining the resolution requirements of both turbulence and chemistry, Poinot [63] expressed the overall resolution requirement for reacting DNS as:

$$\Delta c \Delta x < \frac{I_{cr}}{\sqrt{Re_I Da}} \quad (3.21)$$

with Δx the grid size. I_{cr} is the most critical integral length scale from Equation 2.24 and Re_I and Da are the turbulent Reynolds number and Damkohler number, respectively, as defined earlier in Chapter 2. Δc denotes the number of grid points required to resolve a premixed flame's inner structure adequately. An explicit definition for the flame thickness of a non-premixed flame is ill-posed as the flame is spread throughout the domain rather than

locally. It is a lot more convenient to define the initial flame thickness of a non-premixed setup based on the initial conditions, which is a flamelet in the current study. The initial flame thickness is then defined as in [63], by:

$$\delta_0 = \frac{1}{|\nabla \xi|_{\xi=\xi_{st}}} = \sqrt{\frac{2D_{st}}{\chi_{st}}} \quad (3.22)$$

From Equation 3.8, at the initial condition:

$$|\nabla \xi| = \frac{1}{2} \text{sech}^2 \left(\frac{x - x_0}{2\delta_{z,0}} \right) \left(\frac{1}{2\delta_{z,0}} \right) \quad (3.23)$$

Since in all reacting cases $\xi_{st} = 0.42$ as explained earlier, the initial flame surface is close to the centre plane of the domain, hence from Equations 3.22 and 3.23, $\delta_0 \approx 4\delta_{z,0}$. Poinso [63] states that Δ_c needs to be at least 20 grid points; here, a minimum of 40 grid points span the initial flame thickness in the base case (BC-R-SS:4-8) in Table 3.1 which corresponds with the intermediate resolution in the previous convergence figures. Hence, Poinso and Hawkes's requirements for resolving the chemical scales of this chemical mechanism have been satisfied in all cases considered.

Once more, the condition in Equation 3.21 is formulated for fully turbulent cases and not well defined for developing flows. The convergence of key combustion parameters is studied to observe whether the chemical scales are well resolved throughout the flow development. Firstly, the convergence of the scalar dissipation of the mixture fraction fluctuation is assessed in Figure 3.10. No transport equation of the mixture fraction is solved; however, since the chemical mechanism employed has N_2 as a passive scalar and, therefore, undergoes pure mixing, then the mixture fraction is calculated from N_2 mass fraction in accordance with Burke-Schumann definitions [132]:

$$\xi = \frac{Y_{N_2} - Y_{N_2,o}}{Y_{N_2,f} - Y_{N_2,o}} \quad (3.24)$$

where Y_{N_2} is the mass fraction of N_2 and $Y_{N_2,f}, Y_{N_2,o}$ are the mass fractions of N_2 in the pure fuel and oxidiser streams respectively. The scalar dissipation is then computed as:

$$\tilde{\chi}' = (\widetilde{2D\nabla\xi' \cdot \nabla\xi'}) \quad (3.25)$$

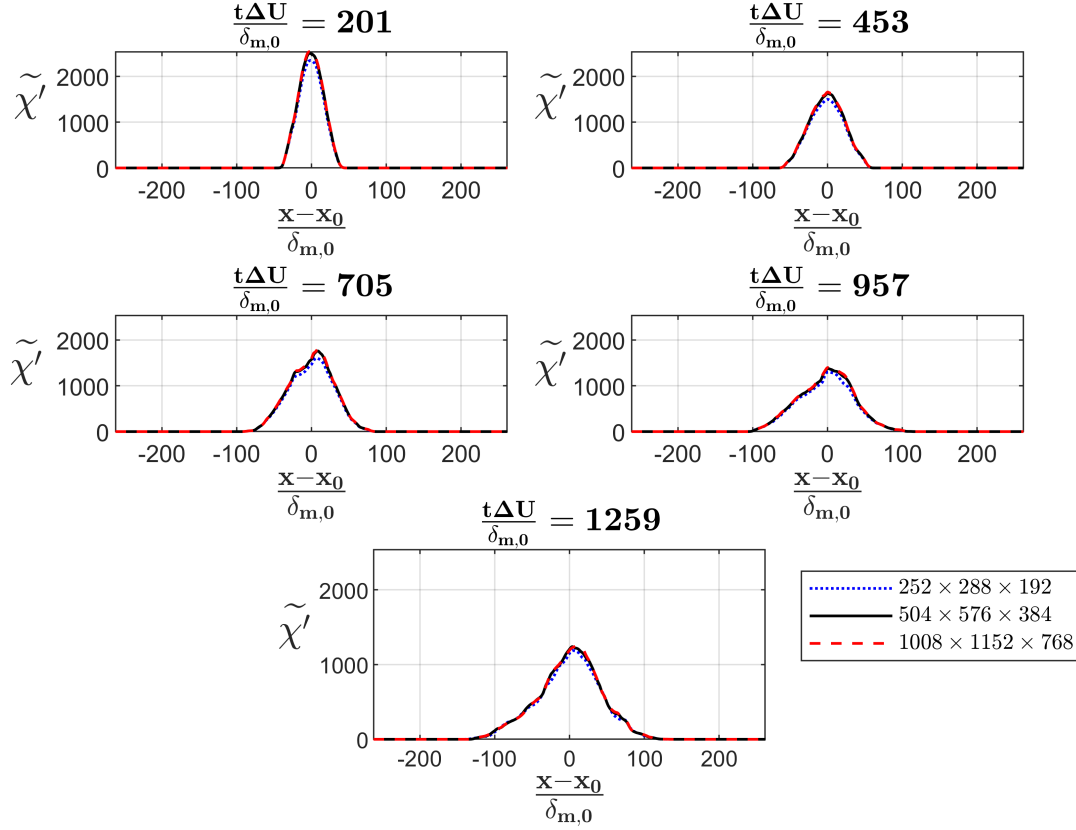


FIGURE 3.10. Mesh convergence of scalar dissipation Reynolds fluctuation across the non-dimensional heterogeneous x -direction for five normalised times and three resolutions of BC-R-SS:4-8 (the base case).

Here, D is the mixture averaged species diffusivity calculated using the mixture viscosity and the Schmidt number as explained in Section 3.2. The behaviour of the scalar dissipation convergence in Figure 3.10 is very similar to that of the kinetic energy dissipation in Figure 3.6, but that is no surprise as they are analogous quantities and are computed using the same numerics and are both converged under the resolutions considered as demonstrated in the figures.

Further convergence of the chemical scales is confirmed in Figure 3.11 by looking at the domain integrated heat release due to combustion Q :

$$Q = \int \dot{\omega}_T \partial V \quad (3.26)$$

where $\dot{\omega}_T$ is the combustion source term in the energy transport equations (Section 3.2) evaluated as:

$$\dot{\omega}_T = - \sum_{k=1}^{11} \Delta h_{f,k}^0 \dot{\omega}_k \quad (3.27)$$

with $\Delta h_{f,k}^0$ is the standard enthalpy of formation for the k th species, and $\dot{\omega}_k$ is the net rate

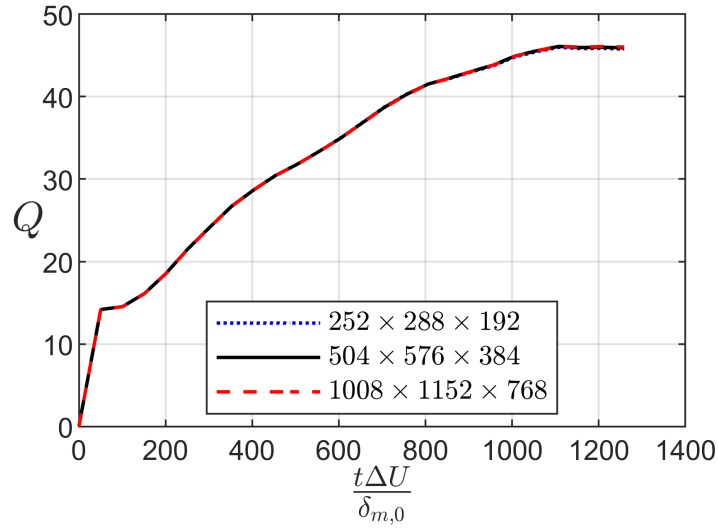


FIGURE 3.11. Mesh convergence of the total domain integrated heat release rate, Q , at three resolutions of BC-R-SS:4-8 (the base case).

of production of the k th species from all the reactions in the chemical mechanism. After a short transition period of $\frac{t\Delta U}{\delta_{m,0}} = 100$ as the flame transitions away from the initial flamelet condition as non-premixed combustion ensures and the heat release rate increases until the flow mixing reaching a stationary equilibrium state at a similar time to that observed earlier in the TKE plot in Figure 3.8. To further ascertain adequate resolution of the flame, the convergence of further reaction statistics are outlined in Figures 3.12 and 3.13. These show that both planar means and RMS, in addition to means and RMS, are conditioned on mixture fraction. The effects of these quantities are cumulative and are therefore based on adequate resolution in previous time steps. Therefore, the convergence of these quantities at a later time step confirms that the flammable regions in the flow are adequately resolved by the intermediate resolution during the development of the shear layer. The lack of observable

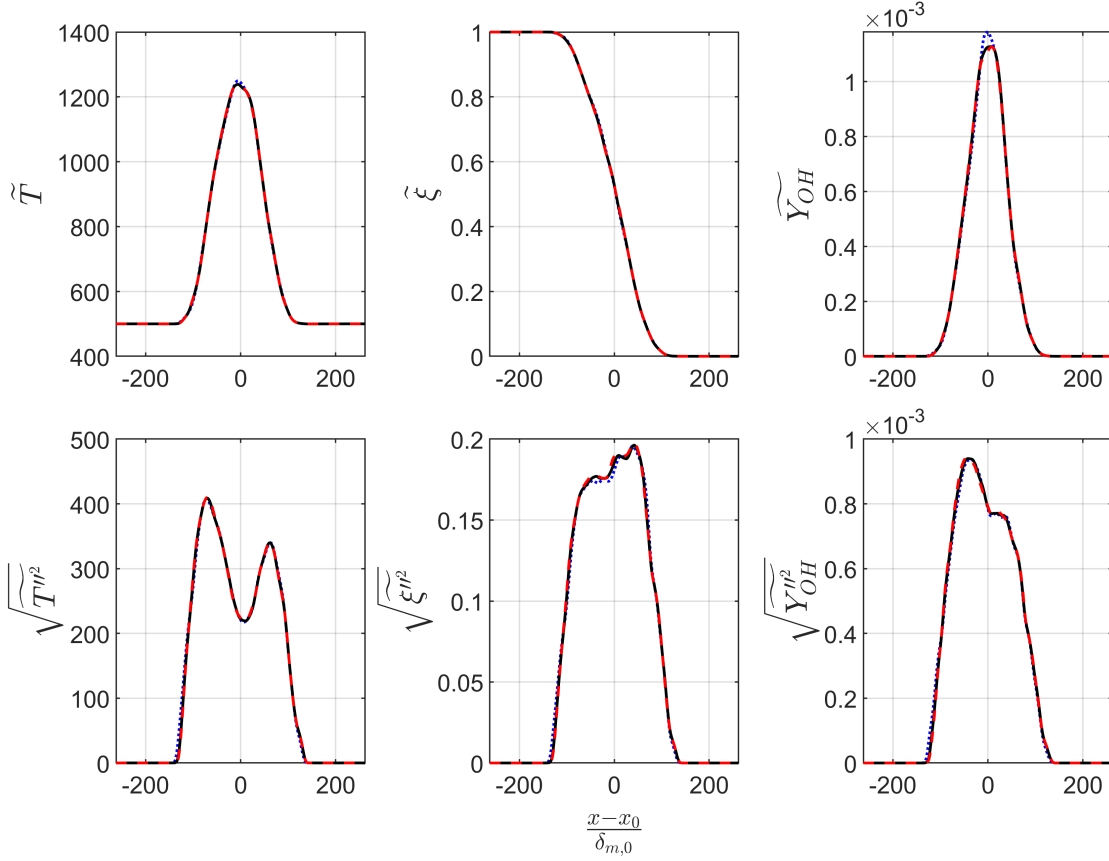


FIGURE 3.12. Mesh convergence of Favre means (top row) and RMS (bottom row) of temperature, mixture fraction, and OH mass fraction from left to right, respectively. The results shown are for the three resolutions of BC-R-SS:4-8 (the base case) at $\frac{t\Delta U}{\delta_{m,0}} = 1259$ and following the same colour schemes as in previous figures.

differences between the intermediate and fine resolution of all the quantities observed in this section confirms this result.

3.6.1.8 Spectral Convergence

Lastly, a strenuous test of convergence is by considering spectral quantities. Here, the three resolutions of the base case are assessed for their spectral convergence using a range of spectral measures. All power spectrum calculations here follow the convolution-based approach outlined in Equation 2.15 while accounting for any adjustments needed to ensure the numerical discretized approach that entails the use of Fast Fourier Transform (FFT) algorithms

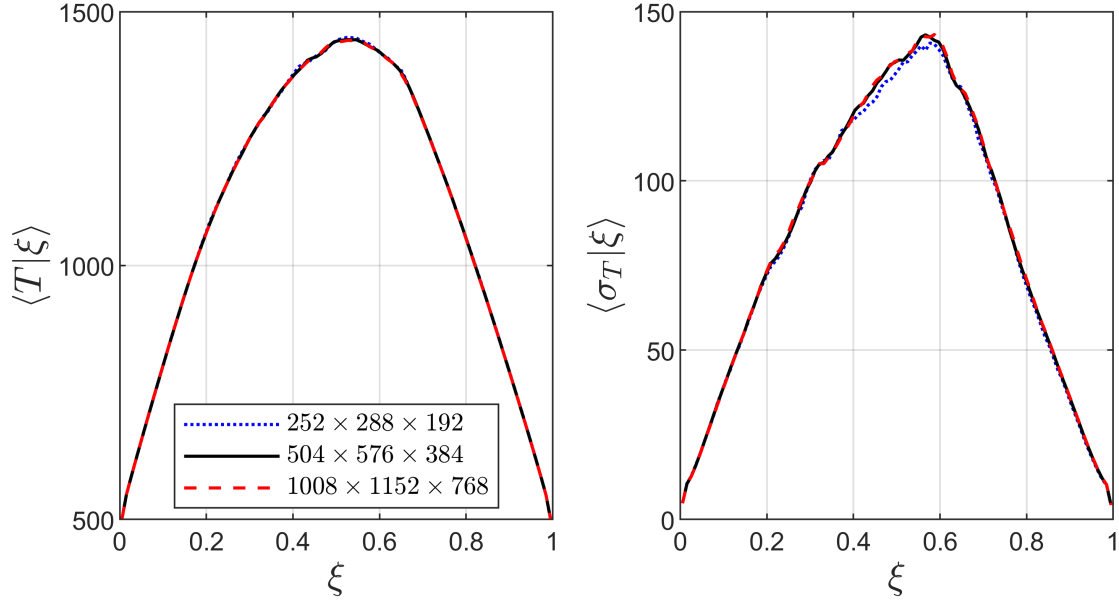


FIGURE 3.13. Mesh convergence of conditional Temperature mean (left) and RMS (right) in mixture fraction space. The results shown are for the three resolutions of BC-R-SS:4-8 (the base case) at $\frac{t\Delta U}{\delta_{m,0}} = 1259$.

continues to satisfy Parseval's theorem as explained in [133]. The most straightforward spectral quantities to compute are the one-dimensional energy spectra commonly measured and reported in turbulence experiments [2]. These are outlined in Figure 3.14.

The one-dimensional spectra for the y and z directions are computed across lines aligned with the corresponding direction in the domain centre plane in the heterogeneous x-direction which is bound by periodic boundary conditions from all four sides. The one-dimensional spectra computed within each line in the plane are then averaged across corresponding wavenumbers to reduce noise and present a more universal statistical representation. For the x-direction spectrum, the plane used is the centre plane in the streamwise y-direction with the same averaging procedure within that plane. The plots above for each resolution have the same minimum wave number based on the domain dimensions that are kept the same between the resolutions. The maximum wavenumber, however, varies between the different resolutions as it is based on the Nyquist limit that depends on the grid size, i.e. $\kappa_{min} = \frac{\pi}{\Delta x}$. This is why the finer case results run for higher wavenumber limits. Overall, the agreement between the intermediate and the fine resolution is maintained in the one-dimensional spectrum. The

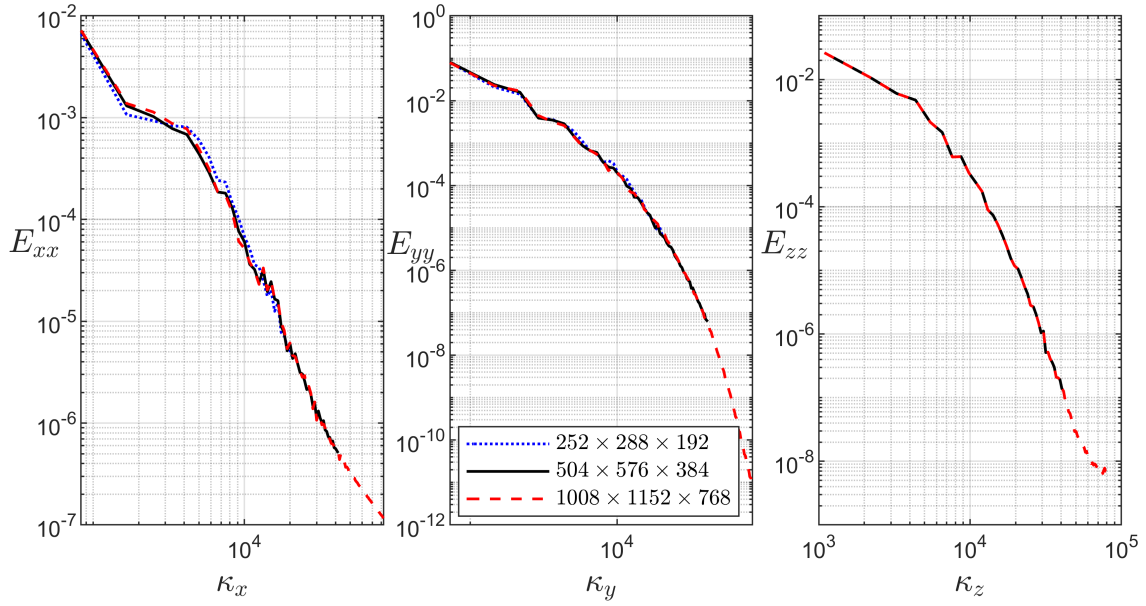


FIGURE 3.14. Mesh convergence of the one-dimensional energy spectrum in all three directions. The results shown are for the three resolutions of BC-R-SS:4-8 (the base case) at $\frac{t\Delta U}{\delta_{m,0}} = 1259$.

consistency between the resolutions is highest in the spanwise spectra, indicating minimal variations in this direction. There are some variations in the main shear flow direction, i.e. the streamwise y-direction, but the most discrepancy between the coarse and the finer two resolutions is in the cross-stream x-direction where the boundary conditions are not periodic. Further two-dimensional spectral convergence assessment was undertaken in the heterogeneous y-z domain centre plane as shown in Figure 3.15 to showcase radial energy spectrum and convergence of chemical and gradient-based spectral quantities.

The results in Figure 3.15 maintain a good alignment between the different resolutions. The largest discrepancies are observed in the entropy and scalar dissipation spectra, which is expected since these look at the spectral distribution of second-order gradients. Interestingly, the largest discrepancy is in the enstrophy power spectra on the largest scales. However, the differences are significantly reduced between the intermediate and the finest resolutions.

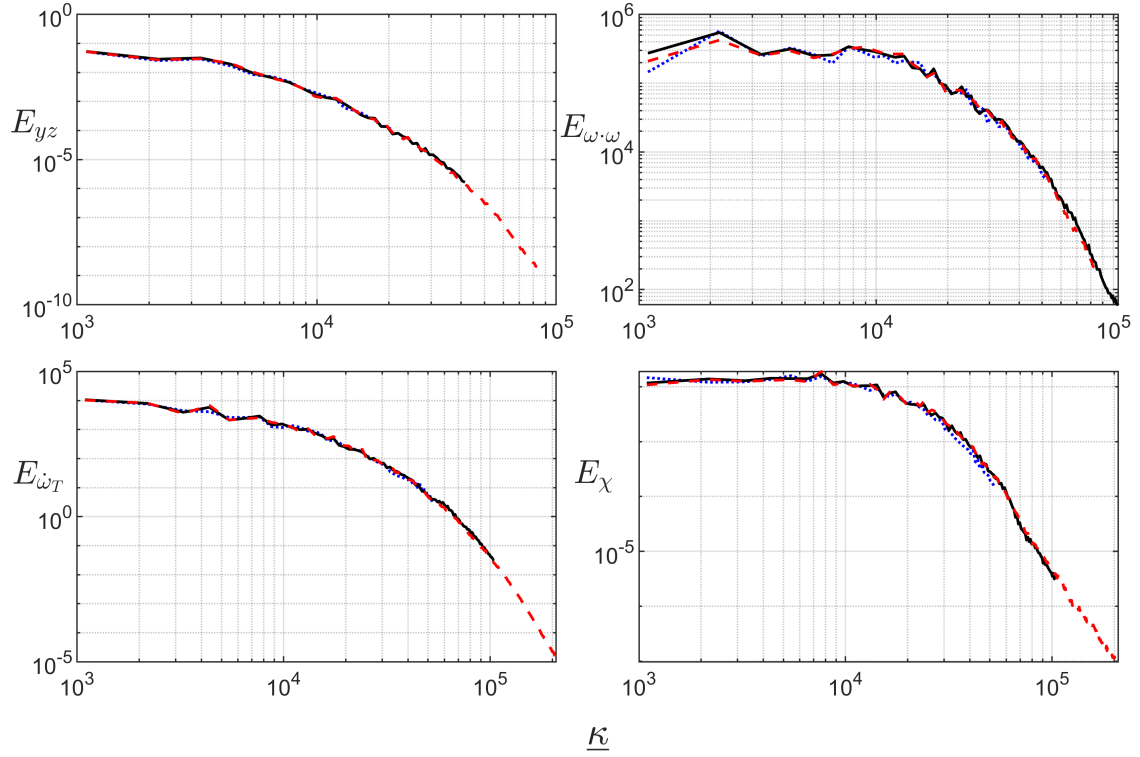


FIGURE 3.15. Mesh convergence of the two-dimensional power spectra in the centre plane of the domain: energy spectrum of the combined (radial) stream and spanwise homogeneous components (top left), the power spectrum of the heat release rate (bottom left), the power spectrum of enstrophy (top right), and the power spectrum of scalar dissipation (bottom right). The results shown are for the three resolutions of BC-R-SS:4-8 (the base case) at $\frac{t\Delta U}{\delta_{m,0}} = 1259$ and are plotted against the radial wavenumber. The same colour schemes used in previous plots in this section are used to denote the different resolutions.

3.6.1.9 Summary

Mesh convergence here is observed for the base case using three different resolutions, doubling the number of cells in all directions for each subsequent resolution. A comprehensive assessment was undertaken, considering both the flow and chemical scales and several gradients and integral-based second-order quantities. Across all measures considered, the discrepancy between the finest and intermediate resolutions is minimal and considerably smaller than those between the coarse and intermediate resolutions, even at earlier times, indicating the results have converged. Therefore, the results of the intermediate resolution were deemed sufficient and were utilised for the rest of this study. Since all the other cases

were parameter adaptations of the base case, the resolution was scaled with the narrow band range used in the initial perturbation for each case. So, for instance, doubling the wave numbers in the initial narrow band perturbation resulted in doubling the resolution (Table 3.1). The Kolmogorov length scale grows with the flow evolution, as reported in other studies [55], [129]. This growth with time is expected for reacting cases due to increased viscosity with temperature - a direct consequence of Sutherland Law. Therefore, the convergence study is completed up to a late enough time to reach the onset of self-similar evolution, covering the stringent initial times that are characterized by sharp gradients rather than just focusing on later times when the resolution requirements are less severe. Table 3.1 outlines the final grid resolution for all cases.

3.6.2 Resolution of the Other Cases and Comparison

The convergence assessment of the base case in the previous section was used to infer the required resolution of the different case setups considered in this study. However, this approach was motivated by feasibility rather than accuracy, so this section is dedicated to assessing the resolution quality of all cases considered in this study. To cover both the large and the small scales, the integral and Kolmogorov scales are both outlined for all cases in Figures 3.16 and 3.17 as they evolve with time under appropriate normalisation for ease of comparison. In both figures, since some of the cases considered vary in their initial free-stream velocities (i.e. ΔU in accordance with Table 3.1), they reach different normalised times before the simulations are stopped due to encroaching boundary effects as the shear layers grow at differing rates. To ensure good visibility in the figure, and since integral scale calculations are time-consuming, particularly for the finer cases, the results of the integral scales in Figure 3.16 are mostly presented for the reacting cases, with only the non-reacting base case included for reference to draw a comparison between the evolution trends of equivalent reacting and non-reacting cases. In this matter, the removal of chemical reactions does not appear to result in any measurable increase of either the streamwise or the spanwise integral scales and, therefore, does not especially require any extra domain size considerations. The streamwise integral scale, however, exceeds the conservative 10% limit recommended by previous studies

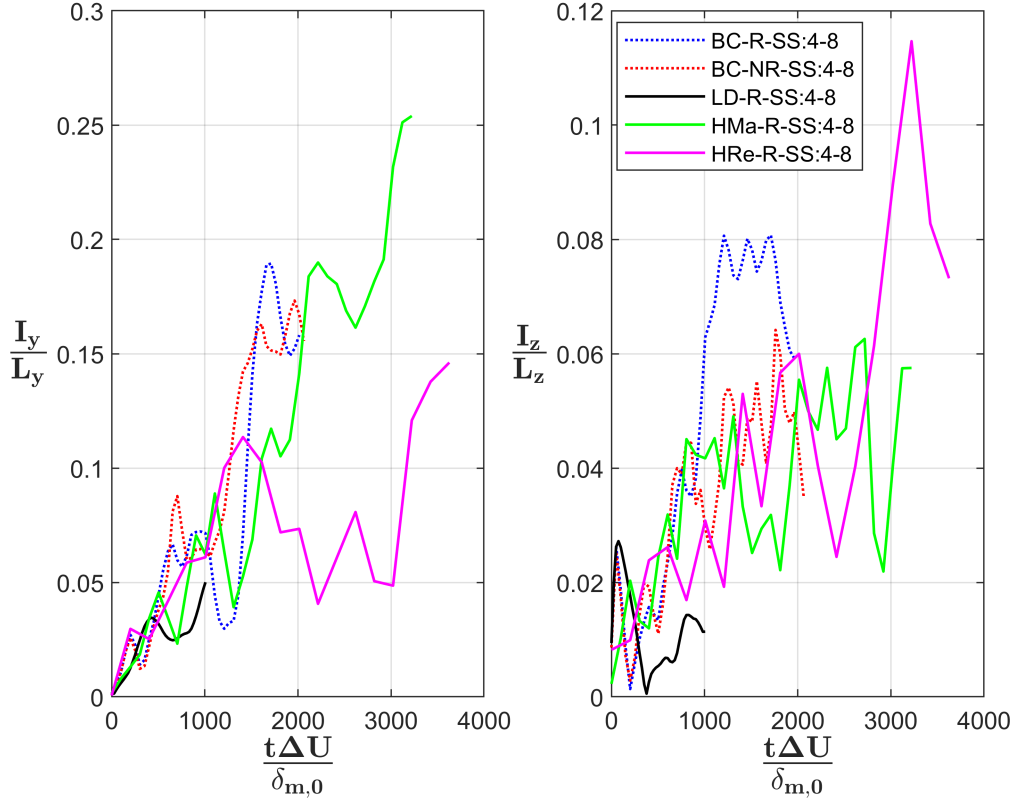


FIGURE 3.16. Comparison of the normalised integral length scales for different cases, where both stream-wise (left) and span-wise (right) integral scales are shown. Time was normalised by the free-stream velocity differences and the initial momentum thickness as commonly done to facilitate comparisons between different studies. The normalisation parameters for both the x and y axes are different between the cases and vary in accordance with Table 3.1.

for several cases past $\frac{t\Delta U}{\delta_{m,0}} = 1500$. Nevertheless, the fact that the streamwise integral scales continue to grow at high rates after crossing 10% of the streamwise domain length proves the lack of undesirable large-scale saturation. For the spanwise integral scale, only the HRe case exceeds 10% of L_z also at $\frac{t\Delta U}{\delta_{m,0}} \approx 3000$ but doesn't continue to grow as in I_y . Therefore, in this study, the 10% recommendation is relaxed to 20% of L_y for the streamwise integral length scale, which is only crossed by the HMa case at $\frac{t\Delta U}{\delta_{m,0}} \approx 3000$. For the spanwise component, the 10% recommendation of L_z is upheld and only crossed by the HRe case also at $\frac{t\Delta U}{\delta_{m,0}} \approx 3000$. Hence, the results of both the HMa and the HRe cases past at $\frac{t\Delta U}{\delta_{m,0}} = 3000$ are excluded from the analysis in this study.

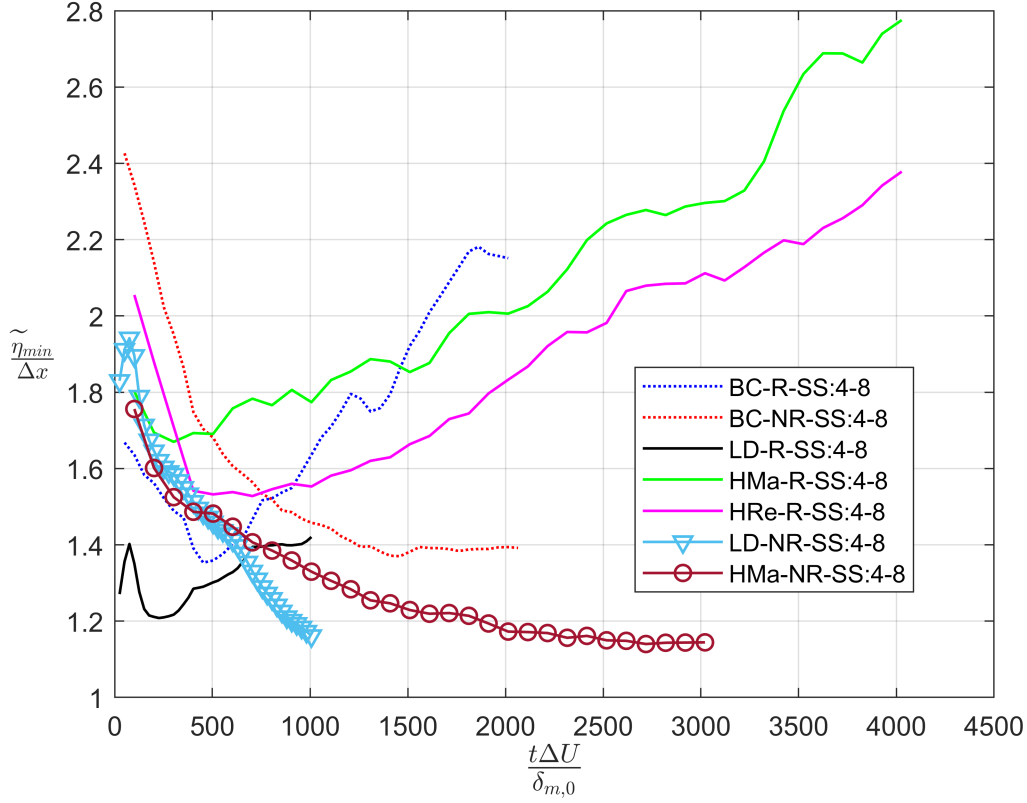


FIGURE 3.17. Comparison of the minimum planar Kolmogorov length scale for the different cases. Time was normalised by the free-stream velocity differences and the initial momentum thickness as commonly done to facilitate comparisons between different studies. The normalisation of the y-axis is with the grid size that varies between the cases in accordance with Table 3.1.

Figure 3.17 shows the Kolmogorov scale resolution for all cases analysed in this thesis. The Favre planar averaged Kolmogorov scale is calculated for each homogeneous plane as defined in Equation 3.17. This is calculated for each time. The minimum planar averaged value at each time is then normalised by the grid size and plotted for all cases. The results show that the Kolmogorov scale is always larger than the grid size at all times and for all cases considered here, confirming they are well-resolved. The trends observed in the Kolmogorov scale variations are largely due to variations in viscosity. For the reacting cases, initially, the flame experiences intermittent extinction where the temperatures fall slightly, and so does viscosity. With less viscous dissipation, smaller Kolmogorov scales are preserved, and the resolution of the smallest scales reduces, as shown. After some time, the flames strongly

re-ignite, and the temperatures increase, raising viscosity and heavily dissipating the smaller Kolmogorov scales. As a result, the resolution of the Kolmogorov scales increases at a later time in the reacting cases. The inert cases have the exact same initial setup as their reacting counterparts with the same initial temperature profiles. Due to the lack of chemical reactions, the temperatures drop, reducing the viscosity and sustaining smaller Kolmogorov scales. This continues until the flow reaches both thermal equilibrium and the flow evolution reaches a stationary stage in which the Kolmogorov scales are still well resolved by the chosen cell widths. This confirms the adequate resolution of the smaller scales in all cases considered for the purpose of the analysis presented in this study.

Flow Development and Turbulence Characterization of Inert Mixing Layers Perturbed by KHIs

4.1 Introduction

Turbulent mixing is a fundamental process that governs fluid flow behaviour in a wide range of natural and engineered systems. The complex interplay between turbulence and mixing is crucial to a myriad of applications, including energy systems that involve either combustion processes, such as in engines and gas turbines, nuclear processes, such as inertial confinement fusion, atmospheric and oceanic dynamics, or even supernovae phenomena.

The challenge of studying turbulent mixing is due to the wide range of the spatial and temporal scales involved and the coupling between the different fluid properties that affect the flow dynamics. With combustion, the complexity is exacerbated due to the interdependence of fluid dynamics, chemistry and heat transfer and the concurrent compositional and fluid property changes. Therefore, understanding the primary turbulent-inducing instabilities and their mechanisms that lead to turbulent mixing is pivotal when optimising and designing for applications where turbulent mixing is critical, such as high-speed propulsion.

Direct numerical simulations (DNS) of temporally evolving shear layers are performed to study the Kelvin-Helmholtz primary instability and its late-time attributes. While KHIs are widely considered the main mechanism by which turbulence develops in shear layers [134], [135], no work has attempted to study the effects of initialising flow fields directly with different KHIs and observing the dependence. The temporal counter-flowing shear layer configuration has been extensively adopted in literature to study shear behaviour, e.g.

[11], [37], [44]. Numerical studies of turbulent mixing focusing on initialising the flow field with a representative initial perturbation to real applications or experiments are relatively scarce. Instead, most numerical studies of turbulent mixing are more focused on the state of self-similarity in fully developed turbulence. Therefore, their choice of initial condition is usually in the form of a broadband isotropic turbulent energy spectrum to allow for the most rapid development of turbulence with little focus on transitional mixing [14], [37], [38] or elements in the seeding perturbation that affect both the evolution and the final state of mixing [51], [135]. The initial conditions commonly used are ones that conform to spectra defined to resemble that of a broadband boundary layer turbulence, commonly characterized by a decay of 4 orders of magnitude with wave number [2], [14], [31], [37].

However, there has been compelling evidence from earlier work that while initial conditions largely have their effects diluted when the flow reaches a state of fully developed turbulence, they still maintain a degree of influence on the self-similar state [134], [135] and not just at the large scales as predicted from linear stability theory but also on the smaller scales and on mixing attributes [44], [50], [51]. For instance, there have been discrepancies between experiments conducted to measure the normalised vorticity thickness in addition to other turbulent statistics in fully developed high Reynolds number mixing layers [47], [136], [137]. Dimotakis and Brown [8] attributed these differences to variable initial conditions between the studies that are only slowly forgotten as the flow tends towards a self-similar state. Furthermore, experimental observations of reacting mixing layers demonstrated a strong dependence of mixing and reactions on the initial perturbation that extended far downstream of the flow and at very high Reynolds numbers [51], [138], beyond the quoted outer thickness based threshold of full turbulence transition established by Dimotakis [9] as discussed in Chapter 2. This has spurred interest in the subject to be investigated numerically.

4.2 Review of Relevant Studies

4.2.1 Numerical Studies

The most significant early numerical studies that focused on the importance of the turbulence-generating initial conditions and the extent to which initial condition effects manifest in late-time behaviour were those of Rogers & Moser [11], [73]. These studies conducted incompressible simulations using this canonical counter-flowing shear-layer setup to study the self-similar behaviour of a non-reacting single fluid mixing layer.

Rogers & Moser completed three different popular studies on the subject. In [73] and [99], instead of initialising the flow field with a broadband turbulent spectrum as common with most numerical studies of turbulence, they initialised their flow with several low wave-number perturbations to correlate with similar experimental investigations, while maintaining a divergence-free initial flow field. These studies emphasized the three-dimensional nature of turbulence and the sensitivity of transitional mixing to low wave number perturbations by examining energy spectra and turbulent kinetic energy in addition to other turbulent statistics. Moreover, they concluded that the three-dimensionality (i.e. spanwise rollers and their pairing events/interactions) accelerates the mixing layer growth and turbulence development. These findings were consistent with the experimental work of [135] that emphasized the role of spanwise vortex pairings and tearings in establishing turbulence development.

In [11], Rogers & Moser instead initialised their incompressible counter-flowing mixing layer (splitter plate setup) with two fully turbulent boundary layers on both sides of the plate. They ran three cases in that study. The first was confined to general turbulent boundary layer initialisation, and the observed qualities were characteristic of fully developed turbulence. The other two cases involved superimposing the turbulent boundary layer initialisation with two-dimensional disturbances of varying magnitudes to observe the effect this has on the transitional structures, the mixing layer growth, and the resulting self-similar state. The logic for including these additional two-dimensional perturbations is to mimic what would occur in splitter-plate experiments where removing the plate between the counter flows or using

trip wires would induce such disturbances. This was also discussed in [139], which, although it investigates Rayleigh Taylor instability, allows for the vorticity-inducing effects of these initially small but important 2D disturbances.

Rogers & Moser's results show that including these disturbances significantly alters the statistics of the final self-similar state with notable changes in the vortical structures at late time to support these changes. It was also found that the structures exhibit a higher sense of two-dimensionality when the additional disturbances are included. Therefore, including these disturbances appeared to prolong transitional features of the mixing layer.

These structural differences meant that the two-dimensional disturbances alter the mechanisms employed in mixing the counter-flowing fluids and, therefore, have serious ramifications for non-premixed combustion and its modelling. Moreover, the higher the magnitude of the disturbance amplitude, the more significant the effect on the late-time statistics. It was also found that the degree of three-dimensionality in the self-similar state directly correlates with scalar mixing, such that the prevalence of coherent structures (more two-dimensional) is characterized by non-marching PDFs of scalars (explained in the next section) and, therefore, enhanced mixing as the prevalent large flow scales continue to entrain the free-streams into the shear layer.

Balaras [31] conducted an LES investigation on the initial condition's effects and the temporal simulation's domain size on the late-time behaviour and turbulence development. The study aimed to extend Rogers & Moser's [11] work to assess whether the domain size influences the persistent 2-dimensionality of the flow structure observed at late time. Like Rogers & Moser, Balaras initialises his simulations with two sets of initial flow conditions, with one resembling that of a turbulent boundary layer, however, obtained through pipe computations rather than through a calculation [140]. Unlike Rogers & Moser, the second set of initial conditions is a random signal rather than amplifying existing 2-D modes in the original turbulent boundary layer profile. Balaras found considerable differences in mixing layer growth rates and turbulent statistics between the temporal simulations of different initial conditions. They concluded that while the effect of the initial conditions is more prevalent in the flow-development stage and self-similarity is reached regardless of the initial conditions, the effects of the initial conditions

still manifest late in the flow evolution. This supports Rogers & Moser's view of a non-unique self-similar state, instead, an initial conditions-dependent one. This study also confirmed that the domain size of a periodic temporal simulation can hinder turbulence development. The domain size restriction results in more prominent two-dimensional flow structures rather than permitting three-dimensionality, a characteristic of established turbulence. In particular, the span-wise domain size seemed to have the greatest effect on prohibiting three-dimensional flow development. The study also found that when considering the early stages of the flow, the choice of a random noise initial condition flattens the energy spectrum of the seeding perturbation and empowers Kelvin-Helmholtz instabilities to exponentially expand the mixing layer thickness and rapidly establish rib vortices. Meanwhile, with turbulent initial conditions, the resilience of the longer wavelengths impedes the growth of the smaller unstable modes, which delays the formation of coherent structures and weakens the significance of subsequent pairings. The study, however, does not consider the influence of the number of pairing events on the achieved self-similar states, which has been popularly conjectured in many previous studies [11], [32], [50], [135], to be a primary factor for full turbulence development.

However, Balaras [31] provides no clear distinction on whether the differences in the self-similar states observed between the small and large domain results are exclusively due to the limitations of the span-wise dimension as claimed or due to the limitations of the stream-wise dimension, which can implicitly affect the wavelength of the most unstable mode in the random noise flow initialisation and hence the number of pairing events. The study includes cases where the domain sizes are only increased in the spanwise directions. Still, the contours and results of these are not presented alongside those for the full domain increase (both streamwise and spanwise extensions) for comparison. Therefore, while Balaras [31] and Rogers & Moser's work highlighted the combined influence of a range of flow initialisation parameters on the three-dimensionality and flow development, these parameters were not considered in isolation to ascertain their individual effects.

Fathali et al. [97] investigated the isolated effects of a range of initial perturbation parameters on the mixing layer flow development. The parameters investigated included the integral length scales and initial spectrum profiles. The study showed that varying these parameters

individually can significantly affect the mixing layer growth rate at early times. The study also stressed the significance of enforcing a divergent free initial velocity field as the initial compressibility effects can prolong the transitional flow development, which has important ramifications for mixing and combustion. It was not outlined by Balaras whether divergence-free initial conditions were enforced, and as demonstrated by Fathali [97] in most studies, the initial velocity field is not directly divergence-free and therefore does not comply with the kinematic condition imposed by the incompressible continuity requirement.

Moreover, while Fathali's investigation provided key insights into some of the parameters affecting transition, the considered parameters are more holistic. They can not be directly attributed to particular elements of the KHIs. Fathali did, however, run a single KHI-induced case, which was initialised using a somewhat similar method to the one adopted in this study. The single case was used for comparison with the other cases, and the paper demonstrated clear KH rollers generated from the KHI-initialised, which had the most rapid mixing layer growth rate compared with all the other cases. Overall, this was another study that showcased the implications of the seeding perturbation on the final self-similar state.

4.2.2 Experimental Studies

Even when considering experimental investigations, the results reaffirm the significance of the initial perturbation on both the flow and mixing evolution and their self-similar state. Oster and Wygnanski [134] studied the large-scale evolution of experimental shear layers with and without forcing. Unforced shear layers are when no perturbation is added to the mean flow, and the shear layer develops based on the initial momentum thickness length scale. On the other hand, the forcing was set up by having a thin flap at the trailing edge of the splitter plate (that separates the two free streams) oscillating at different frequencies. The study reported a clear influence of small amplitude forcing oscillations on the large-scale flow evolution, such as on shear layer spreading rate, momentum thickness, and Reynolds stresses, even at large downstream distances and outer-scale Reynolds number within the order of the transition threshold. The study concluded with the bold statement that mixing layers do not achieve fully developed turbulence due to their retained memory of initial conditions that prevent

a universal evolution of the turbulent scales. This is, however, not entirely accurate, as the universality of turbulence is not at the large scales but in the intermediate to small scales that weren't investigated in that study.

Another interesting finding of this study was the "resonant" effect observed in persistent two-dimensional coherent structures that stabilise (instead of pairing or interacting and breaking down) by feeding on the existing developing turbulence and, in time, reducing it, therefore promoting a perpetual state of transition- exactly consistent with the findings of Roger and Moser temporal simulations when high amplitude two-dimensional velocity perturbations were superimposed on initially turbulent boundary layer interface at the shear layer. In both cases, there is enough evidence to suggest that the forcing frequency of the seeding perturbation is the same (or a harmonic) as that of the most unstable modes in the unforced equivalent shear layer, which leads to resonance. In Oster and Wygnanski, the most unstable mode was related to the initial momentum thickness by spectral analysis of the unforced layer and confirmed by linear theory. In Rogers and Moser, the superimposed two-dimensional velocity perturbations were directly set at the same frequency of the seeding perturbations used to generate the original initial turbulent boundary layer formulated in [140]. This raises a very important implication. Although the boundary layer has already established its full turbulence conforming with the asymptotic state theory (energy cascade, scale separation..etc.), it still somehow retains information about its seeding instability scrambled through its flow information that, when subjected to an additional perturbation of a similar frequency it remembers and resonates, breaking away from the asymptotic state of developed turbulence.

The results of Oster and Wygnanski were commented on by Pope in [2] as divergent from classical turbulent theory and testament to turbulence not being a local state but instead one with a long memory. More importantly, the results of both these investigations showcase a lack of turbulence development at Reynolds numbers at or above the transition threshold, which breaks the popular notion that turbulence increases with Reynolds numbers up to the threshold where independence ensues, and universal turbulent behaviour is observed (Chapter 2 and Figure 2.4). This casts doubt on the simple use of the Reynolds number to judge the level of turbulence or equate the turbulence between different flows developed

from different perturbations and confirms the doubts and speculations raised by Hussain [141] in his comprehensive review of turbulence and coherent structures in 1983. So how exactly is turbulence dependent on Reynolds number if it is not a direct dependence as conventionally believed? Firstly, these studies only considered outer-scale Reynolds numbers and have not disclosed or observed trends in other smaller-scale Reynolds numbers. Secondly, these results do not necessarily imply a lack of dependence altogether but suggest that other seeding perturbation elements also influence. The present study assesses a range of different Reynolds numbers across both turbulence and mixing analysis. The Reynolds numbers are explored as dependent rather than independent parameters across the different case setups. The interdependency between different Reynolds numbers and vortex pairing events is also explored.

Huang and Ho [135] experimental investigation took a much more precise take on assessing the dependence of the seeding instability on turbulence development by assessing the behaviour of the small scales, where the similarity hypotheses are proposed to apply, and investigating a potential mechanism by which transition occurs. They induced fluctuations in the shear layer by acoustic perturbations from loudspeakers at varying frequencies. Their results reaffirm the important role of three-dimensional vortex pairings (of both the spanwise and streamwise structures) as a mechanism of dispersing the large flow scale energy into subsequent intermediate and smaller scales that eventually constitute the energy cascade with a universal equilibrium range ($-5/3$ power law scaling). By monitoring the wavelengths of vortices in the streamwise and spanwise directions, they observed that at least two major vortex pairing events of spanwise structures are necessary for the intermediate to small scales to approach $-5/3$ spectral power scaling and conform to the hypothesized universal behaviour.

This study is also the first to define and correlate a non-dimensional downstream distance with vortex pairing events and, therefore, relate the observed behaviour of the large flow structures to the scale separation process. The normalised downstream distance was defined as a pairing parameter:

$$P = \frac{Rx}{\lambda_0} \quad (4.1)$$

with $R = (1 - r)/(1 + r)$, where r is the freestream velocity ratio since it was a coflowing experiment, x the downstream distance, and λ_0 the initial wavelength of the seeding perturbation. They found that $P = 16$ corresponds to three vortex pairing events and $P = 8$ corresponds to two. It is important to note that although the experiments conducted spanned a wide range of Reynolds numbers, they were all above the transition threshold, so the results do not dispel the Reynolds number independence of classical turbulence theory; just impose an additional requirement of adequate three-dimensional vortex interactions for the universality of the equilibrium range to be realised and stipulate a downstream distance requirement for that to occur.

Building upon this were the experiments of Karasso and Mungal [50] and Slessor et al. [51], who also realised that the turbulence transition is a small-scale phenomenon and focused on that by studying the effects of different perturbation on mixing and chemical reactions that directly correlate with these small scales. These studies were devoted to tracking the mixing transition rather than the turbulence transition. While the two are related, it is important to appreciate that mixing results from flow scale evolution. So, a fully developed mixing state would manifest after turbulence development. Karasso and Mungal assessed the mixing transition, similar to Rogers and Moser [11] by observing the behaviour of scalar PDFs and whether it conforms to marching vs non-marching behaviour. These categorizations are based on whether the most probable scalar mixtures vary with cross-stream (vertical) distance across the shear layer. Non-marching is when the mixing is thorough and characterized by PDFs that stagnate about a constant profile peak- usually close to an intermediate value, e.g. a mixture fraction of 0.5. Marching is when the PDF profile peaks monotonically march with transverse distance, starting from an intermediate value at the centre of the shear layer and either monotonically increasing or decreasing with transverse distance towards the free streams (depending on the scalar value in the free streams). This should not be confused with bi-modal vs uni-modal distributions that consider the entire domain PDF in scalar space rather than depicting the change in scalar PDF distribution across different transverse planes.

Focusing on the effect of the initial conditions, Karasso and Mungal observed that the mixing transition requires initial flow conditions that permit the flow to reach at least $P = 22$ - slightly

larger than the value for small-scale turbulence transition of $P = 16$ reported by Huang and Ho [135]. The results of Karasso and Mungal stress that while two pairing events begin the mixing transition (consistent with Huang and Ho), a minimum of three pairing events are required to realise a fully developed mixing transition. However, the outer-scale Reynolds number of the experiments that attain developed mixing transition in Karasso and Mungal's work is 3-6 times larger than the transition value of Dimotakis [9]. So, while the authors focused on the pairing parameter, P , requirement, it is important to realise that increasing the stream velocities (which allowed higher P values to be achieved in the confines of the experimental apparatus) also increased the Reynolds number.

The studies, however, do not agree on whether the mixing transition after turbulence development constitutes marching or non-marching behaviour. Karasso and Mungal [50] maintain that the mixing transition pertains to marching behaviour, agreeing to an extent with the simulation results of Rogers and Moser [11] and Sharan et al. [44], yet disagreeing with the degree of marching observed and reducing this to a lesser "tilted" depiction. On the other hand, the experimental studies of Konrad [45], Koochesfahani and Dimotakis [49], and Mungal and Dimotakis [46], all found non-marching behaviour at late times of mixing layers with Reynolds number at or past the transition threshold. The significance of marching/non-marching PDF behaviour and how it affects the mixing state are explored in Chapter 5.

Non-marching occurs due to the prevalence and persistence of large-scale coherent eddies that continuously feed parcels of free-stream fluid into the shear layer, whereas marching is when no such coherent structures persist. The prevalence is instead of smaller eddies that improve molecular mixing but also mostly have local effects and result in the mixing with the free streams restricted to the periphery of the shear layer. Consequently, Slessor et al. [51] results that observe dominant two-dimensional behaviour far downstream into a "self-similar" region contradict the expected formation of a marching behaviour at developed turbulence (based off a high Reynolds number characterization). The study also does not consider the significance of downstream P value which could have been used to assess where mixing development is attained. However, they continue to attest to the importance of the seeding perturbation in controlling the mixing state despite reaching Reynolds numbers an order of magnitude

higher than the established threshold! A possible explanation for this is that experimental setup unintentionally produced the resonance behaviour reported by Oster and Wygnanski [134], Rogers and Moser [11], and Hussain [141] as their flow is directed through a turbulence generating honeycomb mesh before the wire tripping which is not the case with the other experimental works.

4.2.3 Effects of Perturbation Wavelength

The effects of the initial wavelength range on the development of turbulence have been indirectly studied previously. For instance, Vreman et al. in [32] thoroughly compared dynamic and non-dynamic subgrid models for the turbulent stress tensor using incompressible large-eddy simulations. In that study, they built up on Rogers & Moser's focus on vortex pairing events as the transition-inducing phenomena in mixing layers by realising that a state of self-similarity is only achieved in their LES if at least three pairing events occur. This finding has indirect implications on the wavelength of the seeding perturbation as that dictates, particularly for temporal simulations, that the most unstable mode of the perturbation should not have a wavelength greater than 1/8th of the streamwise domain dimension if fully developed turbulence is to be achieved. More recently, Baltzer [37] used this finding when setting up incompressible temporal simulations to investigate variable density effects in shear flows. In that study, they ensured the initial perturbation was seeded by 64 wavelengths of the most unstable mode in all their simulations, indicating six different vortex pairing events, i.e. double the number of pairing events suggested by Vreman [32]. This ensured a quick transition to turbulence and clear self-similarity, as demonstrated by their results. Almagro et al. [55] stressed the importance of running different realisations of the same initial conditions used by Pantano [14] for each of the density ratio cases investigated in their study. This was important as they found that small variations of the initial conditions (while still about the same overall spectral profile) affect the turbulent structures and statistics observed, and the effect of that needed to be considered when conducting parameter studies.

Note that in the current setup of this work, a deterministic algorithm is used to generate the initial perturbation, which guarantees repeatability. In the work of Almagro [55] and

Pantano [14] this was not the case and is why they included multiple realisations of the initial condition in their analyses. There is still the case that initialising the perturbation seeded from a range of different random seeds would lead to some variation that could be averaged to focus conclusions and findings, but since it is possible to keep the random seed constant between the cases, the computational resources are best dedicated to investigating the predefined parameter space relating to the KHI eigenvalue.

Recently, the LES work of Sharan et al. [44] studied the effects of different perturbation wavelengths on large-scale evolution and the mixing behaviour using temporal simulations. Their large-scale results agree with Oster and Wygnanski's experiments and trends, and their scalar PDF behaviour exhibits clear marching behaviour after adequate time (the equivalent of downstream distance in temporal simulations). The study concludes that the streamwise wavelength of the seeding perturbation plays an important role in controlling the mixing evolution at both the large and small scales, whereas the spanwise perturbation wavelength is less important. However, the study has some contradictions. It maintains that the mixing PDF transition is insensitive to Reynolds number and P while still quoting a similarly formulated normalised time $tk_0\Delta U$ of 50, after which marching behaviour is observed, where k_0 is the initial streamwise perturbation wavenumber. Also, this formulation is a bit misleading when compared with the definition of the pairing parameter, P , quoted by earlier studies, as it implies a further downstream distance for the mixing transition. Instead, if k_0 is converted to an equivalent wavelength, λ_0 , i.e. $tk_0\Delta U = \frac{t2\pi\Delta U}{\lambda_0} = 50$. Revisiting the pairing parameter P defined earlier for coflowing spatially developing shear layers, and alternate definition needs to be set for temporally developing shear layers in [44]. In a temporal setup with equal free-stream counterflows, the simulation time could be normalised by the initial instability timescale $\frac{\lambda_0}{\Delta U}$, yielding an equivalent pairing parameter of $\frac{t\Delta U}{\lambda_0}$. Taking this into consideration, Sharan et al. results imply a downstream distance of $\frac{50}{2\pi} \approx 8$, which corresponds to two pairing events rather than three as outlined by Huang and Ho [135].

4.2.4 Takeaways and Present Study Focus

As explained in the previous sections, several works in literature surmise that it is the number of pairing events along with the Reynolds number that strictly determines whether a mixing layer attains a state of developed turbulence [11], [32], [135], [138], [142]. But does that mean the Reynolds number is not important to achieve transition? These pairing events are directly a consequence of the seeding perturbation wavelengths and their dimensions relative to the domain size, and no study carefully assessed how variations of these initial perturbations affect the evolution of the different flow scales' development, turbulence, and mixing (as separate aspects). Furthermore, how would these variations in the seeding perturbations simultaneously affect the evolution of the Reynolds number? As explained in Chapter 2, there are different ways to define a Reynolds number, and it is unclear whether all the different definitions are affected in the same way. For instance, linear theory predicts more rapid growth with time of the larger scales by larger seeding wavenumber (small wavelength) perturbations (as confirmed by experiments [134] and simulations [44]), but this does not necessarily extend to the intermediate (inertial range) or smaller flow scales.

It is clear from this review that there is some confusion surrounding the topic. While most studies agree that the effects of the initial perturbation manifest during the transitional development and extend to developed turbulence and mixing, they differ on the extent, the parametric dependencies, and the role and importance of Reynolds numbers. This is because most of the studies only focused on an isolated element of the process and, as a result, produced a partial account. Studies that focused on the large scales and turbulence did not study the smaller scales. Studies examining the transition mechanism through vortex pairings did not explore or track the effects of Reynolds numbers. Studies that explored mixing and chemical reactions either mainly focused on the role of the pairing parameter and downstream distance on the development without reporting on the Reynolds number evolution or have not considered possible effects of resonance and pairing events that may have prevented transition; instead, they focused on achieving a high Reynolds number. For instance, while providing notable contributions, Karasso and Mungal, did not test for conditions of resonance after their flows were observed to fully develop to test if the seeding perturbation information

(beyond the free stream velocities and densities) was truly forgotten as claimed, nor did they investigate more extensive mixing measures like flame structures or conditional PDFs of reactive species to explore discrepancies in mixing from experiments with the same free stream velocities and densities. Furthermore, it is not always possible to explore a parameter space or provide an extensive analysis from experimental investigations compared to numerical ones, particularly when you can artificially control the setup to focus on certain aspects in simulations and accumulate vast stores of flow and chemical data that can be carefully analysed in post-processing.

It is important to draw a further distinction here, as these studies did not explicitly clarify that a self-similar or stationary evolution of statistics towards a later time is not synonymous with fully developed turbulence or mixing. Developed turbulence is characterized by scale separation as explained in Chapter 2, whereas a self-similar final state could be reflective of a stationary equilibrium corresponding to an unfulfilled turbulence transition, which depends on the setup and flow conditions that extend from the seeding perturbations.

The DNS cases outlined in the previous chapter and analysed here aim to explore these physics and address some of the gaps in the literature on understanding the turbulence transition and the correlation with mixing at its different scales, therefore providing a more complete picture. Resonance effects are not explored here, nor are they expected to manifest undesirably (as they did in some of the experimental investigations discussed above) in the results as, by design, the simulations considered do not involve high amplitude two-dimensional perturbations superimposed on an already turbulent flow.

In this chapter, the analysis is restricted to the inert cases, focusing on the flow scales and turbulence. In the next chapter (Chapter 5), the focus is shifted to reacting cases, with the mixing properties and transition analysed. Lastly, the wider extent of the effect of the seeding perturbation on mixing is explored in the final results chapter (Chapter 6) in a more extensive framework than explored in any previous study by considering the evolution of the flame structures in the reacting cases and characterizing their combustion regimes throughout the developing flows.

The present study explores two main parametric variations of the seeding perturbation's eigenvalue: variations in ΔU and variations in the perturbation bandwidth of wavelengths. The latter explores the effect of changing the wavelength ranges of the seeding perturbations (relative to the domain dimensions). Reynolds number is not directly explored as a parametric variation; however, it is tracked in the subsequent analyses and discussions as a dependent variable that varies through the flow development, which was not considered in prior work. Comparisons are then drawn between the developing turbulent statistics and the Reynolds number evolution to assess the previous claims on transition made in the literature.

Case	ΔU	$\frac{\kappa_{min}}{\kappa_0} \leq \underline{n} \leq \frac{\kappa_{max}}{\kappa_0}$	$\frac{L_x}{\delta_{m,0}} \times \frac{L_y}{\delta_{m,0}} \times \frac{L_z}{\delta_{m,0}}$	$N_x \times N_y \times N_z$
LD-NR-SS:4-8	72.5	$4 \leq \underline{n} \leq 8$	$699 \times 1200 \times 800$	$504 \times 864 \times 576$
BC-NR-SS:4-8	145	$4 \leq \underline{n} \leq 8$	$524.2 \times 600 \times 400$	$756 \times 864 \times 576$
HMa-NR-SS:8-16	290	$8 \leq \underline{n} \leq 16$	$524.2 \times 600 \times 400$	$1008 \times 1152 \times 768$

TABLE 4.1. Simulation list and parameters.

The cases studied in this chapter are LD-NR-SS:4-8, BC-NR-SS:4-8, and HMa-NR-SS:8-16 and are summarised in Table 4.1. For easier reference in forthcoming discussions of this chapter, these are referred to as the LD, BC, and HMa cases, as they are all inert. The free-stream velocities are doubled (while ensuring low-Mach conditions), and the absolute wavelength magnitudes in the initial perturbation bandwidth are halved between each subsequent case considered here. The rationale was to keep a constant initial outer-scale Reynolds number between the cases analyzed. Therefore, although LD-NR-SS:4-8 and BC-NR-SS:4-8 have the same normalised wavenumber range, the normalisation is with the domain size, and hence, LD has double the absolute wavelength magnitudes relative to BC. The following sections of this chapter focus on the different flow and turbulence scales to provide a more complete account of the turbulence and flow development and its relation with the seeding perturbation parameters investigated.

4.3 Large Scale Evolution

4.3.1 Contour Visualisation

Figure 4.1 shows the isocontours of the mixture fraction at the latest simulation time for each of the cases analysed in this chapter. While the cases are expected to develop at different rates, inspecting the latest run time should give a preliminary measure of the final turbulent state for each of the cases and help guide subsequent analyses. The axes' dimensions are normalised by the initial momentum thickness (a fixed reference for all cases), and the transverse extent displayed is up to the iso-contour limits (of 0.01 and 0.99) rather than the full domain extent to focus directly on the mixing layer. The choice of using the mixture fraction for this visualisation is to display the three-dimensional turbulent structures. It is also similar to how flow visualizations are conducted in experiments, for instance, by observing dye dispersion due to turbulent mixing.

The three cases above exhibit very different turbulence levels at their latest absolute simulation time, corresponding to similar values in seconds. This highlights different rates of turbulence development between the cases. All three cases exhibit three-dimensional chaotic structures characteristic of turbulence. However, the LD case maintains more coherent structures than the other two cases. The HMA case exhibits the highest level of turbulence, followed by the BC case. While still highly chaotic and three-dimensional, the contours of the BC case in Figure 4.1 indicate some incursion of irrotational free-stream around the $\frac{y}{\delta_{m,0}} = -100$ plane from the lower fuel side which thins the mixing layer at that location and indicates either a potentially persistent large-scale coherent eddy or a deficiency of a range of small-scale eddies around this region even this late in the flow evolution, which holds back further turbulence progression.

4.3.2 Thickness Definitions

The momentum thickness is a conventional measure of free shear layer thickness. It is defined as the thickness the free stream must occupy to compensate for the momentum loss from the

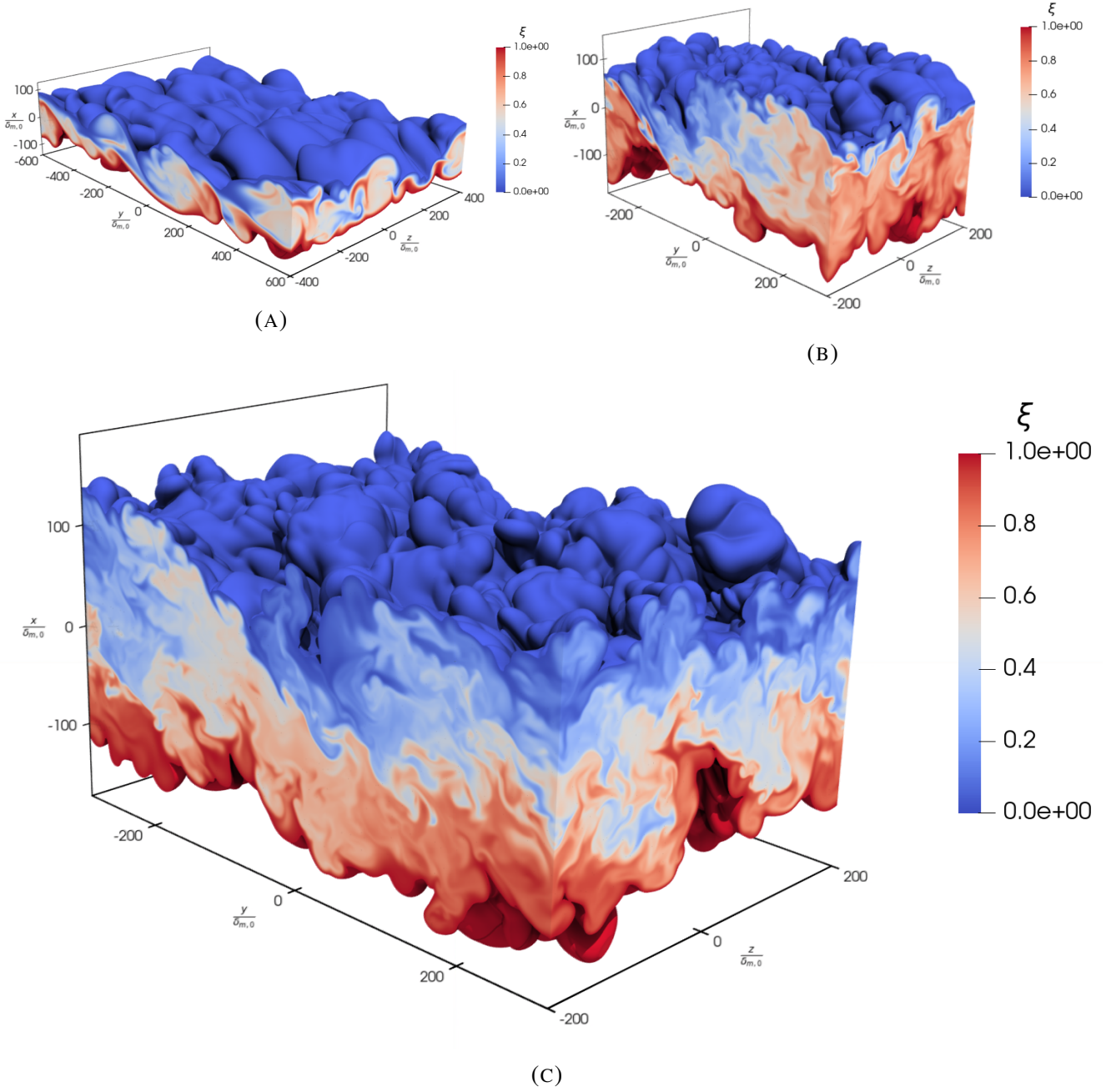


FIGURE 4.1. Isosurfaces of mixture fraction with a cutoff at $\xi = 0.01$ and $\xi = 0.99$ at the latest runtime for each of the cases: LD (A), BC (B), and HMA (C).

total shear viscous dissipation. Based on this, it is expected to increase over time as the viscous dissipation accumulates and drains the free-stream momentum. To maintain continuity, the decelerated fluid layers closest to the shear interface between the two free streams are made to rotate and form vortices that grow with the shear layer. Therefore, momentum thickness

can provide a good measure of the average large vortices diameters throughout the shear layer. The original formulation of the momentum thickness is for boundary layers, but for a shear layer, it simplifies to:

$$\begin{aligned}\delta_m &= \frac{1}{\Delta U^2} \int_{-\infty}^{\infty} \left(\overline{U}_2(x, t) - \left(-\frac{\Delta U}{2} \right) \right) \left(\frac{\Delta U}{2} - \overline{U}_2(x, t) \right) dx \\ &= \int_{-\infty}^{\infty} \left(\frac{1}{4} - \frac{\overline{U}_2^2}{\Delta U^2} \right) dx\end{aligned}\tag{4.2}$$

It is also possible to incorporate density in the definition so that the momentum thickness reflects actual total momentum and considers density variations in the stream. This is particularly useful when drawing comparisons between cases of variable density profiles. However, the cases considered in this study only vary in their initial perturbation and domain size and not in the composition of their free streams, so only the definition of Equation 4.2 is considered here. Using Equation 3.6, which represents the initial mean streamwise velocity, and substituting in the above equation, it can be shown that the initial momentum thickness is indeed half the hyperbolic tangent profile thickness in Equation 3.6 showing consistency with the mean velocity profile definition.

The vorticity thickness is a more direct measure of capturing the thickness of the vortices within the mixing layer. This is conventionally defined using the steepest gradient of the mean streamwise velocity in the cross-stream direction:

$$\delta_\omega = \frac{\Delta U}{\max \left(\left| \frac{d\overline{U}_2}{dx} \right| \right)}\tag{4.3}$$

Such a definition can lead to spurious thickness representation. It can be misleading as it is restricted to limited flow regions (where the gradients are steepest) and, therefore, omits consideration of flow regions where asymmetries are prevalent. Nevertheless, it is still used to provide valuable insights and is commonly used in both experiments and simulations for Reynolds number calculations and to characterize turbulence (e.g. [37], [55]). To improve the smoothness of the vorticity thickness profile, it is possible to include an integration similar to

that in the momentum thickness definition as formulated in [108]:

$$\delta_{\omega_I} = \frac{\int_{-\infty}^{\infty} \left| \frac{d\bar{U}_2}{dx} \right| dx}{\max \left(\left| \frac{d\bar{U}_2}{dx} \right| \right)} \quad (4.4)$$

A third possible measure of mixing layer width that considers the large-scale motions is a threshold distance defined as the transverse thickness in which the main flow velocity stays within a certain threshold relative to the free streams. A common threshold limit for this thickness definition is 90% of the free-stream velocities ([2], [37], [143]), i.e. within 10% variation from the free-streams, and since the free-streams (U_+ and U_-) are each $0.5\Delta U$, then the limits are $U_+ - 0.1\Delta U$ and $U_- + 0.1\Delta U$, hence:

$$\delta_h = \left| x_{\widetilde{U}_y = -0.4\Delta U} - x_{\widetilde{U}_y = 0.4\Delta U} \right| \quad (4.5)$$

The choice of 10% variation from the free streams is more common than smaller thresholds (like 1%) as it provides a smoother measure of the mixing layer at a sufficient distance away from the interface of the shear layer eddies with the free streams. This interface would sporadically vary across the length of the shear layer and as it develops due to the non-linear vortex interactions and turbulence growth.

4.3.3 Thickness Growth

Figure 4.2 shows the evolution of the flow thickness measures in absolute time. The behaviour observed is as expected from linear theory (refer to Equation 2.40), where the cases with higher wavenumber and free-stream mean velocities grow quicker in time. The same observation extends across all three flow thickness measures, confirming the trend with the seeding perturbation variations.

To derive meaningful insights and compare against experimental work, the statistics need to be observed against downstream distance since this is more physically representative of how the flows would naturally evolve. This is also important for assessing self-similarity in relation to the flow dependence on the seeding perturbation attributes explored. To this purpose, it is

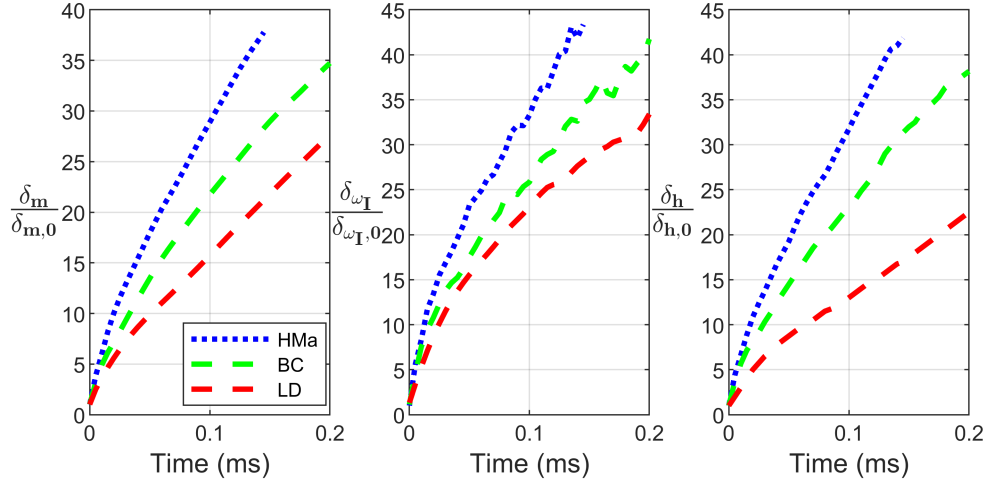


FIGURE 4.2. Flow-based thickness measures and their growth in absolute time: momentum thickness (left), vorticity thickness (middle), and streamwise velocity 10% threshold thickness (right). The y-axes are each normalised by the initial values of the respective thickness measure. The legend entries are shorthand versions such that HMa=HMa-NR-SS:8-16, BC=BC-NR-SS:4-8, and LD=LD-NR-SS:4-8. The full details of these cases are enclosed in Table 3.1.

common to normalise time and observe statistics under a Strouhal number-like normalisation that considers attributes of the initial perturbation frequency. The use of such normalisation was first realised by Vincenc Strouhal in 1878, who defined the Strouhal number to be:

$$St = \frac{fL}{U} \quad (4.6)$$

while observing trends vortex shedding evolution produced by tripping flow with wires at different frequencies [144], where f is the forcing frequency, L is the flow length scale, and U is the bulk velocity.

Here, the normalisation application is different as the present numerical framework is temporal; hence, time correlates to downstream distance in experimental counterparts. Still, the concept of relating the flow development with the seeding perturbation frequency and the bulk free-stream velocity is retained.

Figure 4.3 shows the momentum and vorticity thickness evolution against an equivalent normalised downstream distance. The trends observed here are the opposite of the ones

observed earlier without any temporal normalisation, where here, the net effect of increasing the perturbation wavelengths and simultaneously reducing ΔU leads to more rapid thickness growth. These results are consistent with those observed in experiments (e.g. Oster and Wygnanski [134]) and simulations [44]. This is because, through normalisation, the thicknesses are compared at the same effective downstream distance, which is also observed and assessed in experiments. For example, since the HMA case has four times the free-stream mean streamwise velocity than the LD case, then in the same duration, more of the momentum was utilised to transport the fluid parcels downstream (four times the distance than LD) through convective transport than was absorbed by the growing vortices expanding the shear layer (relative to LD), since the HMA case has higher bulk stream momentum and inertia.

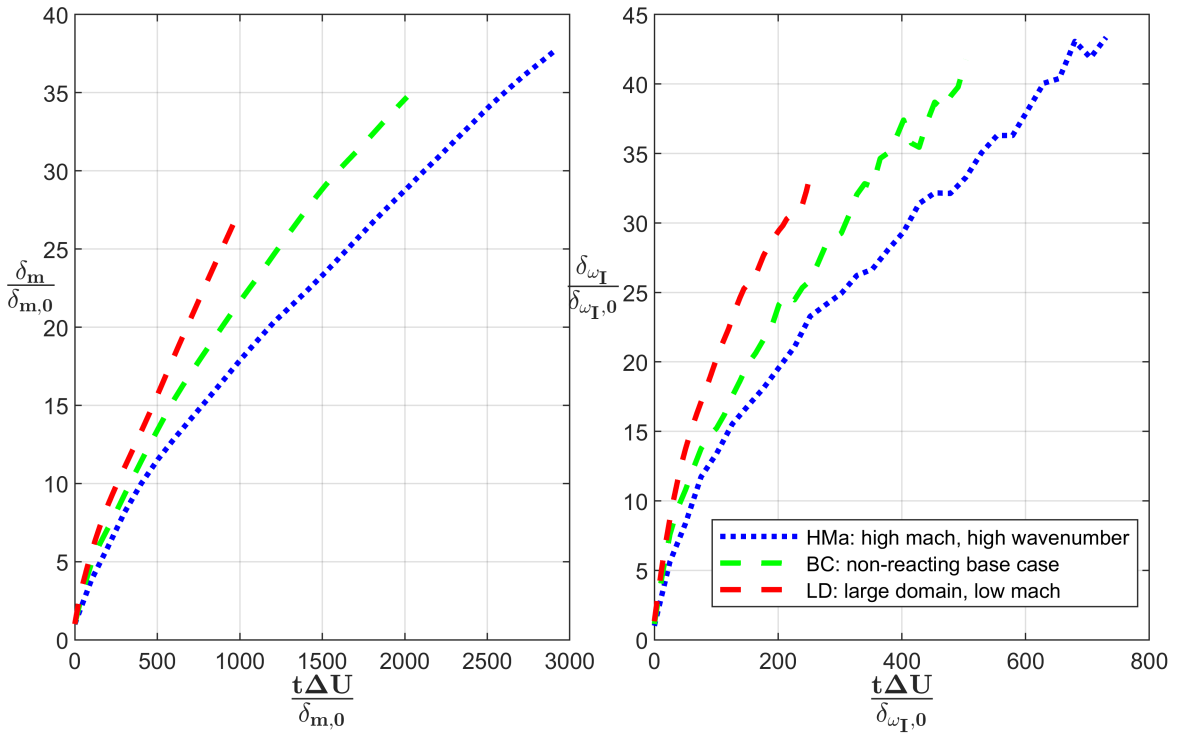


FIGURE 4.3. Momentum and vorticity thickness growths against non-dimensional time. The length scale in the temporal normalisation is the initial value of the respective thickness.

The momentum and vorticity thicknesses are normalised by their initial values in Figure 4.3. The initial vorticity thickness can be shown to be four times larger than the initial momentum thickness [11], [37], and the latter is defined directly in the initial setup of the streamwise

mean velocity as shown before in Equation 3.6. The initial momentum thickness defines the initial velocity gradient, ultimately initiating the vorticity that forms the mixing layer. Experimental setups that strictly rely on the initial momentum thickness without additional artificial forcing are unforced shear layers. The initial momentum thickness defines a natural perturbation frequency for the unforced flow. Most natural and engineered flows, however, involve some level of forcing, whether through obstructions or oscillations. As a result, most experimental work on turbulent shear layers trips the initial flow with wires or acoustic oscillations, resulting in a forced shear layer.

The setup employed in the present study does not utilise physical obstructions or oscillations in the flow pathway but directly applies the flow instabilities that would manifest at the shear interface, i.e., the KHIs. Hence, all cases considered here also have forced shear layers. This explains why no collapse is observed between the different cases in Figure 4.3, as although the same initial momentum thickness was set between the cases to maintain the same shear strain and fundamental mode of perturbation, the different cases have different forcing frequencies owing to their different perturbation bandwidths. So, they separate in accordance with this dependence on the forcing frequency.

The vorticity thickness exhibits more noise than the momentum thickness as it relies on the maximum streamwise velocity gradient, which is prone to fluctuations between time steps, particularly at later times when the flows become more chaotic, as shown for BC and HMA in Figure 4.3 and consistent with the visualisations in Figure 4.1.

Overall, the rate of vorticity thickness growth is higher than that of momentum thickness, judging by the number of times each has grown relative to their respective initial values. This implies a more rapid increase in velocity gradients across the shear layer than the increase in momentum deficit and suggests a lack of direct proportionality between the two, particularly during the early stages of flow transition.

Figure 4.4 shows the evolution of the transverse locations of the mean streamwise velocity thresholds that are used to form the h thickness definition as in Equation 4.5. The growth rate is linear and symmetric for all cases as both free-streams have similar densities (i.e.

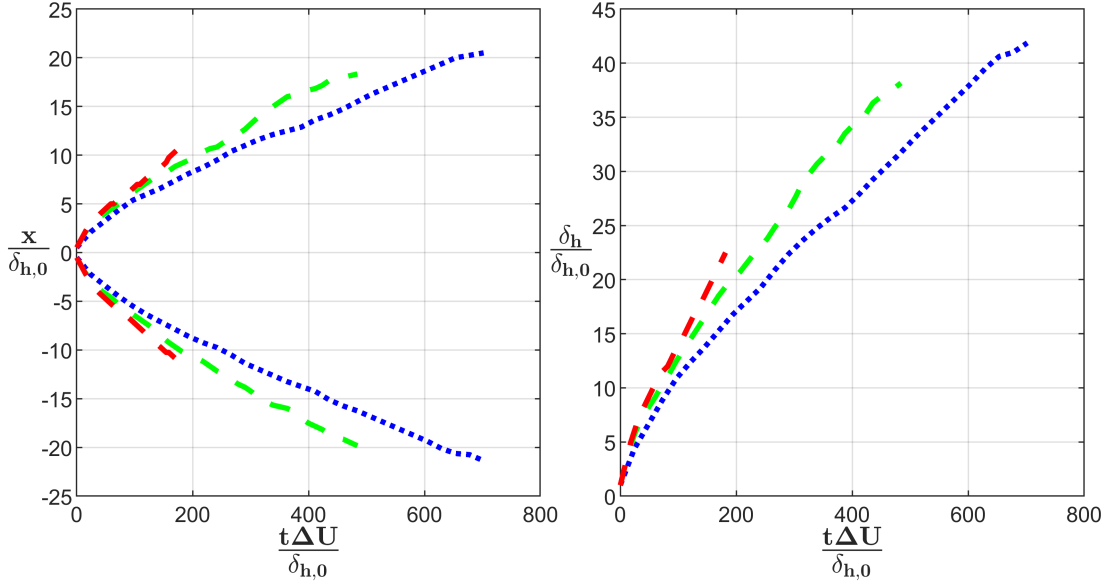


FIGURE 4.4. Transverse locations of the 10% threshold variations of the mean streamwise velocity, $\tilde{U}_y$, from the free-streams (left) and streamwise velocity threshold thickness (right). The initial threshold thickness is used for y-axis normalisation and as the length scale in the temporal normalisation. The colour scheme follows that from previous figures of this section (e.g. Figure 4.3).

low Atwood number) due to dilution of nitrogen in the fuel stream, otherwise asymmetries will manifest as the growth will gravitate towards the less dense free-stream [37], [55]. The trend observed in the threshold thickness evolution are consistent as those in the momentum thickness without significant noise a clear reduction of the growth rate with increasing ΔU and reducing instability wavelength.

To assess the relative growth between the different thickness measures, Figure 4.5 shows the vorticity and threshold thicknesses normalised by the evolving momentum thickness. While there is some noise and variations between the cases, particularly towards earlier times where the initial turbulent and gradient fluctuations are different (owing to the different initial perturbations), there is general agreement in the ratios of the thicknesses. At the initial stages, the growth of the vorticity thickness is larger for larger wavelength perturbations, which can be attributed to their wider-ranging eddies (in the transverse direction) and the resulting larger velocity gradients.

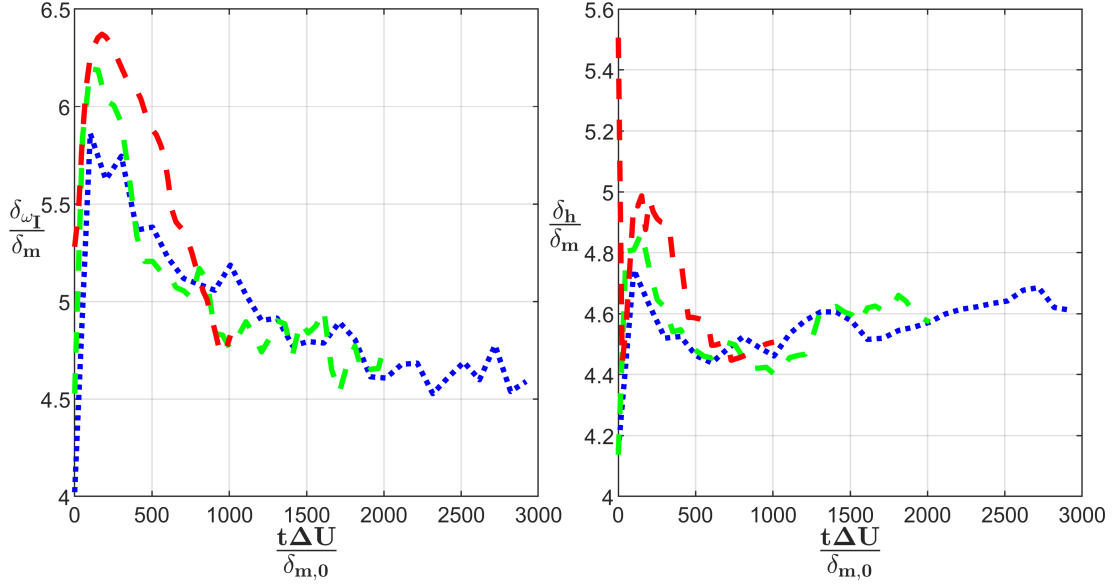


FIGURE 4.5. Ratio of other thickness measure evolution relative to momentum thickness: vorticity thickness (left), and streamwise velocity threshold thickness (right). The length scale of the temporal normalisation is the initial momentum thickness that is constant for all cases. The colour scheme follows that from previous figures of this section (e.g. Figure 4.3).

As previously pointed out, the initial growth of the vorticity thickness is more rapid than either the momentum or threshold thicknesses, reinforcing that increasing velocity gradients leads to all other measures of mixing layer growth. The asymptotic ratio of the vorticity to momentum thickness of 4.5 agrees with the 4.8 average reported by Rogers and Moser ([11]) in fully turbulent boundary layers but is slightly higher than their predicted value of 4 for shear layers initialised from a hyperbolic tangent profile, which was also reported in [37]. Therefore the asymptote observed here is in between the value for developing shear layers and turbulent boundary layers, highlighting an approach towards large-scale turbulent characteristics.

The relative magnitude of the threshold thickness to the momentum thickness also follows the same trend as vorticity thickness, although it fluctuates across a much narrower range. The asymptotic value of 4.6 observed is also very close to that of the vorticity thickness. This shows that it is inappropriate to use the threshold thickness h as a visual thickness when calculating and assessing an outer-scale Reynolds number, as this Reynolds number definition

assumes a visual thickness that scales twice as much as the vorticity thickness [37] which is not the case with the threshold thickness.

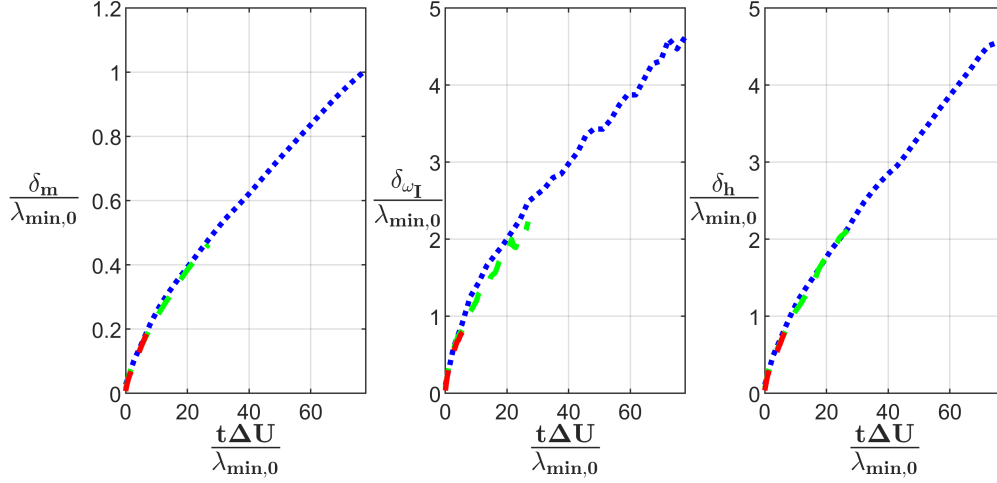


FIGURE 4.6. Self-similar collapse of thickness measures through normalisation by the minimum wavelength of the seeding perturbation. The plot colours follow the legend in Figure 4.3.

Since the previous figures that utilised the initial thicknesses as the length scale for the normalisation failed to demonstrate self-similar collapse, a more Strouhal-representative normalisation is adopted in Figure 4.6 that directly incorporates a fundamental forcing frequency element of the initial perturbation in the form of the minimum initial KHI wavelength. Usually, the most unstable wavelength would be used in the normalisation, but since the initial power spectrum of the instability is constant, any of the initial perturbation wavelengths would yield the same result as long as the choice of wavelength is consistent between the cases. The choice of the minimum wavelength was natural since, from linear theory (Equation 2.40), the minimum wavelength (maximum wavenumber) grows the most rapidly. The resulting temporal normalisation is then a normalised downstream distance that looks at the extent to which the fluid parcels have been convected relative to the initial dominant KHI perturbation dimension. In concept, this is very similar to the pairing parameter P studied in developing flow experiments [50], [135] to assess downstream distance relative to the forcing frequency of the shear layer in an effort to predict and account for vortex merger events as discussed

earlier. For subsequent discussions and figures $\frac{t\Delta U}{\lambda_{min,0}}$ is also denoted by the shorthanded t^* symbol.

The results of Figure 4.6 show a collapse of all thickness measures under this normalisation relative to the previous normalisation. This confirms the dependence of the large flow scale evolution on the seeding perturbation dimensions, in both magnitude and rate of growth- in agreement with linear theory, as the wavelength normalisation is used in both axes. Therefore, in terms of the large flow scales, the dependence extends beyond the initial free-stream velocities and densities, as hypothesized by Karasso and Mungal [50], to the seeding perturbation wavelengths.

Furthermore, this self-similar collapse is not just at late time when turbulence is more developed but is maintained throughout the transitional stages. However, during this self-similar collapse, the BC and the HMA cases transition into a steady stationary growth rate at $t^* \approx 20$, and that is consistent with all thickness measures. Initially, the growth is most rapid as the velocity gradients are highest and the prevalence of large-scale eddies maintain these high gradients, but as vortex pairings occur and the large scales breakdown to form smaller eddies, the gradients reduce to an equilibrium state of lower growth rates. This explanation is consistent with the observations in Figure 4.6 where the gradients of the self-similar profiles reduce first after $t^* = 10$ and then again after $t^* = 20$. It is not possible to ascertain whether this is the same for the LD case as it does not reach $t^* = 20$ before finite domain effects become apparent due to its lower free-stream velocity and larger perturbation wavelength. However, its trajectory is consistent with the BC and the HMA cases that confirm this.

Assuming that t^* values are well representative of the pairing parameter P defined in Equation 4.1 (i.e. R in the definition of P for coflowing configuration is well represented by ΔU for counterflowing setups), these approximate values of t^* that correspond to the gradient change are just slightly beyond the pairing parameter P values of 8 and 16 that were determined by Huang and Ho [135] to correspond to the second and third major three-dimensional vortex pairing events, aligning well with the explanation of the trends presented. The HMA case has a further capacity for a fourth major vortex pairing after a t^* value of 32 since its initial minimum perturbation wavelength was $\frac{L_y}{16}$. However, no clear observable gradient changes

manifest in Figure 4.6 beyond $t^* = 20$, indicating that any subsequent vortex pairings past the threshold of three have less substantial effects on large flow scale growth measures. This confirms the previous observations of Vreman [32], Rogers and Moser [99], and Huang and Ho [135], that required three major three-dimensional vortex pairings to fully trigger turbulence development- at least at the level of the large flow scale evolution.

4.3.4 Large Scale Turbulence

To assess the large-scale evolution of turbulence, the domain integrated turbulent kinetic energy, turbulent dissipation, and the normal Reynolds stress components are analysed in this section. In Chapter 2, Section 2.2.2, the covariances of the velocity fluctuation components have been defined as the Reynolds stresses under the Reynolds averaging convention. Similarly, the Reynolds stresses can also be defined based on Favre averaging. Let $\tilde{R}_{ij}$ be the Favre Reynolds stress, such that:

$$\tilde{R}_{ij} = \frac{\overline{\rho u_i'' u_j''}}{\bar{\rho}} \quad (4.7)$$

Similarly, a Favre turbulent kinetic energy can also be defined as:

$$\widetilde{\mathcal{K}} = \frac{1}{2} \left(\tilde{R}_{11} + \tilde{R}_{22} + \tilde{R}_{33} \right) \quad (4.8)$$

The self-similar collapse observed in Figure 4.7 shows that the dependence of the large scales on the seeding perturbation wavelength range and ΔU is not just restricted to large-scale mixing thicknesses but also includes large-scale turbulence quantities. Alternate normalisation by the initial momentum thickness (instead of the minimum wavelength, while still including ΔU) doesn't lead to the same collapse (not shown here), which emphasises the dependence of the large-scale turbulence on the seeding perturbation rather than just the free-stream velocities as claimed by [50]. While extending to general flow commentary, their claim was, however, based on their analysis of the mixing scales, which are focused on in the next Chapter.

The initial dip in the integrated dissipation was not observed in other reported results, such as in [11], [37], [53], [55]. There are two possible causes for this. Firstly, the initial setup

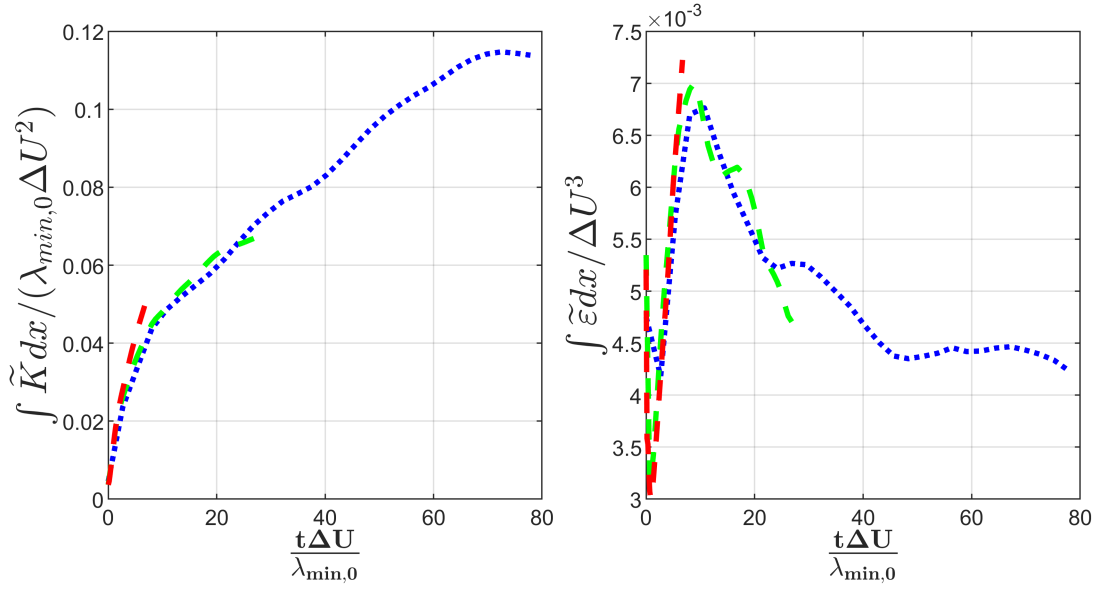


FIGURE 4.7. Self-similar collapse of integrated turbulent kinetic energy (left), and its dissipation. Integration is completed across the entire domain in the cross-stream x-direction, and the length scale used in the normalisation is the minimum wavelength of the seeding perturbation. The plot colours follow the legend in Figure 4.3.

involved a high-temperature profile (for consistency with the reacting cases). The temperature then drops quickly at the start, and due to the application of Sutherland's law, so does the viscosity, which reduces total dissipation. Secondly, the other cases in the literature were initialised with turbulent flow field conditions with pre-existing turbulent fluctuations and Reynolds stresses that more readily dissipate. Here, the initial fluctuations are mostly centred around the shear interface and, therefore, much more limited. These initial fluctuations also constitute the larger eddies, which are still within the energy-containing range and are, hence, less prone to dissipation. The greater initial dip in the integrated dissipation in the LD and BC cases confirms this, as their initial eddies are the largest (relative to the domain size) and hence provide a less vulnerable turbulent fluctuation supply for dissipation than the HMA case. (A consequence of the energy cascade where the effects of viscosity are more prominent in the smaller eddies, which makes their corresponding turbulent fluctuations more prone to viscous dissipation, i.e. more vulnerable.)

Following this dip, the dissipation rises rapidly, along with the turbulent kinetic energy, indicating the prevalence of turbulence-generating mechanisms- likely a series of vortex pairing and amalgamation events. A notable change in gradient in the integrated turbulent kinetic energy occurs at $\frac{t\Delta U}{\lambda_{min,0}} = 4$ followed by a more significant change at $\frac{t\Delta U}{\lambda_{min,0}} = 8$. The peak integrated dissipation also coincides with $\frac{t\Delta U}{\lambda_{min,0}}$ close to a value of 8 for all cases. Coincidentally, these normalised times align with the values of the pairing parameter introduced by [135], as discussed in the previous section, and therefore explain the rise in turbulence around these times and highlight the importance of the seeding perturbation wavelength in predicting the onset of turbulence generating mechanisms.

After $\frac{t\Delta U}{\lambda_{min,0}} = 8$, the turbulent kinetic energy appears to increase at a more uniform rate, indicating less drastic turbulence generating mechanisms occurring, while the integrated dissipation decreases due to decreasing viscosity until it reaches an equilibrium state. Before this, at $\frac{t\Delta U}{\lambda_{min,0}} = 20$ an oscillation is observed in the HMa plot that is not shared with the BC case. This likely indicates a third major vortex amalgamation event in the HMa case. It is only observed in HMa since it is the only case with a small enough minimum wavelength in the seeding perturbation to allow for more substantial three pairings- owing to the greater supply of smaller perturbations in the initial condition. This value of pairing time coincides with the point of stationary linear growth in the mixing layer thicknesses reported in the previous section and lies between the values of 16 and 22, reported by [135] and [50] to coincide with the start of self-similar evolution.

The equilibrium value is only attained by HMa as only this case reaches a late enough $\frac{t\Delta U}{\lambda_{min,0}}$. The stationary evolution is attained in the dissipation before the turbulent kinetic energy at $\frac{t\Delta U}{\lambda_{min,0}} = 50$. The integrated dissipation is not a parameter previously assessed against pairing time (or distance in case of spatially evolving) when it approaches its asymptote for developing flows. Interestingly, this asymptote of ~ 0.0045 is similar to the one observed in [11], [37], [53], [55], which, unlike the present study, didn't exhibit temperature or viscosity variations. This asymptotic value is also attained much later than in earlier studies since they started from turbulent conditions and could attain this equilibrium more readily. Yet, it appears to be a universal asymptote for the large-scale stationary turbulence equilibrium

independent of temperature or viscosity variations. The magnitude of this universal asymptote of the integrated dissipation strictly depends on the initial free-stream velocity, but the onset of this stationary value extends the dependence to the seeding perturbation wavelength.

Furthermore, the integrated dissipation asymptotes before the integrated turbulent kinetic energy and is, therefore, a precursor of the latter by about $\Delta t^* = 20$ - the same pairing time attributed earlier to three pairing events and which was shown here and in other studies to depict the duration (or downstream distance for spatially evolving) from the beginning of the shear instability when self-similar evolution of the large scales is observed. This is interesting as the large vortices should be heavily assimilated into smaller eddies through non-linear amalgamation events this late in the flow evolution. Even more interesting is that the integrated dissipation took another duration of $\Delta t^* = 20$ to reach its asymptotic value from its third pairing event. This observation suggests that the information on the seeding instability is not forgotten by the developing turbulence after the end of the initial transition stages characterized by a linear regime. In fact, increments of $\Delta t^* = 20$ are likely needed for the state of turbulence to traverse across the different stages of transition.

To gain further insight into the directional large-scale turbulence generation, Figure 4.8 shows the evolution of the three normal Reynolds stress components that make up the total turbulent kinetic energy. No collapse is observed between the cases when the normalisation omits the initial perturbation wavelength, even though the streamwise free-stream velocities are retained. (It is implied that a collapse is observed if the normalisation instead includes the initial perturbation wavelength. These stress components constitute the turbulent kinetic energy already shown to collapse in Figure 4.7. Including this normalisation for the integrated normal Reynolds stress components contributes limited additions to the discussion and is therefore omitted).

The trend between the cases is consistent with the earlier observations of mixing layer thicknesses with faster growth in cases with larger wavelengths. The streamwise component attains the largest magnitudes as expected since this is aligned with the mean flow direction, followed by the spanwise component that grows more rapidly than the other two components. The results show growth in both overall turbulence and mixing layer width and highlight

similar trends in the growth dependence on the seeding perturbation wavelengths. A question then arises on how the growth of large-scale turbulence compares to that of the large flow scale thicknesses.

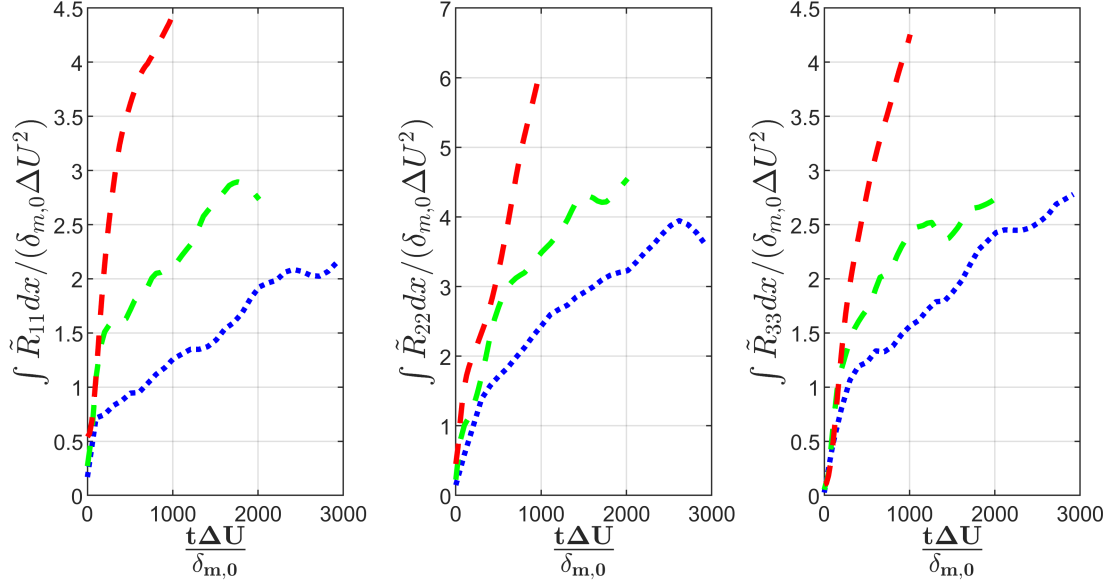


FIGURE 4.8. The evolution of the integrated normal Reynolds stress components: transverse (left), streamwise (middle), and spanwise (right). The plot colours follow the legend in Figure 4.3.

Figure 4.9 shows the integrated normal Reynolds stresses normalised by the evolving momentum thickness and free-stream velocity difference. For the first two figures on the left, i.e. the cross-stream and streamwise normal components, the growth of the stresses is slower than the momentum thickness (highlighted by initial negative gradient rather than the positive gradient observed in earlier work [37]), indicating that the transition of the large flow scales doesn't provide a direct correlation with turbulence generation, which in this case, although also increasing (as shown in Figure 4.8), lags behind. Once more, $t^* = 20$ marks the beginning of asymptotic evolution in all three stress components. The lack of vertical alignment between the different case results is due to the absence of the seeding perturbation wavelength in the y-axis normalisation, but this alignment has already been confirmed in Figure 4.7 with the turbulent kinetic energy that encapsulates all three normal stress components.

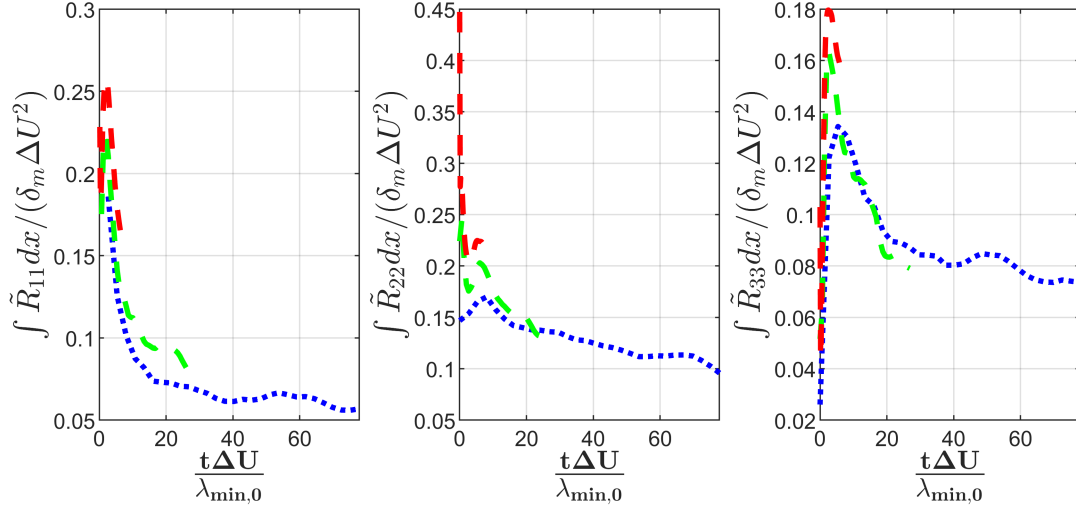


FIGURE 4.9. Evolution of the cross-stream integrated normal Reynolds stresses relative to the growing momentum thickness for all three normal components. The plot colours follow the legend in Figure 4.3.

The integrated cross-stream Reynolds stress has commonly been used in literature to assess the large-scale self-similar evolution of developed turbulence [11], [37], [53], [55]. However, unlike the results presented here, it is common to see this quantity increasing more rapidly than momentum thickness before descending and levelling off. The different initial behaviour observed in the present results can be attributed to the rapid initial decrease in viscosity as the shear layer cools quickly at the start from its initial high-temperature profile. While viscosity dissipates turbulence at the smallest scales, it also provides the shear stresses that roll up the vortices initially and separate them while enhancing the fluctuations, which launches all subsequent turbulence growth. Therefore, it is no surprise that a reduction in viscosity reduces the initial growth rate of turbulence relative to the larger flow scales that define the momentum thickness, which have longer timescales (formed earlier on) and are less sensitive to viscosity changes.

This explanation can also be supported mathematically. Vreman et al. [89] derived a relationship that relates the momentum thickness to the Favre-averaged streamwise velocity component in shear layers:

$$\frac{d\delta_m}{dt} = \frac{1}{\rho_0 \Delta U^2} \int \frac{d}{dt} \left(\bar{\rho} \tilde{U}_2 \tilde{U}_2 \right) dx \quad (4.9)$$

Considering the momentum conservation equation for the Favre averaged streamwise velocity and multiplying that through by the Favre mean streamwise velocity as shown in [37]:

$$\frac{d}{dt} (\bar{\rho} \tilde{U}_2 \tilde{U}_2) = \frac{d}{dx} (\bar{\rho} \tilde{U}_2 \tilde{U}_2 \tilde{U}_1) + \frac{d}{dx} (2\bar{\tau}_{12} \tilde{U}_2) - \frac{d}{dx} (2\tilde{U}_2 \bar{\rho} \tilde{R}_{12}) + 2 \frac{d\tilde{U}_2}{dx} \bar{\rho} \tilde{R}_{12} - 2\bar{\tau}_{12} \frac{d\tilde{U}_2}{dx} \quad (4.10)$$

According to [37], when the right-hand side of Equation 4.10 is substituted inside the integral of Equation 4.9, the first three components of the right-hand side of Equation 4.10 disappear which leaves the last two components. Therefore rearranging:

$$\frac{d\delta_m}{dt} + \frac{1}{\rho_0 \Delta U^2} \int 2\bar{\tau}_{12} \frac{d\tilde{U}_2}{dx} dx = \frac{1}{\rho_0 \Delta U^2} \int 2 \frac{d\tilde{U}_2}{dx} \bar{\rho} \tilde{R}_{12} dx \quad (4.11)$$

Pantano and Sarkar [14] demonstrated that the second term on the right-hand side relating to viscous shear stress is relatively small during stationary self-similar evolution. However, the flow regime examined here is at the early transitional period where the inconsistency in the relative magnitude of the integrated transverse Reynolds stress to the momentum thickness growth is observed compared to earlier work. It is unlikely the second term in Equation 4.11 is small during the initial transitional regime when both the flow and turbulence are rapidly developing. Therefore, with the momentum thickness growth dependent on the seeding perturbation wavelength and free-stream velocities, the rapid initial reduction in the viscosity of the shear layer with the temperature drop stunts the integral shear Reynolds stress that correlates with both the stream and transverse Reynolds stress components and explains the initial drops observed in Figure 4.9.

Surprisingly, although the initial behaviour differs, the observed asymptotic value of the normalised integrated transverse Reynolds stress component is 0.06, consistent with all earlier work, indicating that this is a universal value independent of flow setup provided turbulence has adequately evolved.

The spanwise Reynolds stress component is not included in the above relation. Therefore, it maintains the expected profile, which initially increases much more rapidly than momentum thickness before levelling off. This is consistent with the initially turbulent flow results of [37] in both initial behaviour and asymptotic value. This demonstrates that the spanwise

component is less affected by the viscosity variations than the other two components and likely relies on a more inviscid nonlinear mechanism in its growth. Its rapid growth also reinforces the three-dimensional essence of turbulence and aligns with Huang and Ho [135] observation that spanwise vortex interactions are the main driving force behind turbulence generation.

4.4 Turbulence Transition

4.4.1 Reynolds Stresses

In the previous section, trends for the integrated turbulence across the entire mixing layer were assessed. In this section, the focus is directed towards the local turbulence behaviour. Since the configuration here becomes statistically one-dimensional when stationary evolution is attained, it is common to observe the statistics across the cross-stream direction. Furthermore, an appropriate normalisation of the cross-stream coordinate is required to observe and assess self-similarity between the different cases. Rogers and Moser [11] demonstrate self-similarity by normalising the vertical coordinate by the time-varying momentum thickness for temporal simulations of a counterflowing configuration. This approach is also utilised here.

The first step of assessing turbulence usually involves examining the Reynolds stresses as they provide directional information on the average turbulence fluctuations and intensities. Figures 4.10 and 4.11 show the distribution of the Reynolds stress components at two different t^* values (corresponding to two different downstream distances). The other components of the Reynolds stress are more than an order of magnitude smaller. They are therefore discounted as negligible and omitted in this analysis as consistent with previous studies of shear flows.

At $t^* = 7$, the flows are expected to be nearing the second major vortex pairing. It is also the latest simulation time for the LD case, so it was chosen to compare all three cases. The trends of the peak values across the different stress components are consistent with the previous large-scale observations where larger wavelength (and smaller ΔU) conditions lead to greater magnitudes in the absence of $\lambda_{min,0}$ normalisation. The profiles of the BC case draw closer to

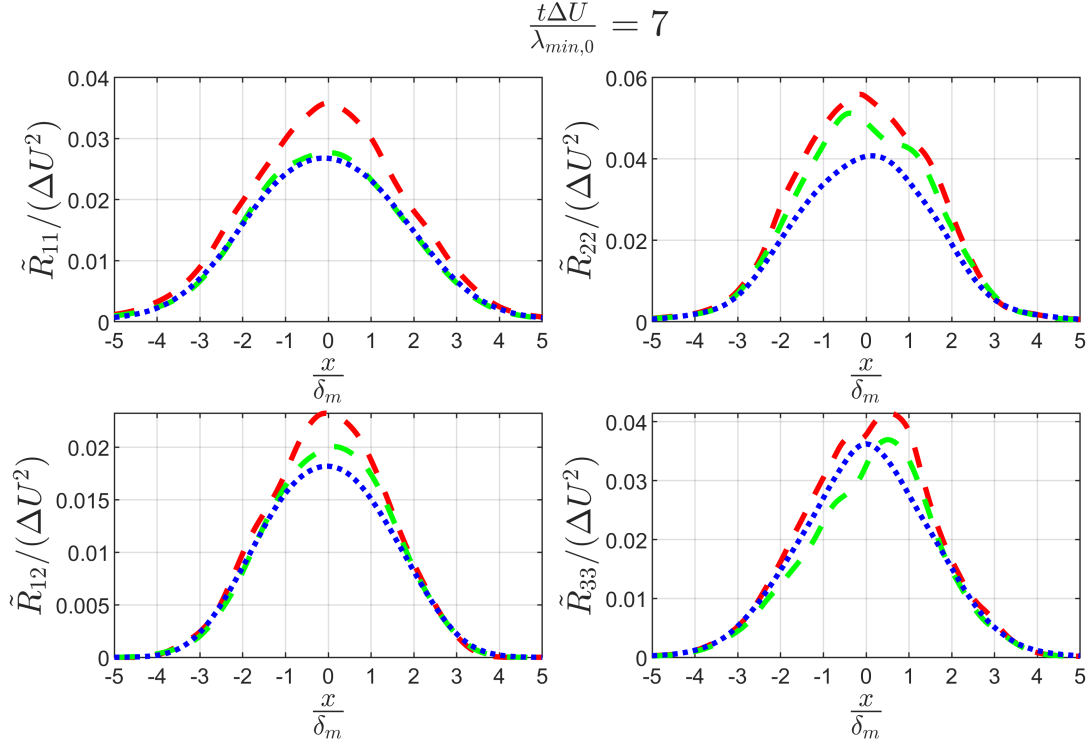


FIGURE 4.10. Normalised Reynolds stress profiles across the transverse direction at $t^* = 7$ for all three cases. The momentum thickness is used in the x-axis normalisation, and the square of the free-stream velocity distance is used for the y-axis normalisation. The plot colours follow the legend in Figure 4.3.

the HMA results, indicating a tendency towards a universal asymptotic profile independent of the seeding perturbation wavelengths.

However, this should not be surprising as the Reynolds stresses depend on velocity scales. Strictly, the appropriate self-similar normalisation should be by the eigenvalue of the KHI as expressed in Equation 3.9, which maintains dimensional velocity units. However, since the densities of the free streams are almost the same due to nitrogen dilution of the fuel stream, and since the streamwise perturbation wavenumber dominates the net radial wavenumber (i.e. $\underline{k} \sim \omega_y$) then $\Phi_0^2 \sim \Delta U^2$ and the dependence reduces to the free-stream velocity without the perturbation wavelengths. This also explains the success of the collapse of the Reynolds stresses observed in multiple earlier works once the flows transition to a stationary turbulent state (e.g. [11], [55]) and explains the lack of collapse in the self-similar Reynolds stress

profiles in [37] since they consider flows with different Atwood numbers without accounting for the density ratio in their normalisation (that also only considers ΔU) which would appear in the eigenvalue terms.

The shear stress components in both figures are positive, but they can also be negative, as in [11] and [37], depending on the mean streamwise velocity profile used. The mean cross-stream Favre turbulent fluctuations (also referred to as turbulent flux) are directed towards the opposing stream as the net effect of the shear instability is simultaneous entrainment from both sides of the shear layer as the vortex structures rotate and mix the initially separate free streams. Therefore, although it is common to observe the magnitudes of $\tilde{R}_{12}$ as negative (e.g. [11], [37]), this is only due to the choice of the mean streamwise flows of both streams. If the lower stream is set with negative mean streamwise velocity, then the shear-stress component will also be negative as in [11], [37] otherwise, if the bottom side flow is set with a positive free-stream mean velocity, then the shear stress components are positive as observed in the present study and [55]. Hence, to compare the universality of the shear stress component, the magnitude is what is of significance and not the direction.

Figure 4.11, shows the normalised Reynolds stress component at $t^* = 27$ which is beyond the transition point reported earlier of 20 to ensure sufficient vortex pairings and that the turbulence evolution is well underway. The LD case does not reach this late normalised time, so only the BC and HMA profiles are presented. Additionally, the time-averaged normalised stress component profiles of the HMA case during its asymptotic self-similar evolution are also presented. This self-similar duration was taken to correspond to $t^* = 30 - 80$. The results confirm that by $t^* = 27$ the Reynolds stress profiles for both cases have significantly approached the normalised asymptotic profiles. Interestingly, the asymptotic profiles in Figure 4.11 are quantitatively well-aligned ($< 5\%$ variance) to the simulation results of Rogers and Moser [11] and the experimental results of Bell and Mehta [145], indicating that under appropriate normalisation, the Reynolds stress profiles conform to universal values in developed turbulent mixing layers.

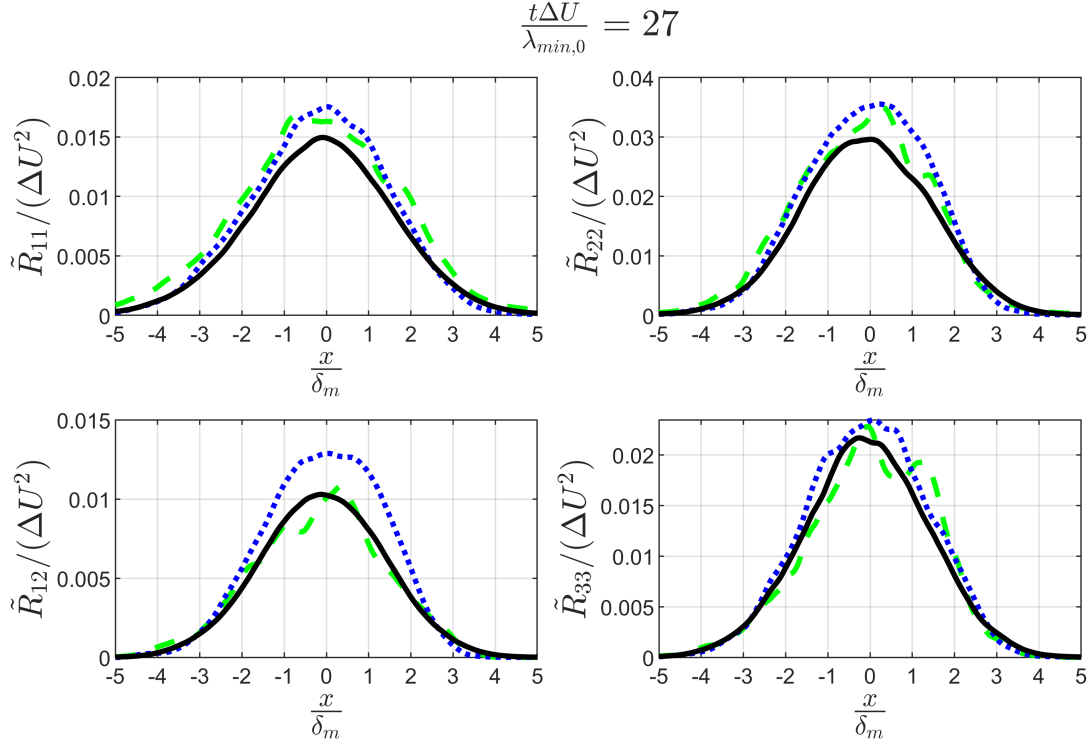


FIGURE 4.11. Similar to Figure 4.10 but at $t^* = 27$. The LD case does not reach this normalised time, so only the BC and HMA profiles are presented. The solid black line represents the averaged Reynolds stress profile for the HMA case during the asymptotic self-similar evolution.

4.4.2 Scale Separation

4.4.2.1 Reynolds Numbers

To derive further insights into turbulence development and its dependence on the seeding perturbation, this section examines the evolution of the different flow scales that constitute the turbulence spectrum. Since the assessment of turbulence is commonly synonymous with evaluating the Reynolds number, Figure 4.12 highlights the evolution of three different Reynolds numbers for all three cases. The formulation for the Taylor and turbulence Reynolds numbers were presented in Chapter 2, Section 2.2.3, along with the formulation for the directional Taylor scales, but since the calculation here involves averaging, they are redefined as:

$$Re_{\lambda_y} = \frac{u_y'' \lambda_y}{\bar{\nu}} \quad (4.12)$$

$$\lambda_y = \sqrt{\frac{\overline{u_y'^2}}{(\partial u_y' / \partial x)^2}} \quad (4.13)$$

$$Re_t = \frac{\widetilde{\mathcal{K}}^2}{\widetilde{\varepsilon} \widetilde{\nu}} \quad (4.14)$$

The planar values of Re_{λ_y} and Re_t are further averaged across the transverse direction within the velocity threshold thickness span (presented in Figure 4.4) and consistent with the notation explained in Chapter 2, Section 2.2.1.2. This provides representative Reynolds number values for the entire mixing layer.

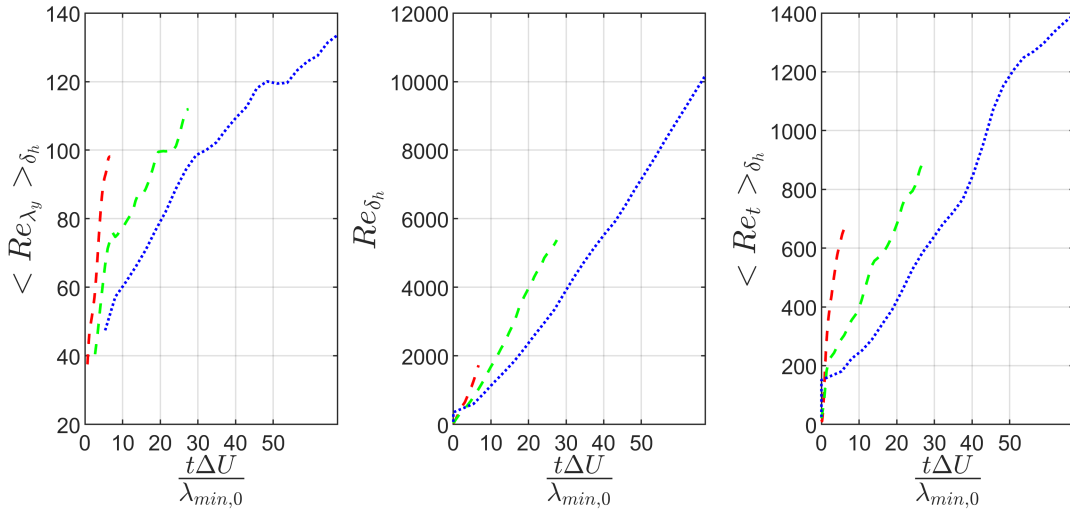


FIGURE 4.12. Evolution of different Reynolds numbers across t^* : the stream-wise Taylor Reynolds number (left), the threshold thickness Reynolds number (middle), and the turbulent Reynolds number (right). The plot colours follow the legend in Figure 4.3.

In order to present a large-scale Reynolds number for comparison, the threshold thickness Reynolds number, Re_{δ_h} , is defined by:

$$Re_{\delta_h} = \frac{\Delta U \delta_h}{\bar{\nu}} \quad (4.15)$$

The trends across all Reynolds numbers in Figure 4.12 are consistent with the observations in all previous sections of this chapter and reinforce the dependence of turbulence growth on the seeding perturbation parameters explored. The Taylor-Reynolds number relies on the gradients of the velocity fluctuations in its calculation, and since the cases are initialised

from laminar profiles with fluctuations only localised at the shear interface, computing these gradient fields is erroneous at the start of the evolution. It is reserved for when the fluctuations are more widespread. This is why the Re_{λ_y} plots do not start from $t^* = 0$, and since the x-axis is normalised time, the same time steps where the fluctuation gradients are calculated correspond to later t^* from LD to HMA.

All cases start from a very similar initial Reynolds number, which validates the choice of parameter variations in the initial perturbations that were designed to achieve this as explained in Chapter 3, Section 3.5. It is, therefore, important when calculating the Reynolds number for assessing turbulence to do so in stationary flow regimes rather than developing ones since the values can change by orders of magnitude, as demonstrated, while the flow evolves.

For all cases and across all Reynolds number measures, the values continue to grow with t^* at different rates depending on the seeding KHI. The growth of Re_{δ_h} is most rapid, which is expected given that the growth of the threshold thickness is more rapid than the turbulent fluctuations, and the free-stream velocities are unperturbed throughout the flow evolution. It then asymptotes to a constant growth rate consistent with the steady growth of the threshold thickness observed when the flows become stationary. The other two Reynolds numbers (the Taylor-based and the turbulence-based) rely on turbulent fluctuations that increase at a decreasing rate, as observed earlier and tend towards a constant-value asymptote. This is reflected in the corresponding Reynolds number profiles. Comparing the turbulent and Taylor Reynolds numbers reveals no direct proportionality as they vary by different factors throughout, where Re_t is between 6 and 10 times as large as Re_{λ_y} .

As demonstrated and discussed in Section 4.3.3, using Re_{δ_h} to describe an outer scale Reynolds number must be exercised cautiously. Based on the earlier discussion, on average, $\delta_h \approx 0.5\delta_{vt}$, where δ_{vt} is the visual thickness used to measure an outer-scale Reynolds number. Therefore, to compare against the transition Reynolds number threshold set by Dimotakis [9] in terms of a visual thickness convention, $Re = 2Re_{\delta_h}$. Based on the results in Figure 4.12, both the BC and the HMA cases cross this threshold of $\sim 10^4$ at their latest time, which is also consistent with their late time Taylor Reynolds numbers that cross the $\sim 10^2$ threshold.

The LD case is also very close to crossing the Taylor Reynolds number threshold but lags behind the threshold of the outer-scale Reynolds number even at its latest time.

Accordingly, cases BC and HMA have transitioned to developed turbulence based on this criterion, consistent with the universal asymptotes these cases have attained in both large-scale turbulent quantities and Reynolds stress profiles. However, these cases only cross the Reynolds number thresholds at their latest simulation times, whereas they reach the universal asymptotic values that correspond to self-similar stationary evolution at $t^* = 20$, as consistently demonstrated in earlier sections. Furthermore, at this t^* value, the BC and HMA cases have different Reynolds numbers. While the BC case approaches the Reynolds number transition thresholds at $t^* = 20$, the Reynolds numbers of the HMA case at this t^* threshold are much lower than the transition criteria. Nevertheless, the correlation between a t^* value of 20 and self-similar asymptotic evolution has been proved on multiple accounts in the previous sections. This points to a discrepancy between the criteria of vortex pairings and the one for Reynolds numbers, as the Reynolds number profiles do not collapse between the different cases at $t^* = 20$, which implies the two conditions are interdependent.

A possible explanation is that both conditions of downstream distance and capacity for vortex pairings, in addition to the Reynolds number criteria, need to be satisfied altogether to allow for a developed turbulence transition. This may explain why in Figure 4.11 at $t^* = 27$, the BC case Reynolds stress profiles are closer to the universal self-similar profiles than the HMA profiles since they have satisfied (or at least closer to satisfying) both requirements at this t^* value. Once the Reynolds number of HMA increases at later t^* , its profiles converge towards the universal values.

4.4.2.2 Evolution of Turbulent Scales

Figure 4.13 shows the evolution of three different turbulence length scales for each case. Each scale was chosen to correspond to different ranges in the turbulent energy spectrum. The largest scale considered is the one corresponding to the large eddy size and lies in the energy-containing range. This was defined earlier in Chapter 2, Equation 2.20 and is redefined

while considering the averaging as:

$$\mathcal{L} = \frac{\widetilde{\mathcal{K}}^{\frac{3}{2}}}{\widetilde{\varepsilon}} \quad (4.16)$$

The streamwise Taylor length scale, defined in Equation 4.13, lies in the inertial range, and finally, the Kolmogorov length scale, defined in Equation 3.17, to represent the dissipation range.

Similar to in the previous section, the length scale values presented in Figure 4.13 are averaged across the transverse extent of the velocity threshold thickness to gain a representative value of the entire mixing layer to aid the comparison between the different cases. The notation used in the figure is consistent with the definitions in Chapter 2, Section 2.2.1.2. All length scales are normalised by the initial perturbation minimum wavelength.

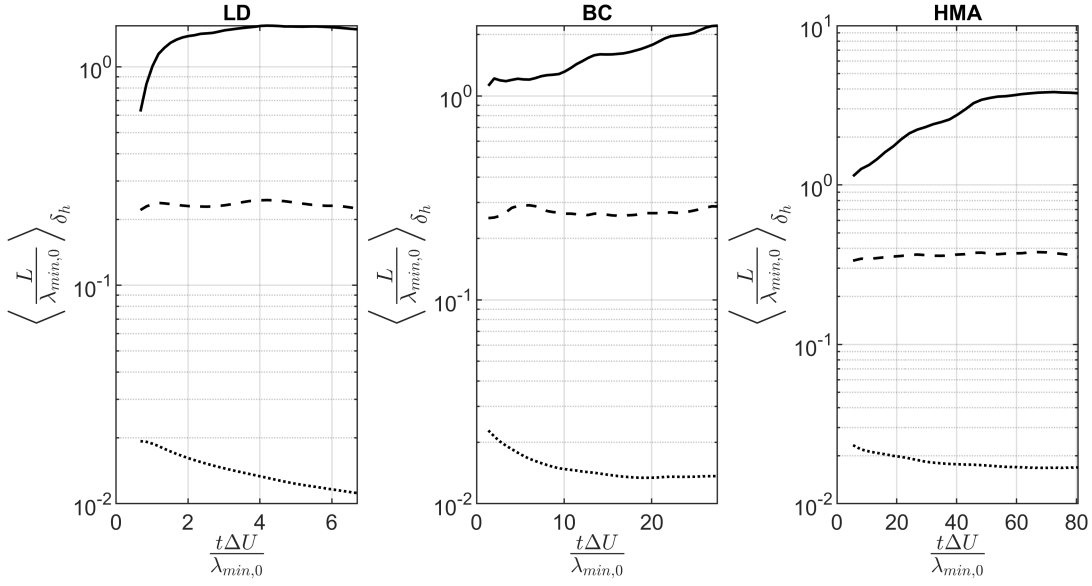


FIGURE 4.13. Evolution of the different turbulent scales normalised by the initial perturbation minimum wavelength, plotted against t^* for each of the three different cases: the large eddy length scale $\mathcal{L}$ (solid black lines), the streamwise Taylor length scale λ_y (dashed black lines), and the Kolmogorov length scale $\tilde{\eta}$ (dotted black lines).

Amongst the three different length scales considered, $\mathcal{L}$ exhibits the greatest change in magnitude over the span of the flow evolution. In fact, the increased scale separation between LD and HMA can be attributed to the more rapid and continued growth of the energy-containing scales. There was also increased separation between the Taylor and Kolmogorov

scales, but not by the same relative order of magnitude. Hence, they were not as conspicuous on the logarithmic scale. Interestingly, the Taylor scales remain steady and appear dependent on the seeding perturbation wavelength. The results in Figure 4.13 therefore highlight the significance of the initial perturbation wavelengths relative to the domain size, as these initial perturbations control the magnitude of the inertial range scales, and without the seeding perturbation set an adequate number of times smaller than the physical domain restrictions, the growth of the large eddies is impeded which affects turbulence transition.

To gain further insight into the scale separation in each case and clarity on the lack of direct proportionality between the Taylor and turbulent Reynolds numbers reported in the previous section, Figure 4.14, shows the evolution of the proportionality constants between the different scales of turbulence that were defined and explained in Chapter 2, Section 2.2.3. These only become constants in stationary, fully turbulent flows and in isotropic, fully developed turbulence, $C_1 = \sqrt{20}$ and $C_2 = \sqrt{30}$.

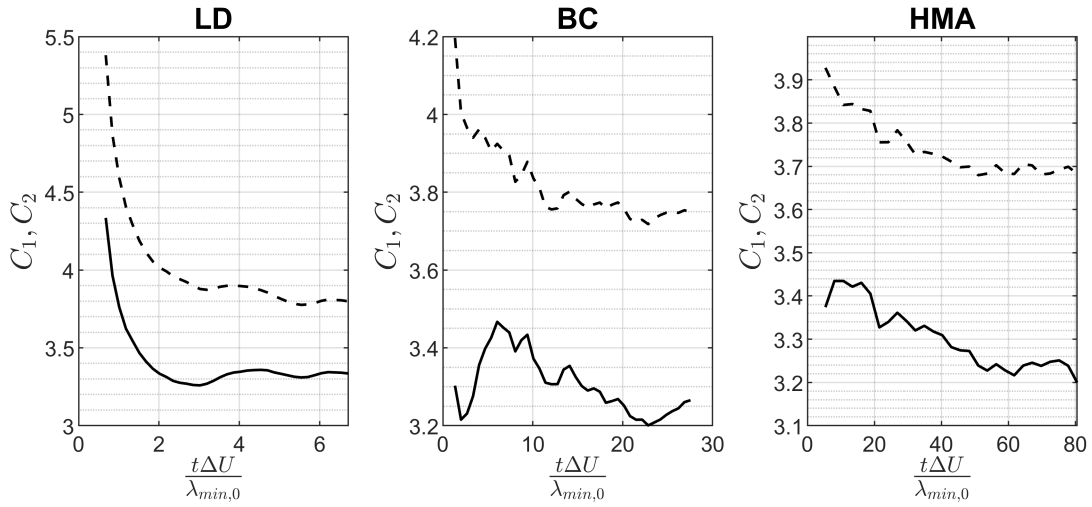


FIGURE 4.14. Evolution of the proportionality constants of turbulent scales: C_1 (solid black line), and C_2 (dashed black line).

Both constants fluctuate and change throughout the evolution, consistent with the lack of direct proportionality between Re_{λ_y} and Re_t . The trends observed with the C_1 and C_2 values do not directly correlate with the normalised time or pairing parameter. They seem more correlated to when the flows reach a stationary state, regardless of whether that state is fully

turbulent, and the cases achieve stationary flow evolution at different t^* values. Although the values for C_1 and C_2 differ slightly from those of isotropic turbulence, C_2 remains larger than C_1 . The three cases agree on the same asymptotic values of $C_1 \approx \sqrt{11}$ and $C_2 \approx \sqrt{14}$ with minor variance.

4.4.2.3 Energy Spectra

Lastly, this section is dedicated to observing the full energy spectra at different t^* values to observe the wavenumber functional dependence. All the spectra calculated here follow the same approach highlighted in Section 3.6.1.8 and use Equation 2.15. Figure 4.15 shows the one-dimensional transverse energy spectra for all three cases at select t^* intervals to showcase the evolution of the spectra with time and vortex pairing events for each case. Appended

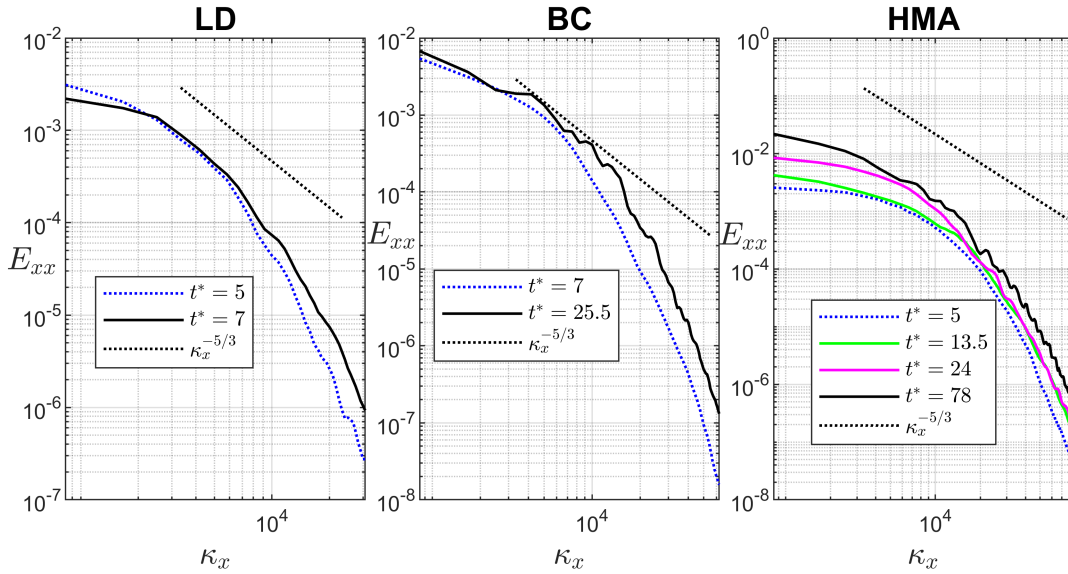


FIGURE 4.15. The one-dimensional transverse energy spectrum for all three cases at different t^* values. The reference $-5/3$ power law dependence is included in each plot (dotted black line) for comparison.

on the same figure is also the $-5/3$ power law that is conventionally used to characterise the inertial range spectral profile in fully developed turbulence as discussed in Chapter 2, Figure 2.4. The results here show a much narrower inertial range for the LD case compared to the BC and HMA results, where the spectra are overall higher, with greater peaks towards the

energy-containing range and more elevated smaller-scale ranges. This elevation of the inertial and dissipation ranges increases with t^* , and for the BC case at $t^* = 25.5$, it is shown to approach the asymptotic $-5/3$ profile. For the HMA case, this alignment is not observed by $t^* = 24$ but is apparent at $t^* = 78$ when the Reynolds number for HMA is also high enough. The spectral profile of HMA at $t^* = 78$ is well aligned with those presented in [55] and [11] of fully turbulent shear layers. Therefore, although a t^* value of 20 was sufficient to mark the development at the large flow and turbulence scales, the finer elements of turbulence development additionally require a later t^* value to show when the Reynolds number is adequately high.

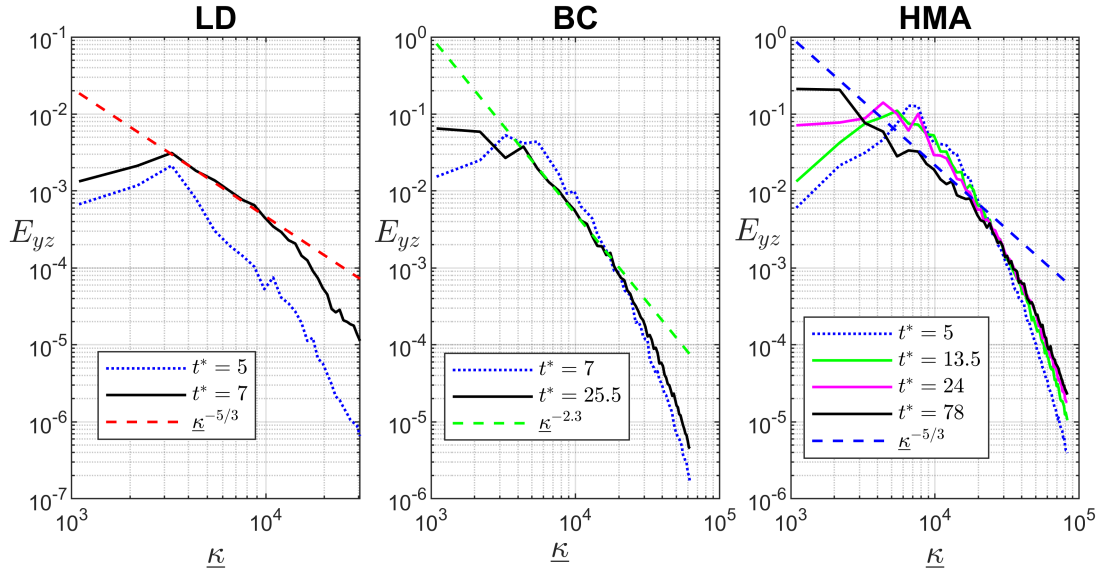


FIGURE 4.16. The two-dimensional radial energy spectra for all three cases at different t^* values. Different power law profiles were appended on each figure for comparison with coloured dashed lines in accordance with the legend entries.

While the transverse spectra provide some insight into the turbulence spectral distribution, the streamwise and spanwise directions hold the most turbulent energy for the shear configuration investigated, as reflected by the Reynolds stress profiles. Figure 4.16 highlights the two-dimensional radial spectral profiles within the $\frac{x}{\delta_m} = 0$ plane that was demonstrated to well-approximate the peaks of the Reynolds stresses in Figures 4.10 and 4.11.

The results show that the energy cascade is only fully realised past $t^* = 20$ as at previous times, there is a small drop in the energy towards the largest length scales. Since the LD case never crosses the 20 threshold, this monotonically decreasing energy profile with increasing wavenumber is not realised. Surprisingly, the LD inertial range aligns briefly with the $-5/3$ power law scaling, although both its Reynolds number and its vortex pairing are below the required threshold for developed turbulence, and as demonstrated by all earlier results, it is the furthest away from asymptotic self-similar evolution compared to the other two cases.

The energy cascade is observed in the BC case by $t^* = 25.5$, although at a more dissipative rate than the $-5/3$ scaling. At this time, examination of the inertial range demonstrates alignment with a -2.3 power scaling with the radial wavenumber- a 40% discrepancy from the hypothesised developed turbulence equilibrium.

The HMA case results demonstrate a transition towards a fully cascading profile at $t^* = 24$, but the inertial range power scaling aligns with the $-5/3$ power law much later, at $t^* = 78$. The results, therefore, collectively indicate that in fully developed turbulence, both a monotonic energy cascade and $-5/3$ power law scaling develop and that assessing these spectrally offers the most stringent test of a developed turbulence regime, as other characterisations of turbulence manifested at both lower t^* and Reynolds number values. Therefore, it is likely that at least an outer scale Reynolds number of 20000 and more than three major pairing events, along with initial perturbation that provides the capacity for such pairings, are needed for turbulence to be fully realised at the spectral level. Overall, the results of Figure 4.16 show that the effects of the seeding perturbation on the turbulent spectra manifest even late in the flow evolution judging by the different functional dependence between BC and HMA cases event at $t^* > 20$.

4.5 Conclusion

This chapter showcased the dependence of different large flow and turbulence scale measures on the seeding initial instability. It then extended this investigation across the different scales, parameters, and spectra of turbulence to fully assess this dependence and characterize

the onset of asymptotic self-similar evolution across the different scales. The dependence on the initial perturbation included both the initial free stream velocity differences (ΔU) and the initial perturbation bandwidth wavelength. This was confirmed by demonstrating self-similar collapse in the different large-scale properties only when both attributes of the seeding perturbation were used in the normalisation in both the x and y-axes quantities. Therefore, unlike the claim made by Karasso and Mungal [50], the present analysis finds that the dependence of the large-scale evolution isn't strictly on ΔU but extends into the wavelengths of the seeding perturbation relative to the domain dimensions, whether numerical or experimental. It also shows that the attributes of the seeding perturbation investigated affect both the downstream time where self-similar asymptotic evolution manifests and the magnitude of the various large-scale quantities.

Furthermore, in the various large-scale quantities explored, a t^* value of 20 has consistently appeared to mark the beginning of stationary evolution, even in turbulence quantities that weren't previously explored against this Strouhal-number-like downstream time. This value lies between the pairing parameter values that demarcate turbulence development, as previously reported in the experimental investigation of Huang and Ho [135] and Karasso and Mungal [50]. This normalised time also aligns with the onset of a third major vortex pairing event previously assigned as the turbulence developing event. Once the flow reaches a self-similar asymptotic state, the magnitudes of the different large-scale turbulence quantities analysed aligned well with previously reported values, indicating a universality of these turbulence quantities regardless of the initial perturbation or flow setup. The only dependence of these universal quantities on the seeding perturbation is in determining the evolution time (or downstream distance if spatially evolving) where large-scale turbulence universality begins.

These results may unintentionally imply that simply a longer evolution time is sufficient for turbulence development to occur, which may support the conventional thinking that at sufficiently high Reynolds numbers and for long enough development time (or downstream distance for spatial configurations), scale separation and turbulence development will evolve (e.g. as in [26]). This, however, would be an inaccurate interpretation of the results presented here. Yes, a collapse between the different cases is observed under temporal normalisation,

but that's only since this normalisation takes into account the seeding perturbation dimension such that the normalised time ($t^* = \frac{t\Delta U}{\lambda_{min,0}}$) can be directly linked to a pairing parameter as in [135]. The time requirement is, therefore, to ensure capacity for pairing events and not just large-scale thickness growth. So if flows that don't have the capacity for additional pairings are left to evolve longer, they'd break away from the self-similarity. For instance, the BC case has $\lambda_{min,0} = \frac{L_y}{8}$ in its initial perturbation bandwidth, which allows a maximum of three major pairing events of the seeding perturbation eddies. Thus, even if the BC flow can evolve past $t^* = 20$, it will break away from the self-similarity compared to HMa since it can't sustain any further pairing events. This can be confirmed by observing the larger discrepancy between the cases towards later t^* in Figures 4.8 and 4.9.

Examination of small-scale turbulence and spectra confirmed the same trends in the dependence on the seeding perturbation parameters but revealed that a t^* of 20 is insufficient for universal asymptotes to be realised at these scales. Instead, both a high Reynolds number and a sufficient t^* value need to be attained for the transition to manifest, with the results suggesting the need for more than three vortex pairing events and a minimum outer scale Reynolds number of 20000.

To conclude, there are three requirements needed for turbulence to fully evolved:

- (1) A mechanism that allows the distribution of flow energy across a range of scales.
- (2) A capacity for such a mechanism to occur an adequate number of times to expand the range of scales.
- (3) An adequate time (for temporal configuration) or downstream distance (for spatially developing flows) to fulfil such capacity.
- (4) A high enough Reynolds number to ensure the longevity of the wide range of scales that would otherwise dissipate.

Since the initial perturbation affects the occurrence of such a mechanism (vortex pairings in shear flows), then it also affects turbulence development and hence, knowledge of the seeding perturbation can help form accurate predictions for the onset of turbulence where normalised parameters can be shown to take universal values. Similarly, this knowledge can also inform

on previously unexplained observed persistence of non-universal flow behaviour, even at high Reynolds number, realised due to unfulfilled adequate pairings and is once more dependent on the seeding perturbation.

While the results show dependence on the seeding instability in the onset of turbulence and the trend of the flow evolution during the transition, they do not conclusively reveal the interdependence between the vortex pairing onsets, which are a function of the seeding instability, and the Reynolds number. This is because the cases that undergo at least three pairing events (i.e., the BC and the HMA cases) also cross the threshold Reynolds number for transition. A wider parameter investigation with more cases seeded from different perturbations and achieving the same late t^* values is needed to further clarify this complex interdependency and understand whether a greater sensitivity manifests towards one parameter over the other.

Mixing Dependence on Narrowband KHIs in DNS of Transitional Reacting Shear Layers

5.1 Introduction

Efficient non-premixed combustion in practical engines is predicated on adequate mixing of fuel and oxidiser at the molecular level. Turbulence is required to achieve the mixing in most applications. However, fuel and oxidiser often enter the combustor as laminar flows and laminar-to-turbulent transition ensues. Most existing research has focused on mixing and combustion in the fully turbulent regime [3], and this knowledge is helpful for many conventional, low-speed applications in which residence times are sufficient and a wide range of instabilities are present. The short-lived transitional flow regimes may be neglected in engine design calculations. The situation in high-speed applications can be quite different, and the critical Reynolds numbers (and t^* thresholds) for complete transition may not be reached within the confines of the physical systems [3], [9]. This might seem counter-intuitive given the high speeds (of order 1000-3000 m/s). Still, short residence times and compressibility effects impede the growth of mixing layers and restrict the growth of length scales that affect Reynolds number [14]. Furthermore, transitional effects can be significant during mixing and combustion stages [10]. Therefore, developing engine designs that control the flow turbulence transition requires a deeper understanding of the transitional mechanisms leading up to turbulence and their effects on mixing and combustion [4], [5].

Combustion in counter-flowing shear layers is predominantly non-premixed, and as described by Poinot [63], non-premixed combustion analysis can be separated into a mixing problem and flame structure problem. This premise is used to organise the analysis in the present study.

The previous chapter highlighted the dependence of flow and turbulence parameters on the initial instability, and the effects of the initial instability were shown to persist towards a later time and affect the growth rate of different turbulence parameters in addition to controlling the onset of the turbulence transition. The analysis in the previous chapter was intentionally undertaken in the inert cases to isolate the turbulence evolution from flow-chemistry effects that would otherwise manifest in the presence of reactions. The subject of analysis in both this and the subsequent chapter is the reacting cases, where the focus is shifted to firstly the mixing attributes that drive the chemical reactions (in the present chapter) and the effects that manifest on the flame structure (in the subsequent chapter).

The analysis in this and the subsequent chapter extends the field in two ways. Firstly, like the previous chapter, it performs fully resolved DNS of shear layers perturbed by KHI of varying narrowband wavelength ranges and free-stream velocities, but unlike the previous chapter, it investigates two other elements of that dependence: the mixing and the flame structure. Secondly, the combustion of syngas co-occurs with the transition, whereas no previous published work has included flow-chemistry interactions simultaneously while studying flow development from fundamental primary instabilities. Moreover, besides providing information on the underlying physics, this chapter and the subsequent one also aim to help inform the modelling of reacting flows in these regimes.

5.2 Simulation Parameters

In this Chapter, the focus is drawn explicitly to reacting cases where the initial KHI narrowband ranges are varied to highlight the effects on combustion. The full numerical implementation and simulation quality details are outlined in Chapter 3. A brief summary is outlined in this section to help focus the results of this chapter.

The main parameter variation between the DNS cases is the spectral narrowband range of the perturbations and ΔU , as specified in Table 5.1 along with other key parameter settings. The naming of the cases considered in these sections is simplified from their full names in the case directory presented in Chapter 3, Table 3.1. For cross-reference, the full name of the

corresponding cases in the Case directory is outlined in Table 5.1. The Mach numbers are increased for Case B and D to maintain a similar visual thickness-based Reynolds number [9] to Case A to isolate the effects of varying the initial narrowband range of the perturbation. Case C maintains the same narrowband range as B but has a higher Mach number (therefore different initial Re) to attain later normalized time for comparison against Case D.

TABLE 5.1. Key model and numerical parameter settings in the DNS cases.

Parameter	Case A	Case B	Case C	Case D
ΔU (m/s)	72.5	145	290	290
Ma_c	0.08	0.16	0.32	0.32
$\frac{\kappa_{min}}{\kappa_0} \leq n \leq \frac{\kappa_{max}}{\kappa_0}$	$4 \leq n \leq 8$	$4 \leq n \leq 8$	$4 \leq n \leq 8$	$8 \leq n \leq 16$
$\frac{L_x}{\delta_{m,0}} \times \frac{L_y}{\delta_{m,0}} \times \frac{L_z}{\delta_{m,0}}$	$699 \times 1200 \times 800$	$524.2 \times 600 \times 400$	$699 \times 600 \times 400$	$524.2 \times 600 \times 400$
$N_x \times N_y \times N_z$	$336 \times 576 \times 384$	$504 \times 576 \times 384$	$1344 \times 1152 \times 768$	$1008 \times 1152 \times 768$
Cross-reference	LD-R-SS:4-8	BC-R-SS:4-8	HRe-R-SS:4-8	HMa-R-SS:8-16
Colour Scheme	— — —	—	— — —	

5.3 Mixing Layer Evolution

5.3.1 Contour Visualisation

Figure 5.1 shows isocontours of the mixture fraction, ξ , for all cases at their latest runtime. The contours demonstrate varying mixing levels and degrees of turbulence, which increase with the increase in initial perturbation eigenvalue (i.e. the combined decrease in perturbation wavelength and increase in free-stream velocities). Case A exhibits coherent structures indicative of large-scale saturation and lack of subsequent breakdown. This level of coherence decreases for Case B, which is still less turbulent than its inert counterpart, as shown in Chapter 4, Figure 4.1. This highlights the laminarizing effect of combustion that impedes the turbulence transition.

Cases C and D appear more turbulent with more rapid mixing layer growth in Case C as highlighted by the wider extent of the cross-stream limits, $\frac{x}{\delta_{m,0}}$, of the ξ contours. Although both Cases B and C have the same initial domain size and perturbation wavelengths, the wider prevalence of small-scale eddies in Case C is striking. It showcases the significance of a higher Reynolds number on the level of turbulence under the same initial perturbation

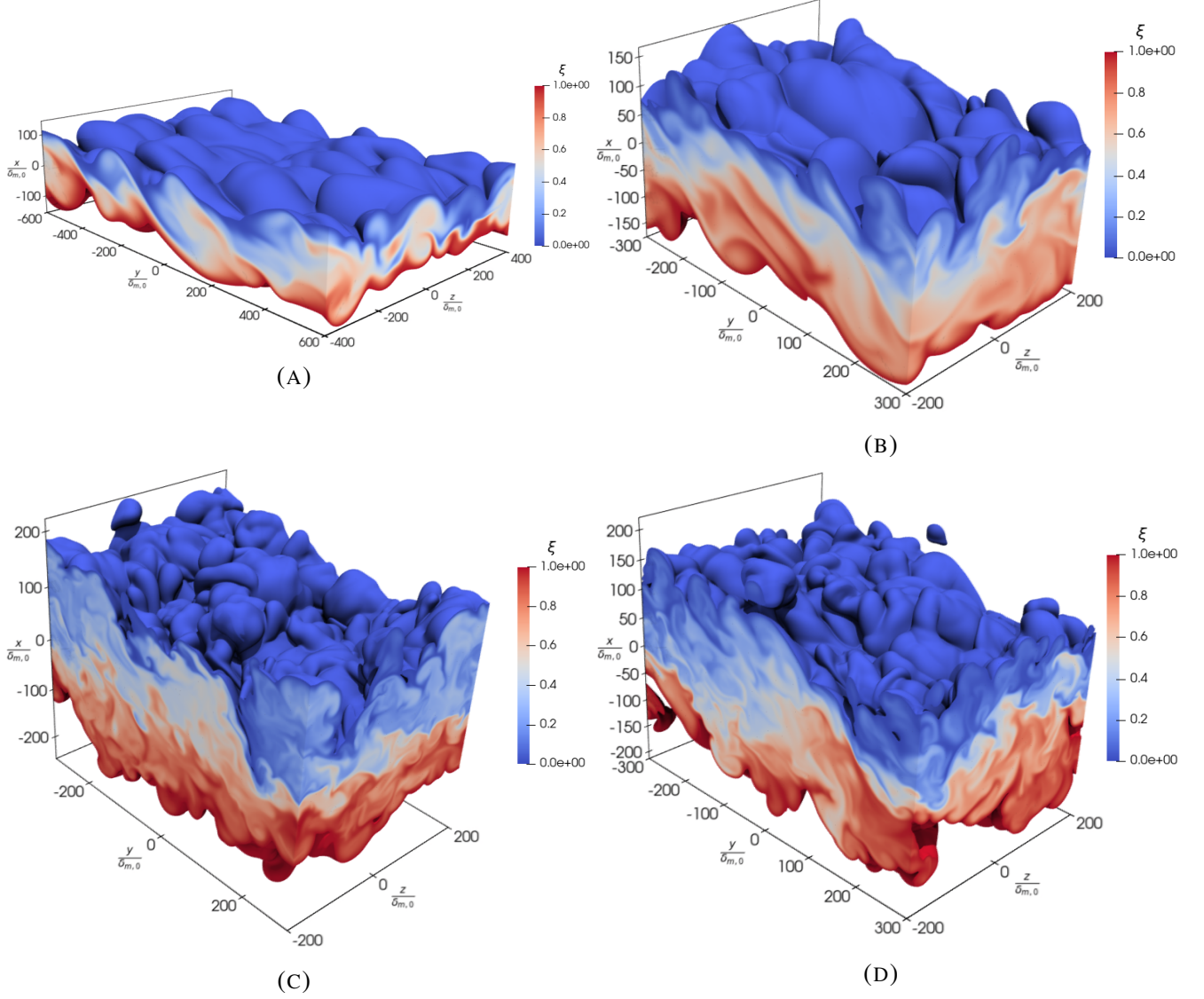


FIGURE 5.1. Isosurfaces of mixture fraction with a cutoff at $\xi = 0.01$ and $\xi = 0.99$ at the latest runtime for each of the cases. The figure labels correspond with the case name in lowercase.

wavelength and domain size. The contours for Case C, however, exhibit a higher degree of coherence and symmetry than Case D, which is apparent when viewed from the x-y plane. This observation is consistent with the conclusions of Chapter 4, as Case D has a higher capacity for vortex amalgamations, given its smaller initial perturbation wavelength relative to the domain size.

5.3.2 Thickness Growth

Figure 5.2 shows the time evolution of two mixing layer thickness measures that are commonly used to characterise shear layer growth [37], [44]; namely, momentum thickness and mixing zone thickness. The momentum thickness was previously defined in Equation 4.2. The mixing zone thickness is also a threshold thickness defined in a similar fashion to δ_h (Equation 4.5) but based on the 1% mixture fraction threshold instead:

$$\delta_z(t) = |x_{[\tilde{\xi}=0.01]} - x_{[\tilde{\xi}=0.99]}|. \quad (5.1)$$

Due to the varying growth rates of the different cases, an appropriate temporal normalisation, as demonstrated in Chapter 4, is required to draw direct comparisons between the cases. In the left-side column of Figure 5.2, the momentum thickness is normalised by its initial value (top) and the mixing zone thickness is normalised by the domain transverse length (bottom). Similar to the trend observed in Chapter 4, Section 4.3.3 and the results of Sharan et al. [44], the results demonstrate reducing mixing layer growth with increasing perturbation eigenvalue, for both thickness measures. Like before, the profiles approach linear growth at later times, marking a transition towards stationary evolution. A closer examination of the evolution (not presented here) reveals three distinct growth stages: an initial stage with exponential growth, followed by two successive stages of linear growth, with a decreasing gradient between both linear growth stages.

Only Cases C and D reach the final asymptotic stage. During the late-time linear asymptote, the normalised momentum thickness growth rate, $\frac{1}{\Delta U} \frac{d\delta_m}{dt}$, for Case C is 0.014, and for Case D is 0.012. Direct dependence of mixing layer growth rates on Mach number has been well-established in previous studies [14], [89], [98], so it is important to note that the Mach number is the same between Cases C and D (so is ΔU) and the discrepancy observed is strictly due to the effects of the initial perturbation that appear to manifest even at late-time.

In the right-side column of Figure 5.2 (top), the initial instability wavelength, $\lambda_{min,0}$ (which varies between the cases), normalises the momentum thickness. Time is also normalised by the instability timescale, $\frac{\lambda_{min,0}}{\Delta U}$, like in the analysis presented in Chapter 4. This normalisation

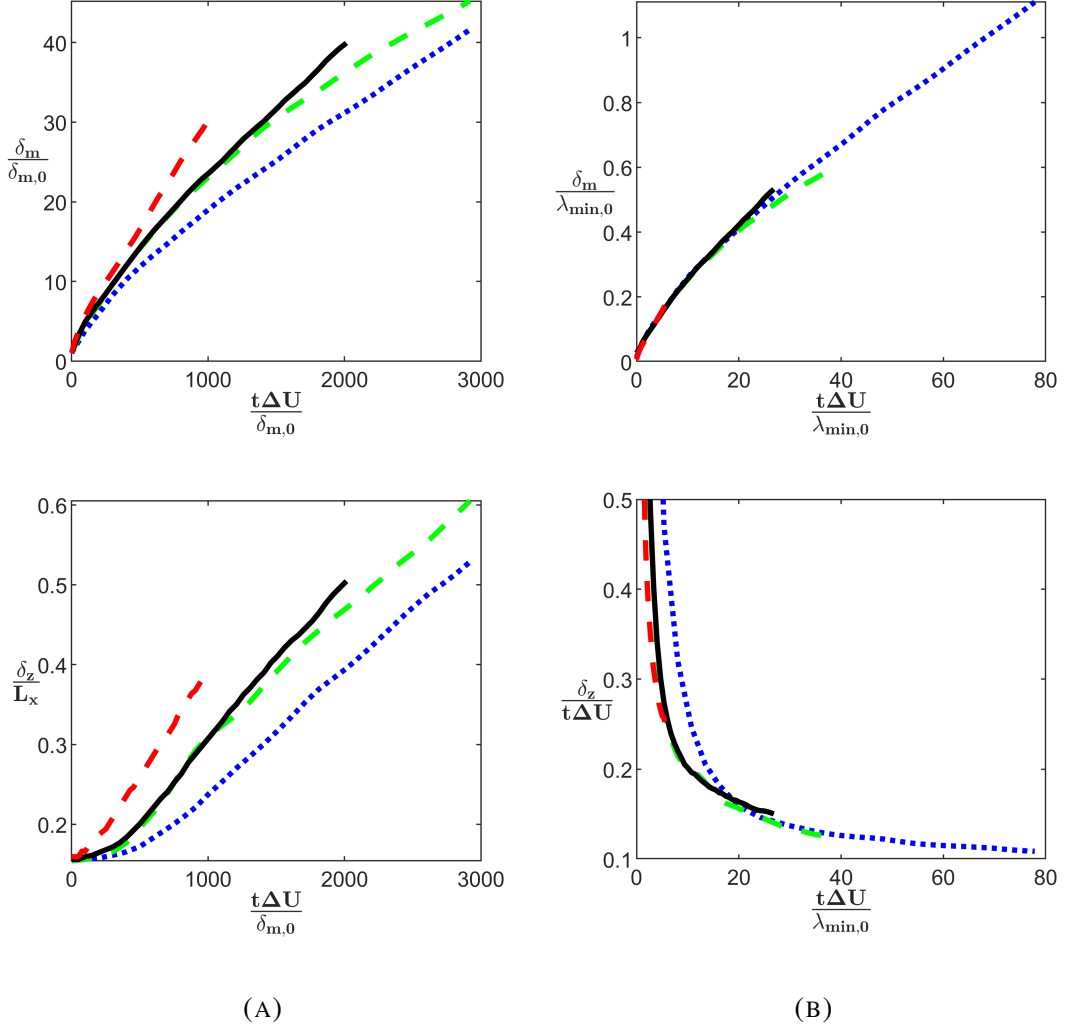


FIGURE 5.2. Normalised momentum thickness (top) and mixing zone thickness (bottom) against different magnitude and temporal normalisations. The colour scheme is specified in Table 5.1.

results in a collapse of the momentum thickness evolution, reinforcing its direct dependence on the perturbation wavenumber even in reacting shear layers. The onset of the final self-similar regime appears to start at $t^* = \frac{t\Delta U}{\lambda_{min,0}} \approx 20$, consistent with the observation of the inert cases in Chapter 4. This consistency of the transition of large-scale thickness growth between inert and reacting cases is further demonstrated within the asymptotic profiles of Cases C and D, whose asymptotic growth rates were only slightly lower than the widely reported range of

0.014-0.0165 observed for both experimental and numerical investigations of inert mixing layers [11], [44], [146].

The overall results indicate some dependence of the mixing layer development on both the perturbation wavenumber and ΔU . These are the main parameters that vary between the cases and directly affect the initial eigenvalue of the perturbation (refer to Equation 3.9). This dependence, however, is expressed to varying extents between the two mixing layer thickness measures explored.

In the momentum thickness profiles, the dependence on t^* is as with the inert cases, where the end of the initially rapid growth is at $t^* = 10$, after which an intermittent relatively high gradient linear growth is observed up to $t^* = 20$, followed by another linear growth profile at a reduced gradient. These observations align with the vortex pairing parameter and show that after two major vortex pairings, the momentum thickness growth becomes linear. After the third pairing, it resumes a linear profile but at a reduced rate. Furthermore, the addition of chemical reactions contributed little change to the key t^* values that characterize flow and turbulence development in the momentum thickness. However, a full comparison between corresponding reacting and inert cases (with the same initial conditions) is required to assess this fully. The explicit analysis of the flow-chemistry interactions across the different flow and turbulence scales is reserved for future work and not undertaken in the present study.

Regarding the mixing zone thickness, the dependence on the seeding perturbation appears more sensitive to the free-stream velocities than the initial perturbation wavelength bandwidth. The vertical separation of the results in the bottom plot of Figure 5.2 (A) reveals a dependence on the initial perturbation eigenvalue as there is no perturbation-relevant normalisation of the y-axis to show self-similar collapse. However, normalisation by the perturbation minimum wavelength (y-axis) against t^* (x-axis) only shows consistency in the final growth rate without an exact collapse (in terms of magnitude), as that observed for the momentum thickness in the top plot of Figure 5.2 (B). (Note that the plots of $\frac{\delta_z}{\lambda_{min,0}}$ are not shown here for brevity). Instead, a collapse (in the y-axis direction) is observed once δ_z is normalised by the convective distance, $t\Delta U$, showing that the dependence of the large mixing thickness is solely on the free-stream velocities in the perturbation eigenvalue rather than also the perturbation wavelengths,

as shown in the bottom plots of Figure 5.2 (B). This is further supported by the lack of collapse in the x-direction when $\lambda_{min,0}$ is retained in the temporal normalisation, as shown in the same figure. In fact, if the same temporal normalisation as in (A) is retained (i.e. $\frac{t\Delta U}{\delta_{m,0}}$), the $\frac{\delta_z}{t\Delta U}$ plots of all cases collapse as they all maintain the same initial momentum thickness (which corresponds to the fundamental natural frequency of shear layer perturbation as explained in the introduction of Chapter 4.).

It is therefore not surprising that Karasso and Mungal [50] claimed that the turbulent mixing dependence and the transition to developed self-similar regimes is strictly on the free-stream velocities, as under the lens of the large-scale mixing effects (which is what they assessed), that is mostly the case. However, as shown in the previous Chapter 4, the effects of different perturbation wavelengths extend to small-scale turbulence and persist to late flow evolution, so it is likely that at the smaller mixing scales, this mixing dependence will also extend to the wavelengths (in addition to ΔU) as will be assessed by studying the flame structure evolution in Chapter 6. Interestingly, however, even at these large mixing scales, the collapse of mixing zone thickness under $\lambda_{min,0}$ normalisation is observed beyond $\lambda_{min,0} \approx 20$ in the bottom plot of Figure 5.2 (B), further indicating that while the dependence of the mixing zone thickness on the initial perturbation wavelength is more subtle than the dependence on the free-stream velocities, it is not entirely forgotten.

5.4 Favre Averaged Statistics

5.4.1 Favre Mean Profiles

Figure 5.3 shows cross-stream profiles of key Favre averaged quantities for select normalised times for all cases, where t^* is set to denote $\frac{t\Delta U}{\lambda_{min,0}}$ for brevity. The smooth reclining profiles for streamwise velocity, U_2 , and mixture fraction indicate developing mixing layers and have been commonly reported. The rate of gradient decrease (due to increased mixing) in these plots is consistent with the trend observed for momentum and mixing zone thicknesses with more rapid gradient reduction with reduced wavenumber perturbation of the KHI such that

Case A shows the most rapid gradient decrease. The cross-stream velocities are an order of magnitude smaller than the bulk streamwise velocities and exhibit a net outward flow from the centre of the shear layer due to the reduced density from combustion. The smaller magnitudes of cross-stream velocities for Case C and D indicate lower flame temperatures and higher densities. The intermittent change in U_1 direction in Case C at $t^* = 8$ close to the domain centre at both sides is likely due to an extinction zone at the core of the mixing layer, causing an influx towards the centre. This zone appears to be enclosed by flammable low-density regions at $x \sim 20\delta_{m,0}$ outside of which the flow reverts outward towards the boundaries. These results, therefore, indicate differences in the mixing and flame distribution between the cases.

The three-dimensional nature of turbulence is apparent in the spanwise velocity profiles, which not only increase in magnitude with time as turbulence develops but also in intermittency to reflect the complex three-dimensional vortical currents of the developing shear layers. The spanwise velocities are also an order of magnitude smaller than the bulk streamwise velocities similar to the cross-stream velocities, except for Case A, where they are smaller by a further order of magnitude due to Case A not transitioning to turbulent mixing as evident from the ordered vortices in Figure 5.1 isocontours. All cases span the same density ranges over time, so different variable density behaviour should persist between the cases and any variations strictly attributed to the initial perturbation parameters highlighted in Table 5.1 and any resulting flow-chemistry coupling. Minimal densities accumulate in the vicinity of the mixing layer with a minimum value consistently at the domain centre due to increasing temperature from combustion and the entrainment of reacting species. The jump in minimum density for Case C at $t^* = 8$ that is not observed to the same extent in the other cases is another precursor for extinction. The width of the density trough in the cross-stream direction is well-correlated with the mixing zone thickness evolution in Figure 5.2.

The last row of plots in Figure 5.3 shows the total scalar dissipation rate, $\chi = 2D(\nabla\xi)^2$ across time for all cases normalised by χ_q , the quenching scalar dissipation for laminar diffusion flame, obtained from solving the steady flamelet equations in mixture fraction space. All cases have the same initial χ profile as δ_z is fixed throughout to maintain the focus on the effects

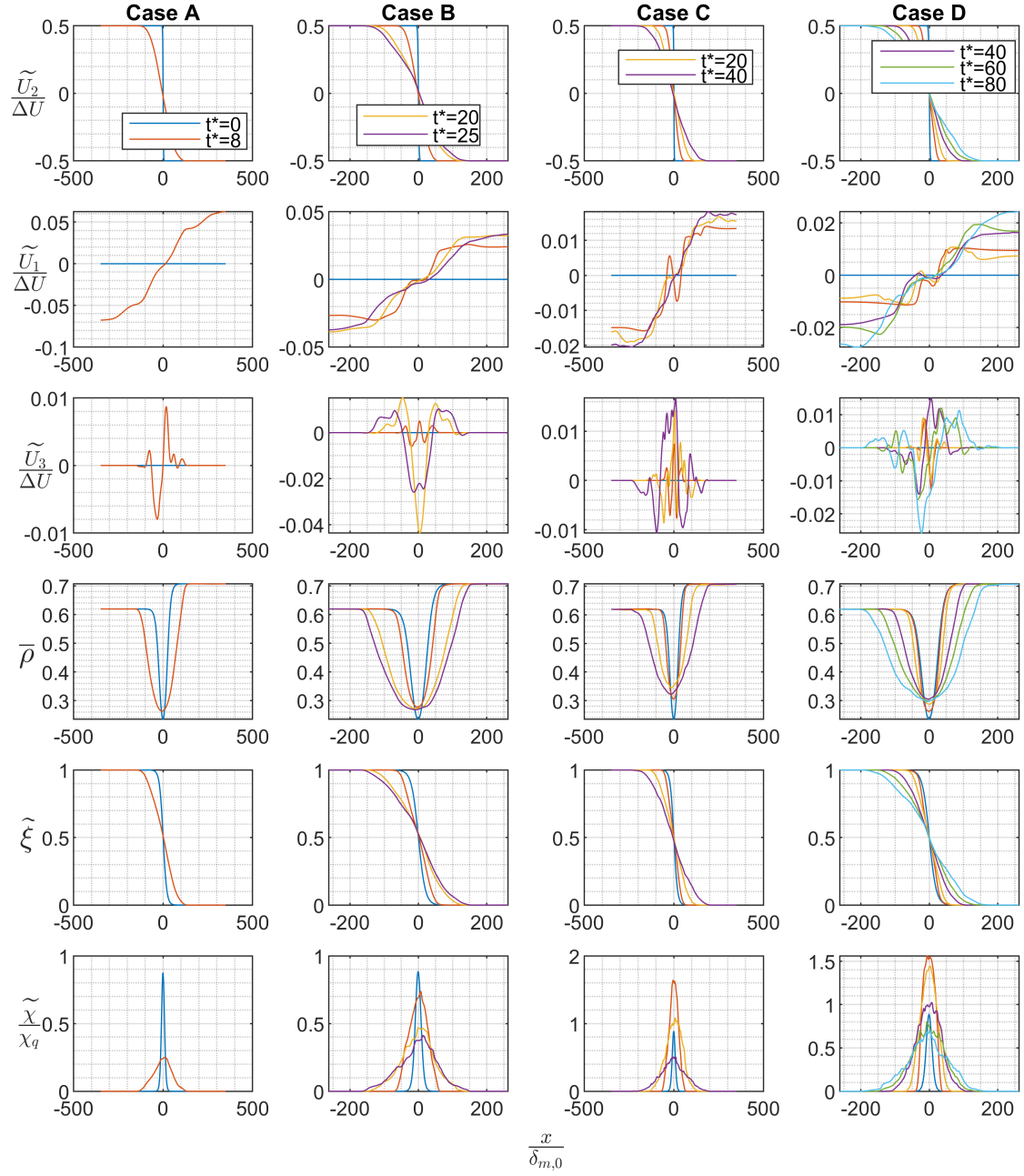


FIGURE 5.3. Favre averaged key quantities at different normalised times, $t^* = \frac{t\Delta U}{\lambda_{min,0}}$. The x-axis is the cross-stream dimension normalised by $\delta_{m,0}$. Velocities are normalised by ΔU and scalar dissipation by χ_q . To prevent obscuring the figure, only legend entries corresponding to new times are added from Case A to D. Therefore, for all figures, $t^* = 0$ is blue, $t^* = 8$ is red, and $t^* = 20$ is yellow (if present).

of the initial perturbation. For reacting non-premixed flames, the peak scalar dissipation coincides with the centre of the shear layer where the highest scalar gradients exist, along with the compressive stress from the density drop due to reactions. With time, this peak should

reduce, at a decreasing rate, in the presence of a steady flame as better mixing ensues, reducing the gradients. This is what's observed in Cases A and B. However, the scalar dissipation increases considerably in Cases C and D before eventually decreasing. This behaviour is characteristic of prominent chemistry-turbulence interactions. χ values greater than χ_q do not necessarily imply complete flame blow-out, as non-premixed flames can intermittently sustain higher strain rates than those that would otherwise quench a steady laminar flame, as the unsteady flame endures a response time to transition to the higher strain [147], [148]. However, the rapid decrease in the peak χ value for Case C between $t^* = 8$ and $t^* = 20$ once more indicates extinction that leads to a steep relaxation of the gradients. More analysis of the flammability of the cases is presented in Chapter 6.

5.4.2 Mixture Fraction Variance

Figure 5.4 shows the mixture fraction variance against cross-stream location normalised by the mixing zone thickness. The normalisation of the horizontal axis produces a good alignment of the variance profiles between the cases. Two different normalised time instants are shown; the first corresponds to the latest time achieved by Case A, which is also close to the normalised time quoted to mark the onset of the mixing transition in [44]. The second time instant corresponds to the start of the transition's second linear growth rate stage identified earlier. At $\frac{t\Delta U}{\lambda_{min,0}} = 8$, all cases demonstrate a scalar variance profile that resonates with early-time mixing behaviour. It is predicted that two vortex pairing events would have occurred for all cases by this time. The profiles manifest two distinct peaks and a trough towards the centre due to fuel and oxidizer streams going towards the centre of the shear layer, where mixing is most rapid and sharp scalar gradients are still maintained.

By $\frac{t\Delta U}{\lambda_{min,0}} = 20$, δ_z has grown to almost double the size of the earlier time in all cases (except Case A, which doesn't reach this time); however, the span of the core of the mixture fraction variance appears to maintain the same normalised width. This shows that the large-scale mixing zone width correlates quite well with the mixture fraction variance. Furthermore, since the mixing zone thickness dependence on the seeding perturbation is clear and predictable, as demonstrated earlier in Figure 5.2, this suggests that information about the seeding KHI

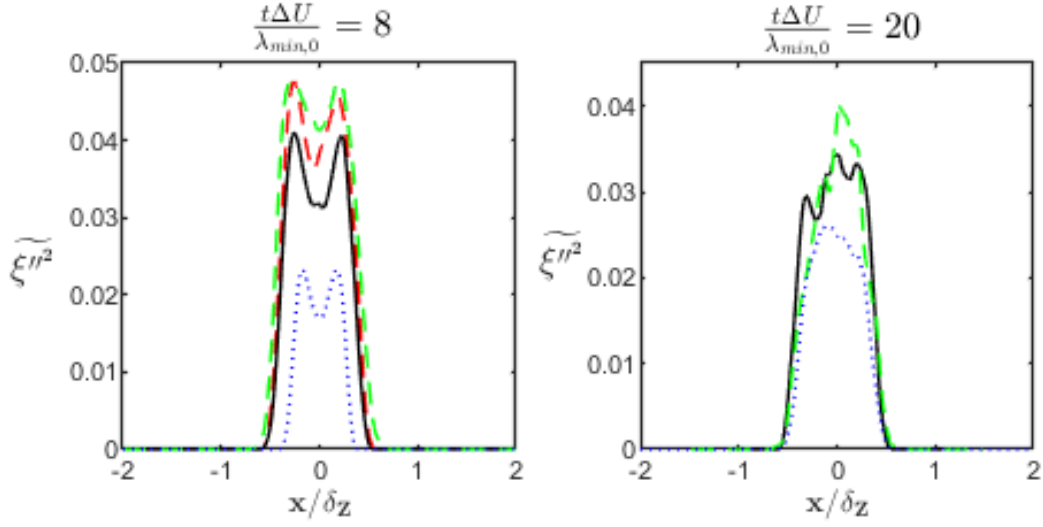


FIGURE 5.4. Favre mixture fraction variance at two normalised times. The colour scheme is specified in Table 3.1.

attributes can be used to track mixture fraction variance profiles, $\tilde{\xi}''$, which carries some significance for combustion modelling (where the mixture fraction variance transport is solved).

A reduction of the overall scalar variance magnitude is observed at the later time, as the flow is at a more mixed state. For Cases C and D, the two variance peaks have merged into one, as expected at the onset of the mixing transition. Case B, however, hasn't established a well-defined single peak variance profile, which indicates it is still transitional. This result highlights that factors other than the magnitude of the initial streamwise instability wavelength and ΔU may affect the mixing transition, and allowing the shear layer to evolve to a later normalised time alone doesn't guarantee the onset of turbulent mixing.

Moreover, although Case B and C attained higher integral mixing thicknesses and growth rates in Figure 5.2, they do not demonstrate effective mixing at the smaller scales, where Case D is seen to mix more rapidly than both Cases B and C. Therefore, observing the transition at the larger mixing scales doesn't necessarily guarantee it on the smaller scales. In fact, although the momentum and mixing zone thicknesses collapse between these cases under appropriate normalisations, they exhibit different mixing profiles, as shown in Figure 5.4 at $\frac{t\Delta U}{\lambda_{min,0}} = 20$.

Besides the small deviation of Case B, these results reinforce the temporal limit of $\frac{t\Delta U}{\lambda_{min,0}} = 20$ to mark the transition on both mixing measures. Since both Cases B and C have the same KHI wavelength range, the reason why Case C attains better mixing at $t^* = 20$ than B must be due to different ΔU . However, this further branches into two possible reasons. Firstly, a higher ΔU in Case C leads to a higher Reynolds number, which provides more support for small-scale structures that enhance mixing, even at the same t^* value. Secondly, since both are reacting cases, a higher ΔU in Case C leads to a higher flame strain, which reduces flammability in Case C relative to B. Less combustion in Case C leads to less dissipation of the small-scale turbulence, which leads to better mixing [61].

Therefore, it is likely that both these reasons together lead to better mixing in Case C than B. However, since the analysis presented in Chapter 4 consistently reinforced the significance of the $t^* = 20$ in characterizing the transition, it is more likely that the flow-chemistry interactions are the main reason behind the discrepancy of Case B as they are an added element of variability that was not previously accounted for. Nevertheless, since the current focus is on the mixing rather than the flame structure or flow-chemistry interactions, the next section examines the Reynolds number.

5.5 Reynolds Number Evolution

Two different Reynolds number definitions are employed to characterise the differences in turbulent mixing between the DNS cases. The first is based on the streamwise Taylor microscale, Re_{λ_y} which is re-defined as:

$$Re_{\lambda_y} = \left\langle \frac{u_2'' \lambda_2}{\bar{\nu}} \right\rangle_{\delta_z} \quad (5.2)$$

where $u_2'' = \sqrt{\overline{(U_2 - \widetilde{U}_2)^2}}$ is the streamwise velocity RMS, and the streamwise Taylor length scale is given by:

$$\lambda_2 = \sqrt{\frac{\overline{u_2''^2}}{(\partial u_2' / \partial x_2)^2}} \quad (5.3)$$

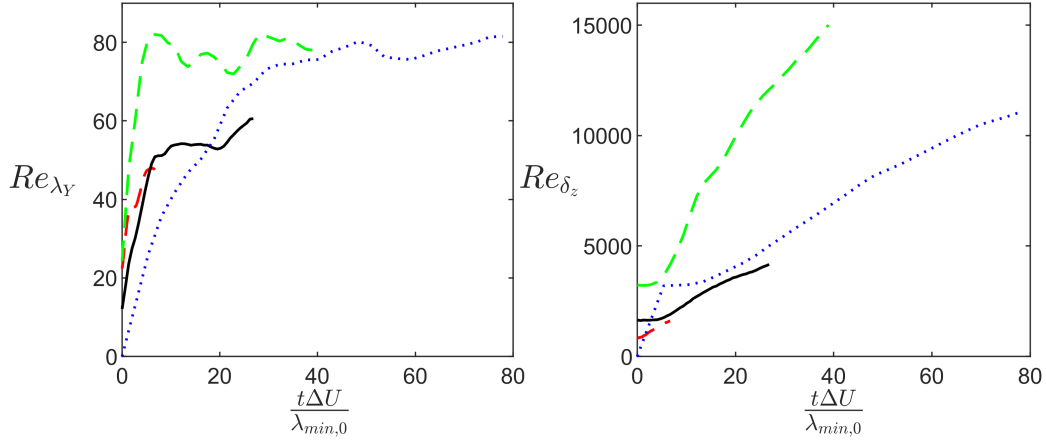


FIGURE 5.5. Taylor Reynolds number calculated within the mixing zone (left), and shear layer thickness Reynolds number based on the mixing zone width (right). The colour scheme is specified in Table 5.1.

This definition is used as it accounts for the anisotropy of the flow configuration and since Taylor Reynolds numbers have been universally used to characterize the onset of fully developed turbulence [2]. Full details on the averaging notations employed are disclosed in Chapter 2, Section 2.2.1.2.

The second Reynolds number definition is based on the mixing zone thickness to obtain a large-scale mixing Reynolds number measure for comparison:

$$Re_{\delta_z} = \frac{\Delta U \delta_z}{\bar{\nu}}. \quad (5.4)$$

The evolution of both Reynolds numbers with t^* is reported in Figure 5.5. Unlike the results of the inert cases in Chapter 4, none of the present cases cross the $Re_{\lambda_y} = 100$ threshold, highlighting the effect of the flow-chemistry interaction.

Since the mixing zone corresponds to a large length scale (judging from its normalised value relative to the domain size in Figure 5.2 (A)), it is safe to count it as a visual thickness and hence $Re_{\delta_z} \approx Re$. Only Cases C and D cross the 10^4 Re_{δ_z} threshold (as discussed in Chapter 4). Although Case C crosses this threshold just after $t^* = 20$, the Taylor Reynolds numbers for both Case B and D are the same at this t^* value (both well below the 100 threshold). Since Case D has the most homogenized mixture fraction variance profile in Figure 5.4 while having the same Reynolds number as Case B, which shows less homogenization, this confirms the

discrepancy between Cases B and C in Figure 5.4 is not due to the Reynolds number of Case B being lower, but due to flow-chemistry interactions as initially proposed.

In Figure 5.5, Re_{λ_y} stabilizes and reaches a maximum at different normalized time instances depending on the initial perturbation wavenumber, with Cases A, B and C all saturating prior to Case D in normalised time. This is contrary to the observation with the inert cases in Chapter 4, Figure 4.12, which supports that this saturation is an artefact of flow-chemistry interactions. This highlights an inverse relationship between the initial perturbation wavelength and the time at which Re_{λ_y} saturates, which is somewhat consistent with the trend of mixing layer thickness growth rates reported earlier, as cases with larger initial perturbation wavelengths grow faster and hence saturate quicker. Still, the alignment of the saturation points between cases of the same initial perturbation wavelength is striking. Cases A-C, which has the same normalised initial perturbation bandwidth as shown in Table 5.1 saturate at the same t^* whereas Case D, the only case that has a smaller initial perturbation wavelength bandwidth (shown by larger wavenumber in Table 5.1), saturates at a later t^* value.

Moreover, the results show that the magnitude or final saturation of the Taylor-Reynolds number depends not solely on the initial perturbation wavelength but on the initial free-stream velocities, which once more points towards the effects of flow chemistry interactions. Since all cases have the same initial momentum thickness, then Cases with higher ΔU have a higher mean effective flame strain rate and are therefore able to sustain a higher level of turbulence before the laminarising effects of combustion prevent any further turbulence growth, i.e. an equilibrium is reached. Therefore, the growth rate of the Taylor-Reynolds number is controlled by the initial perturbation wavelength, whereas ΔU controls its maximum equilibrium magnitude. The same saturation is not observed in Re_{δ_z} as the free-stream mean velocities remain unperturbed throughout the flow evolution, and δ_z grows at a rapid rate, far exceeding the rise in viscosity with increased temperature due to combustion.

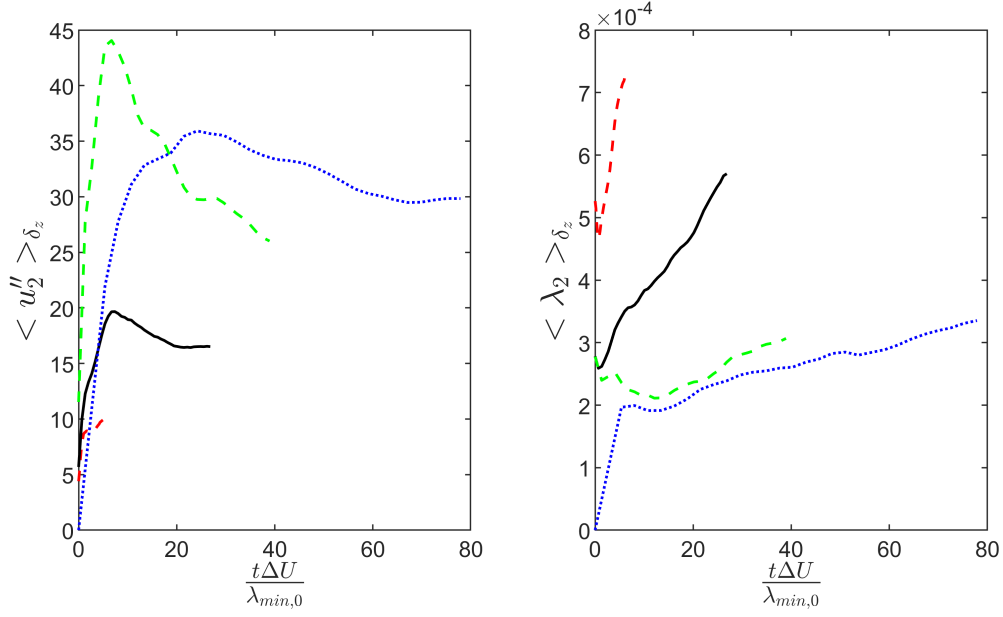


FIGURE 5.6. Streamwise velocity RMS calculated within the mixing zone (left), and streamwise Taylor length scale within the same region (right). The colour scheme is specified in Table 3.1.

To gain further clarity on the trends observed in Re_{λ_Y} , a closer inspection of its constituent streamwise velocity RMS and Taylor length scales is presented in Figure 5.6. Both quantities are averaged within the confines of the mixing layer (as was done with Re_{λ_y}) for consistency and to reduce statistical noise. The results show that for Cases B and C at $t^* = 7$ the streamwise velocity RMS reaches its peak and starts decreasing afterwards.

This t^* value marks their Re_{λ_y} saturation corresponding with the point where the cases exhibit a sharp drop in their RMS velocity, marking the increased turbulence dissipation from combustion. The trends in Taylor length scale growth align with the previous observation of the large-scale mixing layer thickness, showing higher lengths and growth rates for reducing perturbation eigenvalue. The profiles of both Cases C and D are closest in both the velocity RMS and the Taylor length scale, supporting why their Re_{λ_y} reach similar asymptotes.

It is also worth noting that since the cases examined here maintain the same domain sized as their inert counterparts (or even larger for Case C), which did not exhibit this saturation in Reynolds number (as shown in Chapter 4, Figure 4.12), the effects observed and analysed in

this section are not due to domain limitations. This is further supported by the integral length scale assessment in Chapter 3.

5.6 Mixing Scales and Asymptotic Behaviour

5.6.1 Integrated Scalar Dissipation Rate

With this chapter mostly concerned with the mixing aspect of non-premixed combustion, scalar dissipation is discussed next since it plays a pivotal role in tracking the physics of non-premixed regimes and, hence, their modelling [149], [150]. This warrants exploring the effects of the initial perturbation on its temporal evolution. Since flames in these mixing layers develop into a statistically one-dimensional profile at late time, a measure of the integrated scalar dissipation rate in the heterogeneous cross-stream direction is expected to converge to a constant value. Here, the normalised integrated scalar dissipation rate is defined as

$$L_\chi = \frac{1}{\Delta U \left\langle \widetilde{\xi''^2} \right\rangle_{\delta_z}} \int_{x_0 - \delta_z}^{x_0 + \delta_z} 2D \widetilde{(\nabla \xi'')^2} dx \quad (5.5)$$

From classical flamelet theory [151], scalar dissipation measures the normal strain subjected to a diffusion flame by considering the scalar gradients. Since the overall normal strain is proportional to ΔU in shear layer configurations, the normalisation here is dimensionally sound and will allow direct comparison between the cases.

Although there was significant variation in both the directional evolution and magnitude of Favre averaged total scalar dissipation values in Figure 5.3, Figure 5.7 (left) indicates a potential asymptotic stabilisation at $0.33 < L_\chi < 0.38$, considering the different equilibrium levels of Cases B, C, and D.

This behaviour in the reacting flows considered is similar to the reported stabilisation of turbulent dissipation in inert flows as observed in Chapter 4 and consistent with the results in [11], [37], [55], and is indicative of mixing evolving in a self-preserving state. This asymptotic evolution is also observed to transpire around $t^* = 20$ rather than coinciding with the t^* values

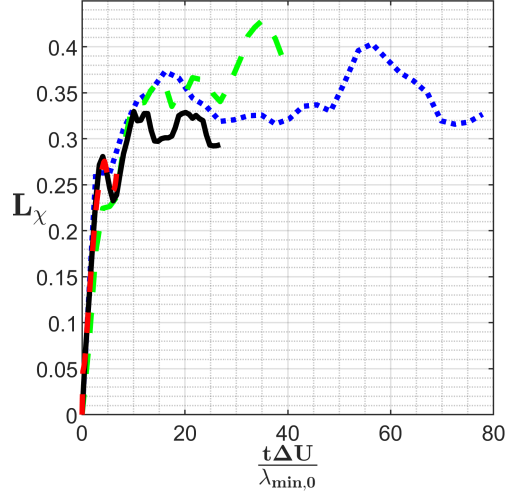


FIGURE 5.7. Evolution of the normalised integrated scalar dissipation rate for Cases A-D. The colour scheme is specified in Table 5.1.

that corresponded to the plateau of Re_{λ_y} in Figure 5.5, supporting that it is indicative of an asymptotic mixing state rather than the product of turbulence-chemistry interactions. Note that due to flow-chemistry interactions, the turbulent kinetic energy dissipation is affected by combustion and its integrated value for reacting cases doesn't conform to the self-similar profile observed in Chapter 4, Figure 4.7.

5.6.2 Mixture Fraction Variance Transport Budget

In conventional steady diffusion flames, diffusive transport significantly dominates over convective [92]. To verify if this is the case in developing shear layers, the Favre averaged mixture fraction variance balance equation is considered [63]. This equation is widely used to calculate $P(\xi)$ in combustion models (usually a β -function). Assuming the molecular diffusion terms are negligible compared to the other terms and omitting them:

$$\frac{\partial \widetilde{\rho \xi''^2}}{\partial t} + \frac{\partial (\widetilde{\rho U_i \xi''^2})}{\partial x_i} = -\frac{\partial}{\partial x_i} (\widetilde{\rho U_i'' \xi''^2}) - 2\widetilde{\rho U_i'' \xi''} \frac{\partial \widetilde{\xi}}{\partial x_i} - \widetilde{\rho \chi''} \quad (5.6)$$

The dissipation term in the above equation constitutes $\widetilde{\chi''} = 2\widetilde{D(\nabla \xi'')^2}$ which appears inside the integral in Equation 5.5. Since the means are computed across the homogeneous planes and omitting the unsteady term (validity of this will be assessed from the budget total

as observed later), only the cross-stream spatial derivatives remain. Dividing by $\bar{\rho}$ across Equation 5.6 and integrating in the cross-stream direction within the mixing zone yields:

$$\underbrace{\int_{x_0-\delta_z}^{x_0+\delta_z} \frac{1}{\bar{\rho}} \frac{\partial (\bar{\rho} \widetilde{U_1 \xi''^2})}{\partial x} dx}_C = - \underbrace{\int_{x_0-\delta_z}^{x_0+\delta_z} \frac{1}{\bar{\rho}} \frac{\partial}{\partial x} (\overline{\rho U_1'' \xi''^2}) dx}_{TT} - \underbrace{\int_{x_0-\delta_z}^{x_0+\delta_z} 2 \widetilde{U_1'' \xi''} \frac{\partial \widetilde{\xi}}{\partial x} dx}_P - \underbrace{L_\chi \Delta U \langle \widetilde{\xi''^2} \rangle_{\delta_z}}_D \quad (5.7)$$

The term on the left side is the convective term (C), and the right side constitutes the turbulent transport (TT), production (P), and dissipation terms (D), respectively. Stationary self-similar mixing evolution manifests when the above terms balance to render the unsteady term zero, as shown in Figure 5.8, where this also coincides with $\frac{t\Delta U}{\lambda_{min,0}} = 20$ for Cases B and C. This is not the case for D, where the total reaches zero much later at $\frac{t\Delta U}{\lambda_{min,0}} = 50$ due to a persistently large magnitude of the production term, potentially due to varying levels of flow-chemistry interaction for this Case that alters the flow composition and delays the steady mixing evolution.

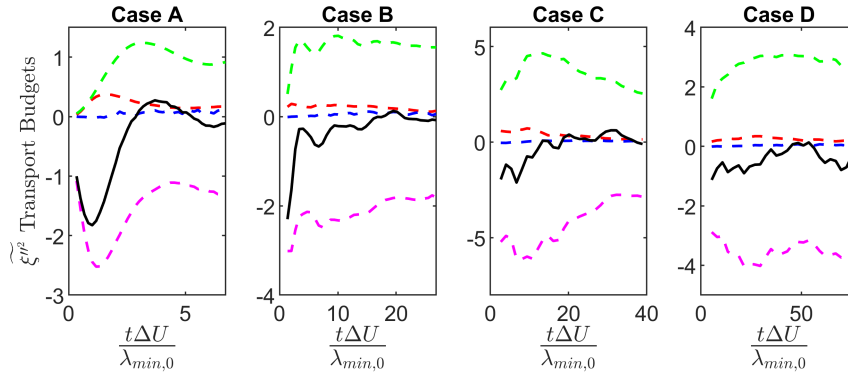


FIGURE 5.8. Mixture fraction variance transport budgets, with C (dashed blue), TT (dashed red), P (dashed magenta), D (dashed green), and total (solid black) shown for all cases across normalised time.

Since the total dissipation constitutes a sizeable portion of the mixture fraction transport budget, it's sensible that its pseudo-stabilisation is indicative of steady mixing evolution as proposed. Compared to steady diffusion flames, the results show that while the diffusive transport is significant, it almost mostly balances the production term that results from the

growing transverse flux as the shear perturbation evolves. The results also show prominent unsteady effects until at least $t^* = 20$.

5.6.3 Mechanical-to-Scalar Mixing Time Scale Ratio

With a prominent disparity between the mechanical and mixing behaviour (discussed above) and with the importance of the interaction of these two scales in combustion modelling, the mechanical-to-scalar mixing time scale ratio is defined as:

$$r_z = \left\langle \frac{\widetilde{\mathcal{K}}}{\widetilde{\epsilon}} \middle/ \frac{\widetilde{\xi''^2}}{\widetilde{\chi''}} \right\rangle_{\delta_z} \quad (5.8)$$

The evolution of this ratio is shown for all cases in Figure 5.9, where r_z is shown to stabilize at late time. The clear stabilisation of r_z to an order of unity is consistent with previously obtained results for turbulent non-premixed combustion [93], [123], [152]. The asymptotic evolution is more apparent in cases that reach later nondimensional times. The stabilisation of L_χ and r_z in Cases C and D indicates a balanced mixing between streamwise convective and cross-stream diffusive mixing. The discrepancy between the r_z profiles before $t^* = 20$ foreshadows the mechanical and mixing behaviour imbalance and shows dependence on the seeding instability during the transition process.

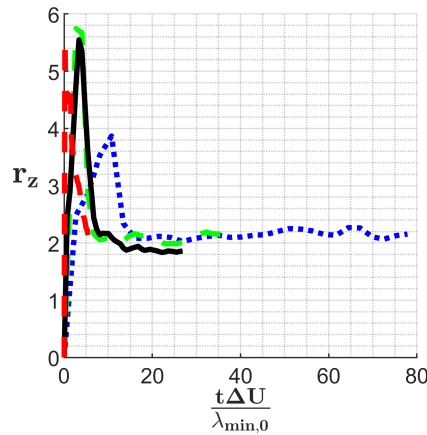


FIGURE 5.9. Evolution of the mechanical to scalar mixing time scale ratio for Cases A-D. The colour scheme is specified in Table 5.1.

In fact, Figure 5.9 shows that the higher the wavenumber of the seeding perturbation, the more delayed the peak r_z even under temporal normalisation by the instability timescale. Furthermore, the trend in the t^* value when the plateau is reached is consistent with the observations of the Taylor Reynolds number in Figure 5.5. Cases A-C maintain the same KHI wavelength bandwidth level at $t^* = 7$, whereas Case D, with the smaller perturbation wavelength (relative to the domain size) level at double the downstream distance at a $t^* = 15$. Unlike Re_{λ_y} , however, the magnitudes of the asymptotes are almost identical between the cases, which indicates that the impact of the free-stream velocities on the stationary Re_{λ_y} value is due to the feedback of the chemistry on the flow through viscosity (rather than scalar dissipation rate), and since viscosity does not directly affect r_z , the impact on the magnitude is more subtle in Figure 5.9.

The results, therefore, confirm that the effects of the initial perturbation wavelengths manifest at the small mixing scale and control both the transitional evolution and the onset of the equilibrium state. However, unlike with flow and turbulence development analysed in Chapter 4, the onset of stationary evolution is not universal between the cases explored at $t^* = 20$ at the varying mixing measures investigated owing to the added variability of flow-chemistry interactions.

5.7 Mixture Fraction PDF Evolution

To explore whether the turbulent transition impacts the PDF profiles of the flows, the PDF of the mixture fraction is analysed for all cases at different planes in the heterogeneous cross-stream direction. This is also undertaken to assess whether additional variabilities manifest between Cases C and D since these are the ones that attain a clearly developed state as evidenced by both the contours and the asymptotic statistics. Results for three different normalised time instants were chosen for the comparison as shown in Figure 5.10. Assessing whether $P(\xi)$ exhibits marching/non-marching behaviour is a useful diagnostic to determine the mixedness state of the flow throughout the shear layer as discussed in [11], [44]. These categorizations are based on whether the most probable scalar mixtures vary with cross-stream

(vertical) distance across the shear layer. Non-marching is when the mixing is thorough and characterized by PDFs that stagnate about a constant profile peak. Marching is when the PDF profile peaks monotonically march with transverse distance- either monotonically increasing or decreasing with transverse distance towards the free streams (depending on the scalar value in the free streams).

Non-marching behaviour implies a more homogeneous fuel-oxidiser mixture across the span of the shear layer in the heterogeneous direction and results from persistent large-scale eddies that heavily entrain the shear layer and introduce the free streams towards its centre. Non-marching behaviour is more characteristic of small-scale structures that localise mixing at the periphery of the shear layer with less drastic entrainment of the free streams.

Marching/non-marching profiles carry significant implications for combustion, as marching behaviour implies a direct correlation between the heterogeneous coordinate and the mixture fraction field. Moreover, a marching profile induces a flamelet-like behaviour where the stoichiometric surface is mostly restricted within a single plane in the heterogeneous direction. This may indicate that flamelet closure approaches are highly relevant in such flow conditions consistent with classical diffusion flame behaviour. Therefore, understanding the dependence of the mixture fraction PDF on the seeding perturbation is fundamental to choosing the most appropriate combustion modelling approach for LES and RANS studies.

However, the literature has no consensus on whether turbulent mixing layers universally manifest marching or non-marching behaviour. A large number of experimental investigations of mixing layers attaining high visual-thickness based Reynolds numbers (over the turbulent threshold outlined by Dimotakis [9]) provide conflicting PDF behaviour as outlined in the review presented in [44]. This supports that a visual thickness-based Reynolds number alone is an insufficient predictor of a final state of mixing, consistent with the discrepancy observed between different Reynolds number definitions as discussed. Instead, consideration of the initial perturbation (the forcing function of the mixing layer) and the resulting mechanism of energy transfer is explored in this section to outline correlations.

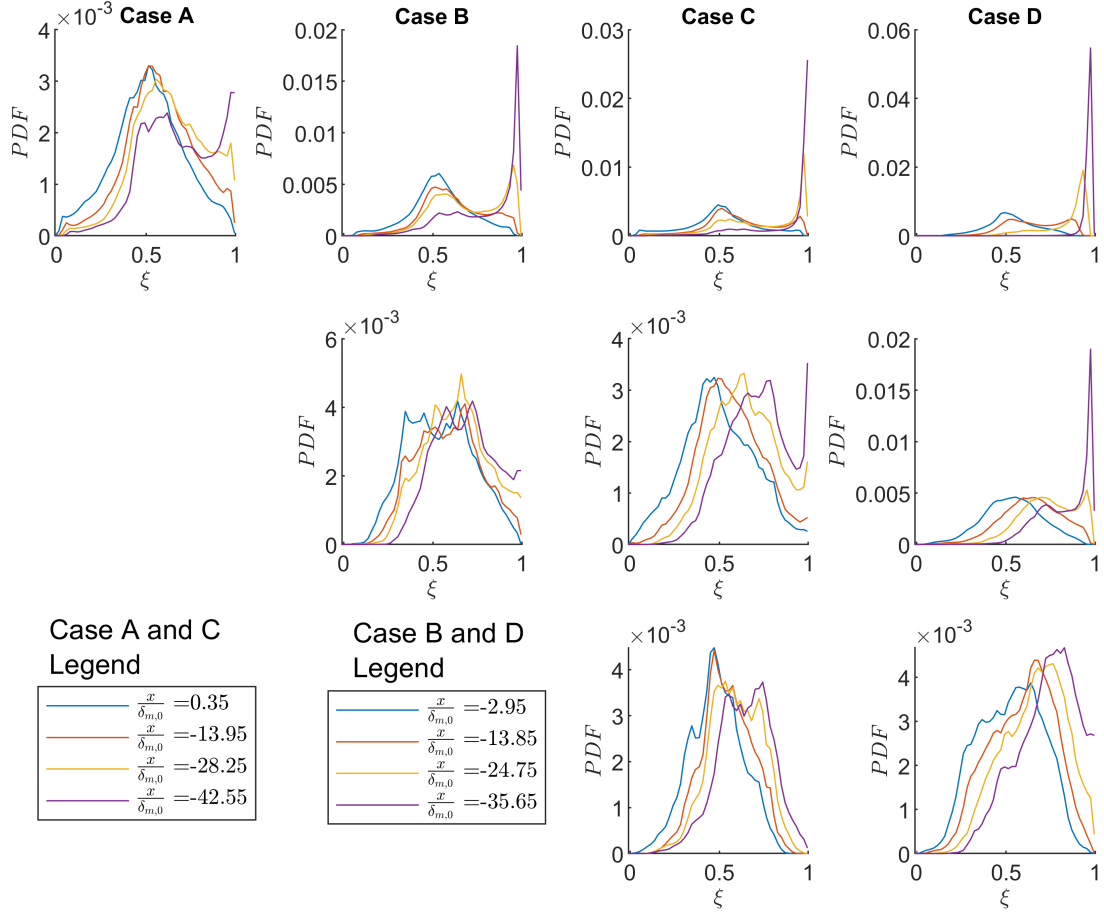


FIGURE 5.10. $P(\xi)$ throughout different planes in the heterogeneous direction (transverse) for Cases A-D and at three different normalised times, $\frac{t\Delta U}{\lambda_{min}}$: 8 (top), 20 (middle), and 40 (bottom). Cases A and C have the same legend entries, while cases B and D have another set of legend entries that are both outlined in the bottom left of the figure.

To track $P(\xi)$ across the heterogeneous planes, two legends are provided in Figure 5.10. Cases A and C have the same transverse domain extent as outlined in Table 5.1, and therefore maintain the same increment across the $\frac{x}{\delta_{m,0}}$ bins. Thus, the plots of Cases A and C follow the same legend. The same applies to Cases B and D, which have the same transverse extents and thus follow the same separate legend. The transverse spatial increment in the PDF profiles demonstrated were chosen based on proximity to enable better comparison. Contours are presented only for a single direction away from the centre plane (towards the fuel side) as the results are symmetric about the shear layer centre and follow the same trend on either side.

Figure 5.10 shows a consistent non-marching behaviour for all cases at $\frac{t\Delta U}{\lambda_{min,0}} = 8$ as a second vortex amalgamation has not yet homogenised the large scale eddies in any of the cases. By $\frac{t\Delta U}{\lambda_{min,0}} = 20$, Cases C and D begin showing marching behaviour but to varying extents. Case D exhibits stronger PDF marching owing to its smaller initial perturbation bandwidth, which leads to a higher prevalence of small-scale eddies. This is further confirmed by comparing the PDF of the peripheral plane between Cases C and D (i.e. $\frac{x}{\delta_{m,0}} = -42.55$ for C), where for Case C it shows greater mixing due to the large scale eddies that entrain from the free-streams. Conversely, the profile of Case D on this plane remains largely comprised of fuel. The PDFs of Case B at $t^* = 20$ exhibit clear non-marching behaviour. This is consistent with the contour visualisations in Figure 5.1 that correspond to $t^* = 20$ (only for Case B) and demonstrate a large extent of coherent structures. This also agrees and explains the inhomogeneous mixture fraction variance profile for Case B at $t^* = 20$ in Figure 5.4.

Interestingly, however, by $t^* = 40$, like Case B at $t^* = 20$, Case C reverted back to fully non-marching behaviour after showing some marching tendency at $t^* = 20$. Conversely, Case D maintains its marching behaviour at $t^* = 40$. These observations are consistent with the ones made earlier in Section 5.3.1 regarding the level of turbulence in the mixing contours of Cases C and D at their latest simulation time. The results reaffirm the importance of the seeding perturbation wavelength range in controlling the state of mixing even when both cases attain similar mixing Reynolds numbers. This further verifies that the effect of the initial perturbation on mixing manifests at a late time and is not just important during the transition process.

5.8 Conclusion

This chapter assessed the effects of the initial fundamental primary shear instability on the mixing evolution in developing flows. While Chapter 4 assessed inert mixing layers for their flow and turbulence development, reacting cases were considered in the present chapter to derive a direct correlation with the resulting flame behaviour in the subsequent chapter. While the flow and turbulence scales are directly related to the seeding velocity fluctuations, mixing

effects are more buffered through transport properties and flow composition. Nevertheless, the results directly correlate the seeding perturbation eigenvalue parameters and the mixing evolution.

At large mixing scales, the mixing evolution depends more on the free-stream velocities than the initial KHI wavelengths, consistent with the earlier experimental investigations of Karasso and Mungal [50]. However, assessing finer mixing scales and Reynolds numbers reveals a further dependence on the initial perturbation wavelength bandwidth (relative to the domain dimensions). These are reported and analysed across various mixing parameters. Furthermore, the larger the KHI wavelength bandwidth, the quicker the onset of an asymptotic mixing state, even at different Reynolds numbers, consistent with the larger and more rapid normalised growth rates of these larger wavelengths that were previously reported on in Chapter 4.

The results of this chapter emphasize the importance of accounting for the effects of the initial perturbation when attempting to characterize the onset of the turbulent mixing transition or the steady-state mixing state. For instance, even though Cases C and D attained the same Taylor Reynolds number asymptote, they exhibited different final PDF behaviour due to the distinct states of their final eddy structures and distribution. This consideration of the initial perturbation and the downstream distance from the onset of the seeding instability should extend to mixing closure models in combustion modelling approaches.

Unlike the trends observed with the inert cases in Chapter 4 that revealed a consistent t^* value of 20 to correlate with the asymptotic self-similar evolution of various flow and turbulence parameters, the mixing attributes explored in this chapter did not maintain the same consistent dependency on a unique t^* value. This was systematically assessed across several mixing parameters and was determined to be due to the added variability of flow-chemistry interactions that were not present in the inert cases. The explicit assessment of the chemical behaviour that reveals deeper insights into this flow-chemistry interdependency is undertaken in Chapter 6.

Flame Structure Dependence on Narrowband KHIs in DNS of Transitional Reacting Shear Layers

6.1 Introduction

The previous chapter highlighted how varying the initial perturbation affects turbulence development and mixing. Since the shear layers investigated predominantly undergo non-premixed combustion, the cases are expected to exhibit varying levels of extinction and reignition due to the different extent and timing of flame-turbulence interactions in Cases A-D. Since the strain imposed by turbulence on the flame can promote extinction, and since the onset of turbulence is correlated to the initial perturbation scales as demonstrated in the previous section, the question is then whether a similar direct link manifests between the initial perturbation and the flammability and whether that is expressed through different combustion regimes of the mixing layer. In fact, assessing the flame structure evolution between cases initialised from different perturbations provides a stringent diagnostic of the small-scale mixing attributes of the transition and their dependence on the initial instability. This is, therefore, the subject of the present chapter, which analyses the same cases presented in Chapter 5 and whose parameters are outlined in Table 5.1. Besides informing on the flame structure dependence on the seeding instability, this chapter also aims to provide some combustion modelling for developing flows.

6.2 Qualitative Flame Behaviour

Figure 6.1 presents the temperature contours at the latest simulation run time for Cases A-D. The stoichiometric surface and regions of high scalar dissipation are also marked. The total

scalar dissipation, χ , rather than the fluctuation scalar dissipation χ'' , is presented to compare directly with the dissipation in steady laminar flamelets.

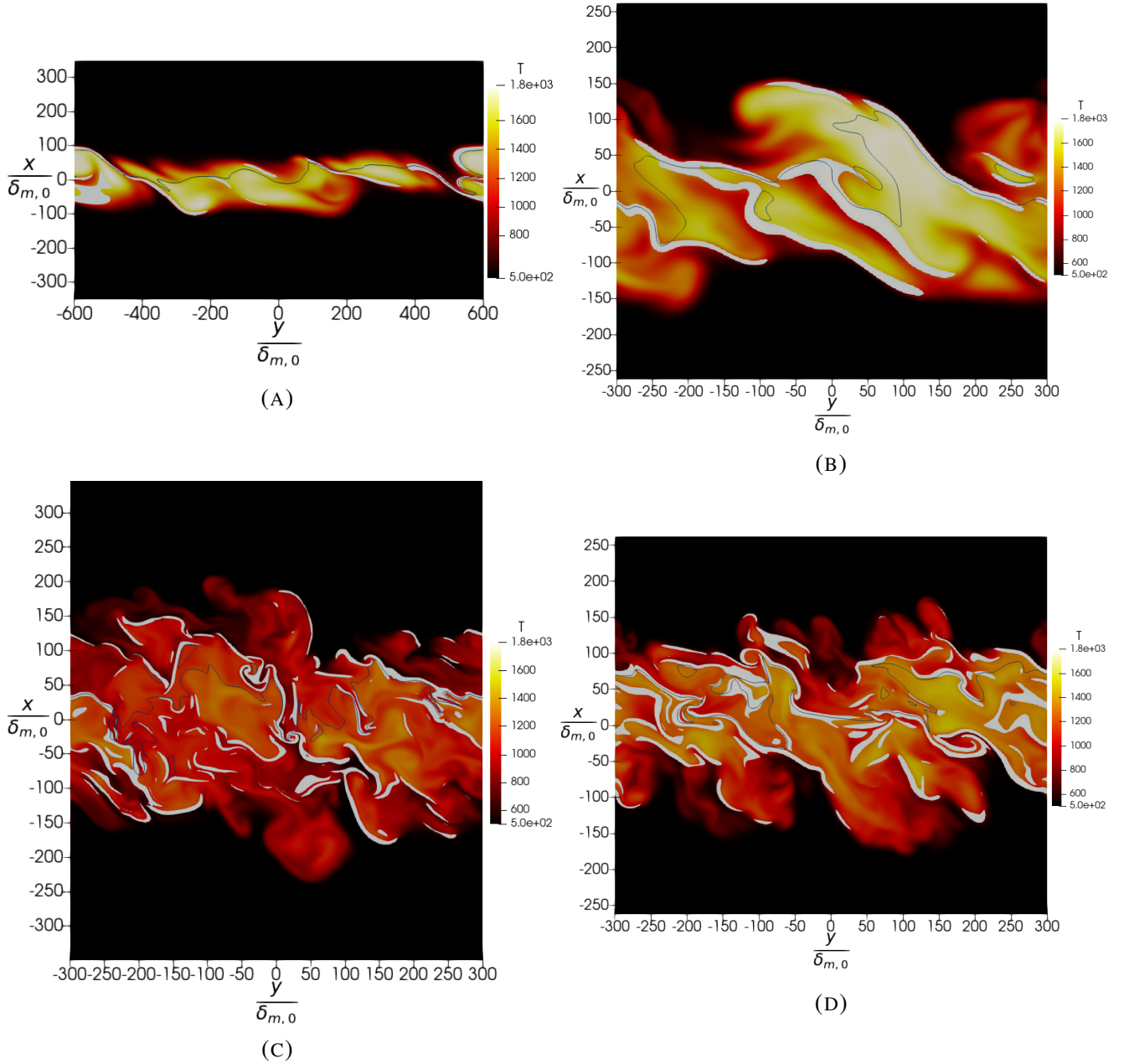


FIGURE 6.1. Instantaneous temperature contours at the latest run-time for each case overlaid with the stoichiometric surface ($\xi_{st} = 0.42$) in black, and $\chi > 50\% \chi_q$ in white. The cases correspond with figure labels. In terms of t^* values, these correspond with $t^* = 7$ for Case A, $t^* = 27$ for Case B, $t^* = 40$ for Case C, and $t^* = 80$ for Case D.

Usually, however, $\chi \approx \chi''$ at a late time, as mean gradients are small compared with the fluctuation gradients at this stage of the flow evolution. This is not the case at early times when the flow is still laminar or at early transitional stages, as fluctuations would not be sufficiently developed.

Turbulent mixing is essential for non-premixed combustion. However, the strain induced by the turbulent flow field and the mixing layer growth can significantly stretch and contort the stoichiometric surface, leading to increasingly high scalar dissipation rates and extinction. This is observed in Figure 6.1, where the more turbulent cases (C and D) show the most distorted reaction zones and high extinction levels, as evident from the lower temperatures in the flammable regions. At the time instants shown, Case C has the lowest temperatures, characteristic of extensive local extinction, followed by Case D.

In Cases A and B, flammable regions are localized and entrapped within large and relatively more organised vortical structures. As shown in Case B, the flame surface appears discontinuous between these structures, as indicated by thick zones of high scalar dissipation rate. The increased strain in these regions thins the local entrainment braids of the reactants from the free streams, which increases local mixing timescales and reduces flammability consistent with the findings in [153]. The prevalence of smaller vortices and their nonlinear interactions penetrate and merge the flammable regions in Cases C and D. Out of all the Cases, D is the only one that maintains a continuous and ignited flame surface confined to the centre of the shear layer without being clearly associated with large organised vortices. In addition to the flammable regions near the continuous stoichiometric surface, Cases B-D also show dispersed flammable kernels within the mixing zone as indicated by the ξ_{st} contours. The size of the kernel scales with the prevalent vortical sizes in each case.

6.3 Mixture Fraction Dependent Statistics

6.3.1 Significance

Reduced order manifolds are commonly endorsed in combustion modelling to capture the chemical behaviour in flow regimes with significantly reduced computational cost. With these approaches, only the transport equations of the defined manifold parameters are solved, and these parameters can then be used to directly evaluate the remainder of the thermochemical state. One of the approaches to defining these manifolds is empirically by applying principal component analysis (PCA) and/or multivariate adaptive spline regression (MARS) to experimental and DNS datasets [154], [155].

Alternatively, these manifolds can be physically derived from observing the governing equations and making suitable assumptions based on experimental and/or DNS observations [156], [157]. Both flamelet modelling and conditional moment closure (CMC) fall under the physically derived approach. Recent work through both approaches (empirical and physically derived) has concluded that two appropriately defined parameters, namely the mixture fraction and a progress variable, are adequate to close the flame structure problem more generally in combustion modelling [150], [155], [158]. The appropriate choice of these two quantities allows all combustion modes to be accounted for, so do not restrict the application to premixed or non-premixed regimes.

All cases presented here are predominantly non-premixed. For non-premixed flames, while low dimensional manifold equations retain their dependence on the progress variable at the non-premixed limit, this progress variable behaves like a time variable rather than a conditioning variable. The present focus is therefore diverted to conditional statistics in mixture fraction space to derive relevant fundamental insight into the effect of the seeding instability on the flame structure and support future model development efforts. Discussions in this section help evaluate the adequacy of this conditioning variable in capturing the thermochemical state in transitional flow regimes.

6.3.2 Extinction and Flame Strain Evolution

To illustrate the temporal patterns of the chemical state between the different cases, Figure 6.2 (a) shows the maximum ensemble Favre averaged temperature against absolute simulation time. Good alignment is observed between the cases without any temporal normalisation, and the varying extents of extinction and reignition observed are consistent with previous observations. This is contrary to the observations of the flow and mixing development in previous chapters that required appropriate temporal normalisation by the seeding instability timescale to demonstrate alignment between the cases. Figure 6.2 (b) shows the conditional mean scalar dissipation rate within the stoichiometric surface, which can be used to quantify the normal strain subjected to the stoichiometric flame surface. All cases have the same initial scalar dissipation rate as was shown previously due to the same initial momentum thickness profile. However, the scalar dissipation increases at varying rates and reaches different peaks for each case. Higher free-stream velocities are directly linked to increased normal strain on the mixing layer and increased scalar gradients, which result in higher peaks for Cases C and D. The trend of the scalar dissipation evolution is consistent with that of extinction in Figure 6.2 (a) where the cases with the highest $\langle \chi | \xi_{st} \rangle$ peaks are the ones with the most extinction. While Case A briefly brushes against χ_q in its peak at a similar time to which it shows maximum extinction, the peaks of the other cases sustain significantly higher scalar dissipation values (up to $4 \times \chi_q$ for Case C) and occur earlier than the instant of minimum $(\tilde{T})_{max}$.

Doubling the initial convective velocity between Cases A and B and again between B and C also doubles the peak scalar dissipation, showing a direct proportionality accounted for in conventional finite-rate combustion models. Meanwhile, increasing the wavenumber of the initial perturbation while increasing the convective velocity only increases the peak 1.5 times, thus somewhat attenuating the jump in normal strain. However, it is important to note that the trends in scalar dissipation are not just due to turbulence and Reynolds number effects but also due to feedback of chemistry on the flow, as Pantano [123] demonstrated how heat release reduces scalar dissipation, and hence the increase of χ in Case C can be attributable to more extreme extinction that isn't realised in the other cases.

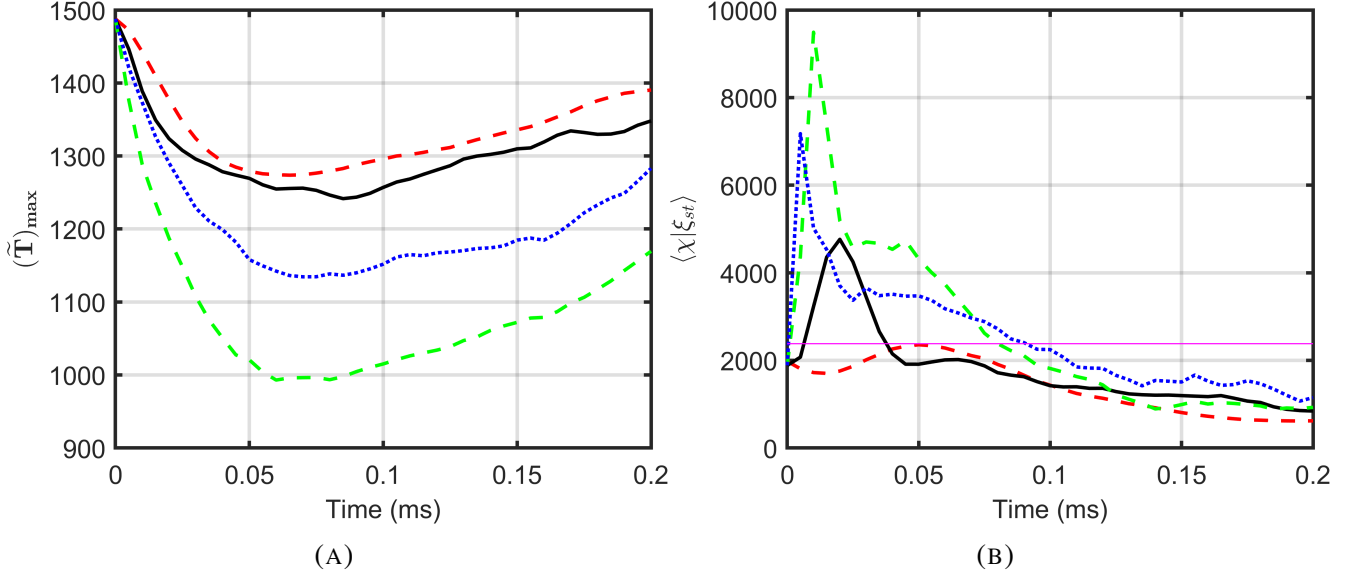


FIGURE 6.2. (a) shows the maximum of the cross-stream Favre averaged temperature profiles over time, (b) shows the stoichiometric scalar dissipation, which is the conditional mean of χ within $\xi = \xi_{st}$ contour. χ_q is indicated by the horizontal solid magenta line. The colour scheme is specified in Table 5.1.

Extinction was shown to increase not only the peak of the scalar dissipation but also the width of the profile [61], reinforcing how local extinction aggravates strain rates. Increasing the wavenumber and the convective velocities expedite the onset of the peak dissipation rate, with Case D reaching its peak at the earliest. Case C exhibits the steepest extinction, as previously pointed out, due to both the higher convective velocities that steepen scalar gradients and also the relatively more rapid growth of the mixing layer (as shown earlier in Figure 5.2). This is due to its lower initial perturbation wavenumber relative to Case D, which further stretches the flame surface and amplifies the normal strain. After 0.1 ms, the scalar dissipation rate for all cases converges to 40% of χ_q at a steady rate of decrease while interestingly aligning themselves in order of wavenumber magnitude. This highlights an essential deficiency of classical flamelet approaches when studying such flow-dependent reacting flows, as these strictly rely on scalar dissipation measures to gauge the level of strain subjected to the flame, which for transitional flows like the ones considered, would be insufficient as although at the late time all cases exhibit similar steady χ profiles they maintain drastically different flame structures as highlighted in previous statistics and the regime diagram.

6.3.3 Temperature and Heat Release Rate

Figure 6.3 shows the conditional temperature and heat release rate Favre means and r.m.s of Favre variance for all cases with conditioning on ξ . The temporal coordinate denotes absolute simulation time since, unlike mixing, normalisation with the instability time scale showed no significance or correlation between the cases in their flame profiles. The conditional mean temperature results show all cases exhibit extinction and reignition across time, albeit to varying extents. For Case A, extinction mainly manifests as a reduction in high-temperature bandwidth in mixture fraction space, with ignition becoming more centred around stoichiometry. In other cases, extinction is more severe with a drop in the temperature profile. The more turbulent cases have lower temperatures and more extreme extinction, consistent with previous observations. The temperature RMS for Cases A, B, and D are low at the start and increase with reignition, with the profiles centred slightly above stoichiometry at intermediate ξ values. Case C shows different behaviour with the highest temperature RMS building up before extinction and reducing after while maintaining relatively high values above stoichiometry around $\xi = 0.5$.

Contours for heat release rate show different behaviour than temperature, where the highest conditional means of $\dot{\omega}_T$ are before 0.05 ms for all cases with peaks towards slightly richer mixtures than the stoichiometric value. Case C exhibits the most drastic drop in heat release, which swings back up gradually afterwards. For the other cases, $\dot{\omega}_T$ remains either steady or gradually decreases after extinction. Both temperature and heat release rate standard deviations are an order of magnitude smaller than the respective means. The RMS for heat release is highest initially in leaner regions of the mixture in Cases B-D and only shifts to richer regions in cases B and C. The close similarity in the magnitudes of heat release rate between all the cases indicates similar chemical time scales, which is expected due to the same compositional initialisation in each case. The differences are, therefore, mainly due to the varying mixing rates and flow strains. The results confirm that the chemical profiles evolve temporally independently of the initial instability time scale due to the good alignment observed in the results of the different cases in absolute time. The varying degrees of extinction between the various cases result in a snowball effect that aggravates the disparity

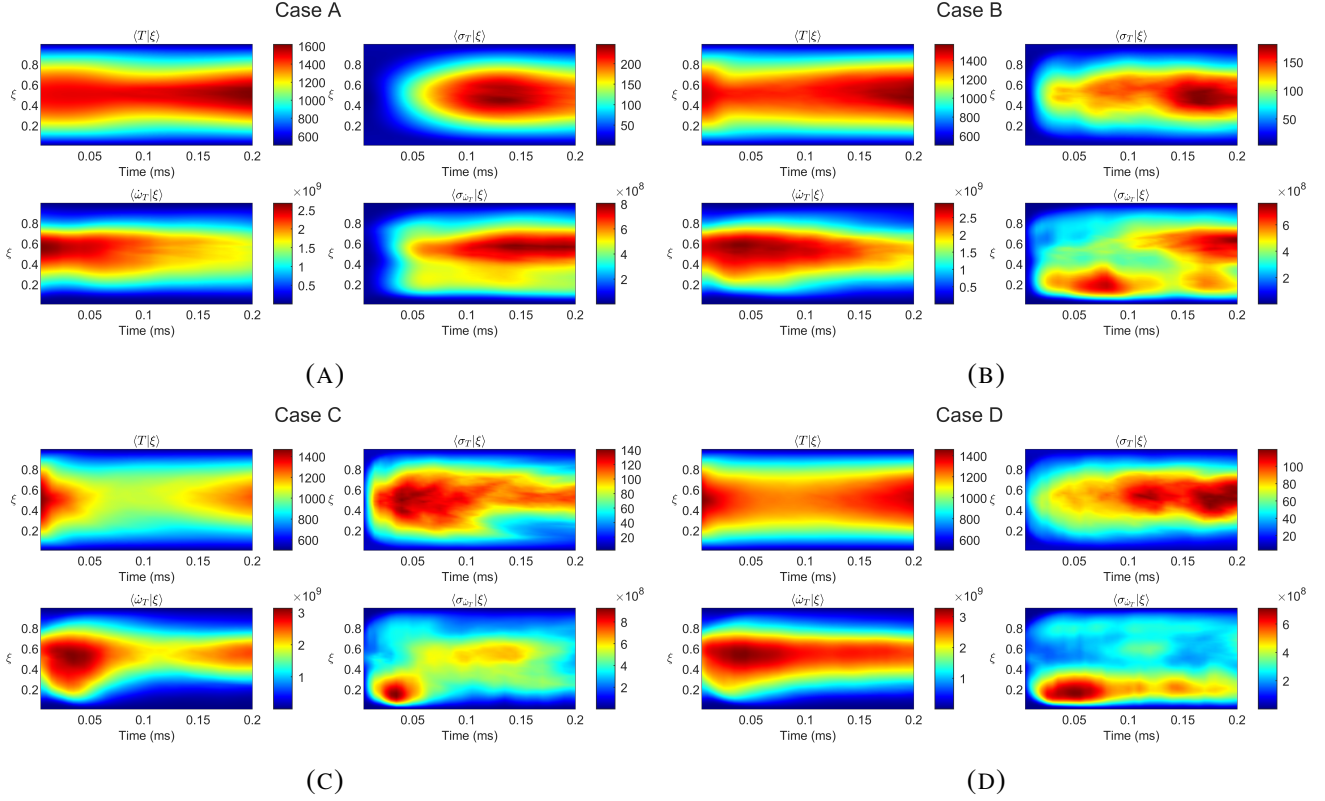


FIGURE 6.3. Temperature (top) and heat release rate, $\dot{\omega}_T$, (bottom) means (left) and r.m.s. (right) conditioned on mixture fraction for all cases across absolute simulation time.

in the flame behaviour between the cases at later times. More aggressive extinction results in better mixing.

The lack of alignment of heat release rate and temperature in time is because temperature is not necessarily a direct measure of chemical reactions but the accumulated effect of heat transport due to both chemical reactions and flow effects. Extinction effects increase scalar dissipation, and higher scalar dissipation has been correlated with increased heat release rate, as shown in Pantano's work [159]. This increase, however, still occurs after a lag due to the reaction timescale owing to unsteady effects, as reinforced in the prior discussion of the scalar dissipation mean conditioned on the stoichiometric mixture fractions (Figure 6.2 (B)). Therefore, the peaks of heat release can correlate well with points in time of maximum extinction, albeit after a time lag.

6.3.4 Hydroxyl Radical Conditional PDFs

As with the mixing evolution, comparing the different flame behaviour between the cases needs to consider the varying mixing and chemical rates and whether an appropriate temporal normalisation would draw similarities or highlight dependence on the initial instability. Figure 6.4 outlines the flame-marking OH radical mass fraction PDFs conditioned on the mixture fraction field. The results provide a qualitative insight into the flame behaviour over time instants normalised by the instability time scale over which mixing was shown to depend. For a steady diffusion flamelet behaviour, the highest conditional PDFs would accumulate around the conditional means. This is very clearly observed up to $t^* = 20$ for Case D and somewhat observed up to $t^* = 8$ for the other cases. The large discrepancy in the profiles between the cases is expected, given limited universal alignment between the cases at unique t^* values was observed in the mixing evolution analysis of Chapter 5. The results in the Y_{OH} profiles exhibit stark differences with no clear dependence on t^* .

For Cases B and C at $t^* = 8$, the flamelet-like profiles appear to disintegrate with increasing dispersion of Y_{OH} around stoichiometric mixture fraction. Case B ignites further with time at $t^* = 20$, judging by the rise in the conditional mean curve relative to the extinction profile (more OH production), with an increased dispersion and accumulation of OH above the conditional means, indicating a change in the combustion regime around stoichiometry and disconnect of the flame surface into large flame pockets which aligns with the observations made in the temperature contours. On the other hand, Case C heads towards extinction with a concentration of OH radicals below the conditional mean, which is entirely below the extinction profile. At $t^* = 40$, Case C shows evidence of reignition behaviour with an increase in the conditional mean and re-accumulation of OH around the conditional mean profile, indicating a reconnecting flame surface. Case D shows that smaller wavenumber perturbation helps keep the flame surface intact across the mixture fraction range. These results indicate that varying the initial perturbation has significantly altered the extinction rate, combustion regime, and likely the reignition mechanisms. Moreover, it puts into question whether the same temporal normalisation is appropriate for tracking the chemical evolution, as no clear correlation can be drawn between the profiles for the different cases at the same

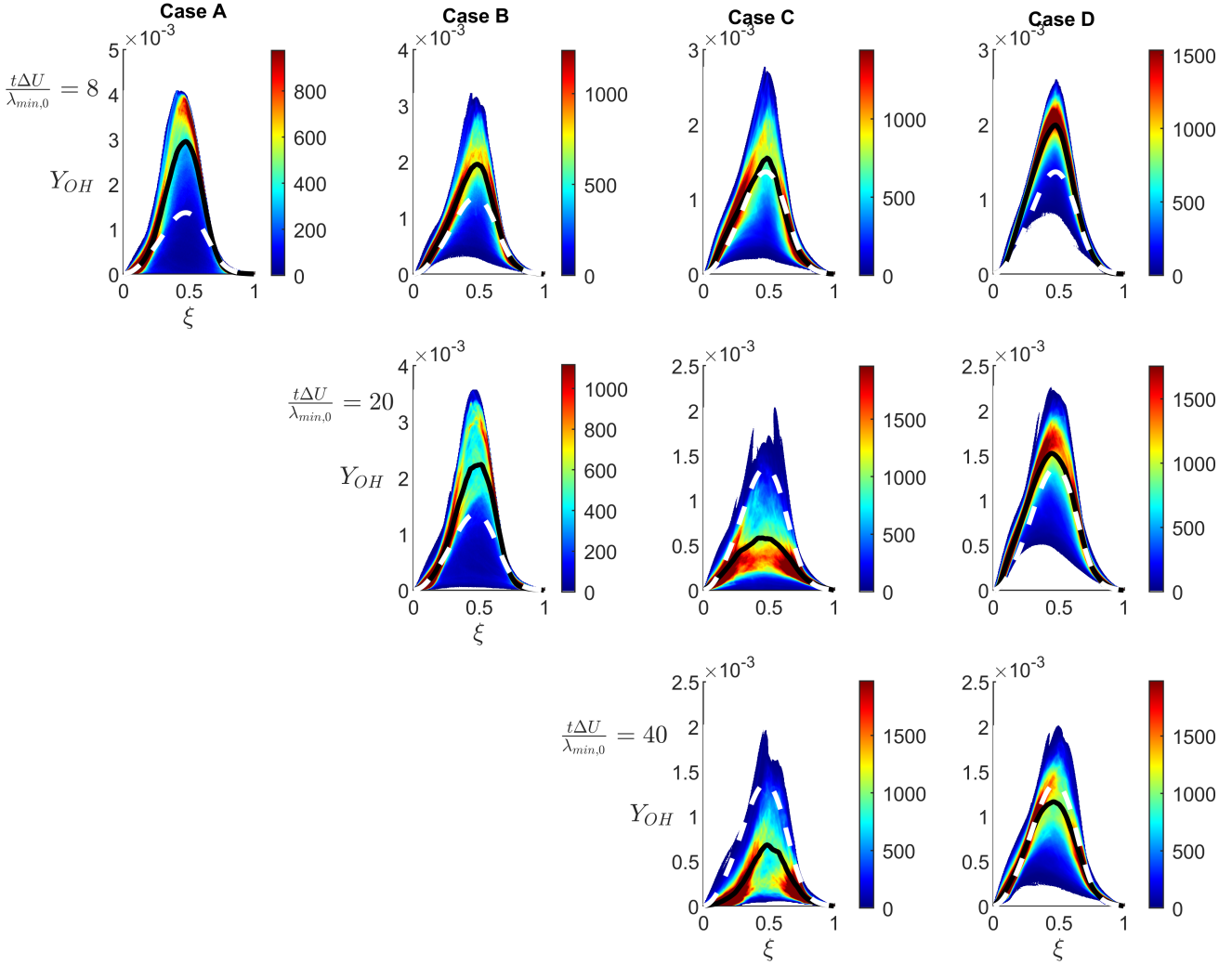


FIGURE 6.4. Conditional PDFs (contours) and conditional means (black lines) of OH mass fraction in mixture fraction space at three normalised times, $t^* = \frac{t\Delta U}{\lambda_{min,0}}$. The dashed white lines denote the OH mass fraction profile at a steady flamelet close to extinction with $\chi = 99\%\chi_q$.

t^* . Since all cases have the same fuel and oxidizer compositions and the same initial scalar dissipation profiles (Figure 5.3), the differences can only be attributable to the variation in the initial perturbation and how that drives different mixing behaviour and varying degrees of turbulence-chemistry interactions.

6.3.5 Transverse Vorticity Evolution

Turbulence in shear flows is directly driven by vortex structures and their pairing events [32], [73]. Moreover, previous studies have shown direct correlations between combustion product concentration distribution and vortex morphology [153], as vorticity was demonstrated to impose varying levels of strain on the flow field while also affecting the entrainment of reactants into the shear layer. Vorticity can induce tangential gradients along a flame surface, leading to varying levels of normal strain along the same mixture or flame surface and promoting curvature effects. Here, the initial perturbations directly influence the array of eddies and vortex scales that transpire with flow development and, in turn, influence mixing rates. Figure 6.5 shows the conditional Favre mean cross-stream vorticity. This is the component of the vorticity that considers both the stream and span-wise velocity components within which the initial instabilities are set. It is also aligned with the heterogeneous direction where ξ mean profile is observed, providing a measure of the rotational motion tangential to the flame front.

The results in Figure 6.5 show a direct correlation with the temperature and heat release profiles, where flammable regions in mixture fraction space have negative vorticity and more dispersed positive vorticity regions. Outside the flammable regions in mixture fraction space are heavily strained mixtures with large positive vorticity. The correlation between the vorticity contours and the temperature RMS in Figure 6.3 shows strong alignment between high-temperature RMS and negative ω_1 means or dispersion of positive vorticity regions. This supports the role of curvature effects in modifying the flammability across ξ iso-contours as was explained in Section 6.4.

An interesting observation is how the most heavily extinguished case (Case C) is the one where large positive vorticity values have penetrated the flammable mixture fraction range without a clear accumulation of negative vorticity around stoichiometry. This variation in vorticity magnitude and direction in reacting flows has been previously reported across several studies [124], [148] and is due to changes in the strain field due to combustion. The opposing shear strain indicated by the switch in the direction of transverse vorticity, particularly around

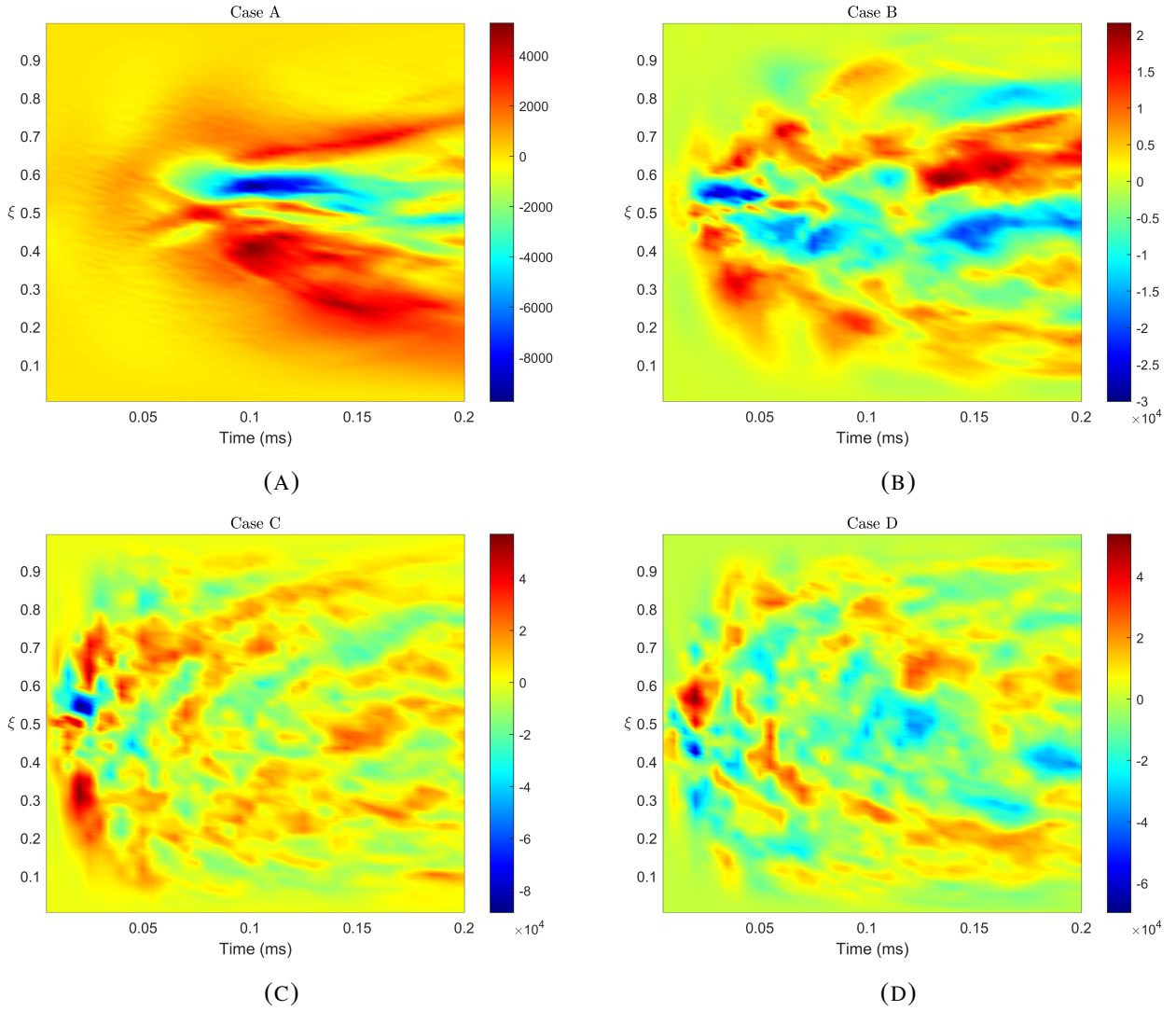


FIGURE 6.5. Cross-stream vorticity (ω_1) mean conditioned on mixture fraction for all cases across absolute simulation time.

stoichiometric conditions as observed, has been previously shown to support re-ignition and flame stabilisation [124]. These observations warrant extended analyses and discussion in future work as they provide some insights on the underlying flow-chemistry coupling: 1) the dispersion of the positive high vorticity regions could be indicative of curvature effects and help support their modelling 2) the feedback of chemistry on the flow may correlate with changes in the sign of transverse vorticity fields, i.e. vorticity aligned normal to the shear layer.

6.3.6 Chemical Species Distribution

Figures 6.6 and 6.7 present the conditional means and RMS in mixture fraction space for each of the 11 species in the studied chemical mechanism. N_2 is included here for completeness to demonstrate that it is indeed passive in the current implementation and confirm its linear relationship with ξ , which it is used to define. The relatively low RMS for many species validates the accuracy of the conditional means in representing the chemical profile and the suitability of ξ as a conditional variable for non-premixed combustion configuration as is conventionally endorsed. However, the RMS is still large relative to the means in several species, particularly ones involved in critical reactions. The fluctuation of mean profiles at different times for the same case correlates with the unsteady flame behaviour which is why it is most evident across all species for Case C.

Intermediate species involved in OH -based reactions, namely OH , O , and HO_2 , maintain fluctuations of comparable magnitude to the means in some cases. These sizeable fluctuations also extend to H_2 in leaner mixtures and O_2 in richer mixtures, likely owing to their relative scarcity, reducing statistical convergence. Case C exhibits the highest fluctuations in these species since it remains in high Reynolds number regimes for most of the simulation duration compared to all the other cases and, as a result, endures significant flow-chemistry coupling and unsteady flame behaviours.

Although ΔU is the same for Cases C and D, increasing the perturbation wavenumber in Case D leads to a better conditional mean representation of the chemical state with relatively lower RMS. This reinforces that understanding the seeding instability is important for characterizing and optimising combustion performance and that two flows at the same high Reynolds numbers do not necessarily maintain the same chemical state if they are seeded by a perturbation of a different length scale due to the different historical evolution of the mixing process between the two cases.

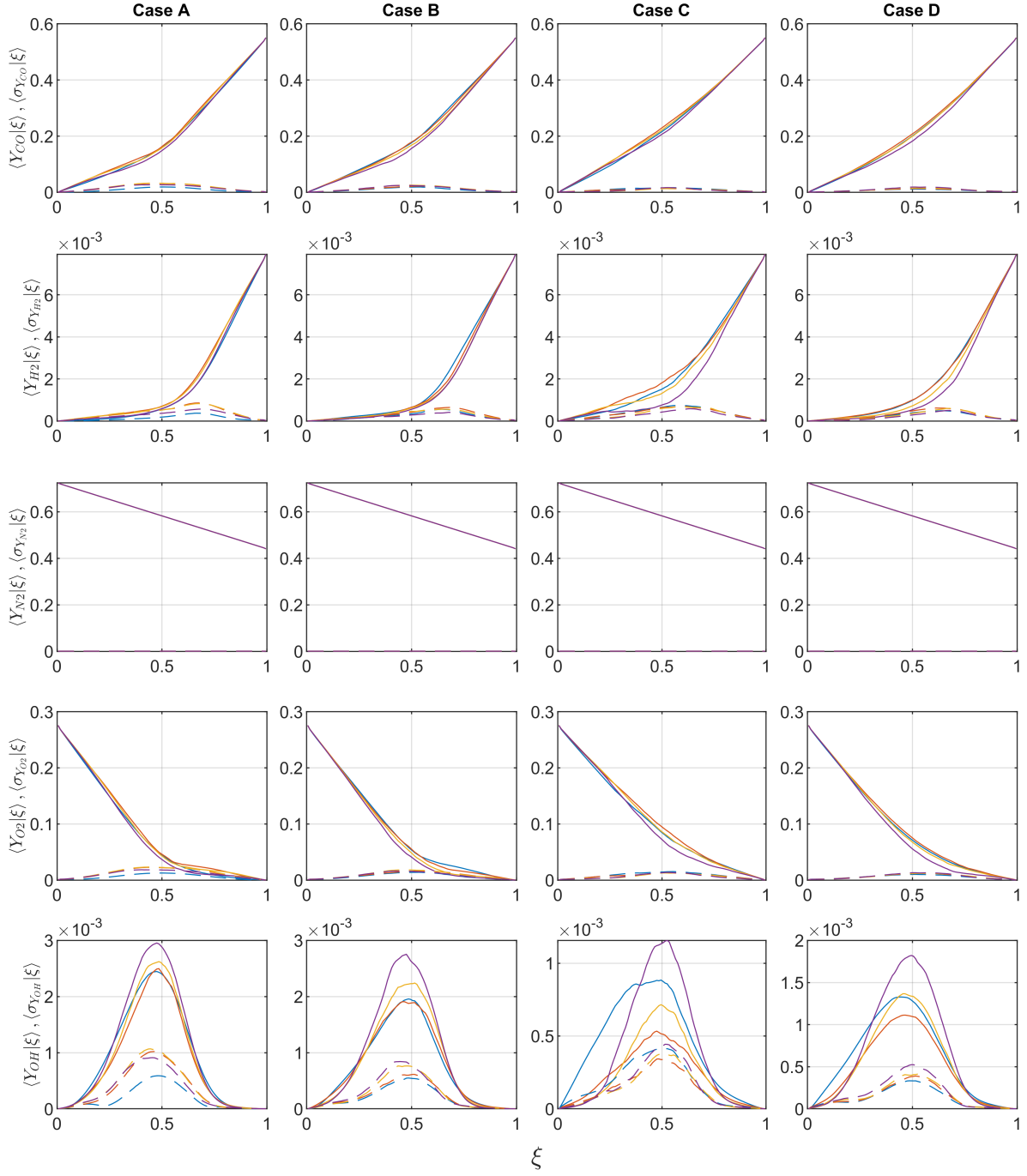


FIGURE 6.6. Mixture fraction conditioned statistics for reactant species and hydroxyl radical at different times: 0.05 ms (blue), 0.1 ms (orange), 0.15 ms (yellow), and 0.2 ms (purple). Both means (solid lines) and RMS (dashed lines) are shown for each species.

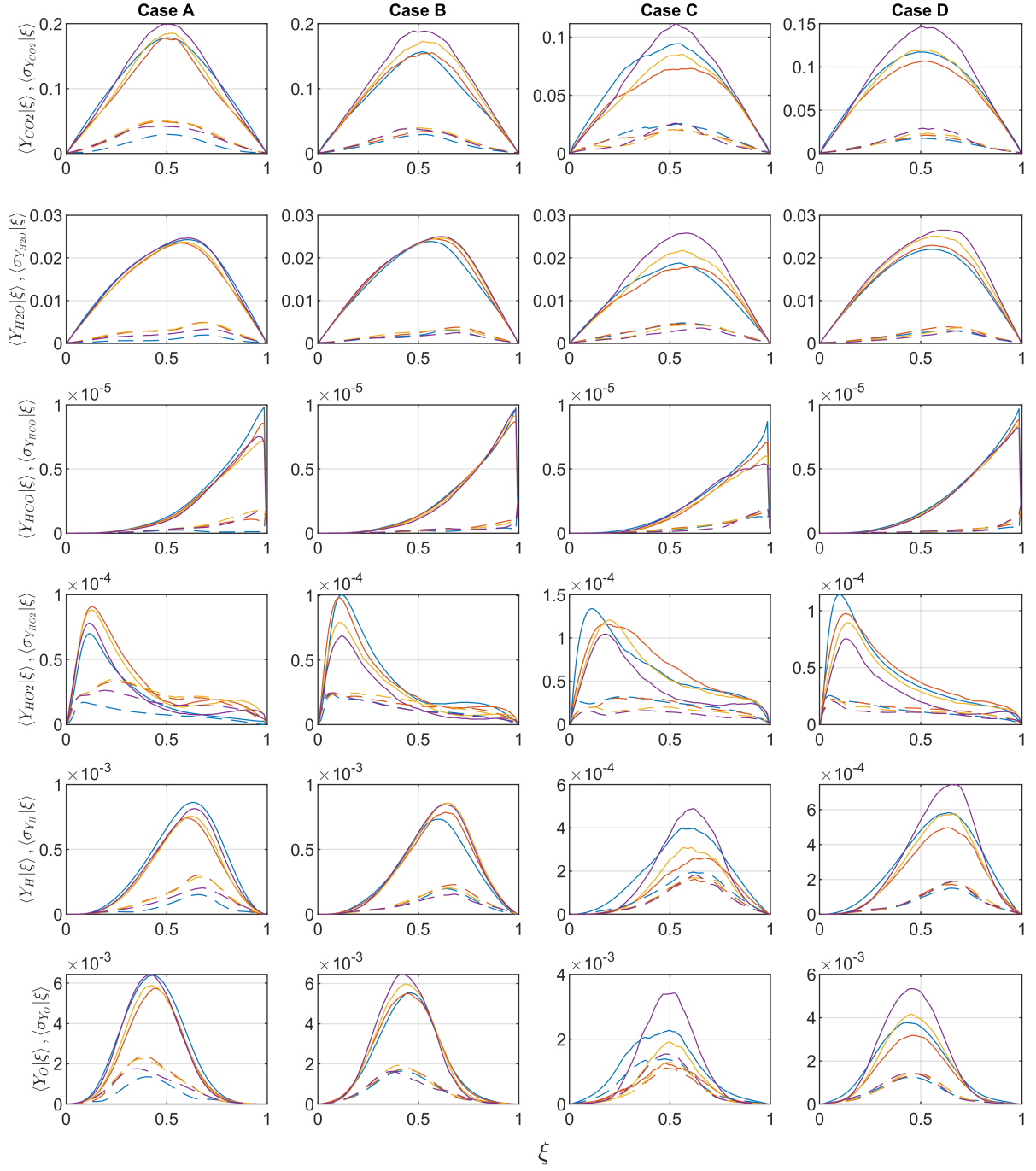


FIGURE 6.7. Mixture fraction conditioned statistics for remaining product and intermediate species of reaction mechanism studied at different times: 0.05 ms (blue), 0.1 ms (orange), 0.15 ms (yellow), and 0.2 ms (purple). Both means (solid lines) and RMS (dashed lines) are shown for each species.

6.3.7 Scalar Dissipation

Figure 6.8 shows how scalar dissipation conditional means and RMS vary in mixture fraction space at different times for Cases A-D. Once more, the high magnitude of the RMS relative to the means highlights a large extent of fluctuations within mixture fraction isocontours, as is visually confirmed in Figure 6.1. Scalar dissipation is a function of the flow dynamics and the mixing evolution, so it is unsurprising that it varies across ξ iso-contours in developing flows. This is why conventional combustion modelling requires the independent closure of scalar dissipation using the mixing time scale, which varies between the cases considered and across time for each case. Given the trends observed in mixing profiles with initial perturbation variations, it is predicted that consideration of the initial perturbation time scale will play a role in modelling scalar dissipation evolution in developing flows, as the trends have shown a direct dependence on the seeding instability in Figure 6.2.

Moreover, the discussions presented in earlier sections foreshadow that modelling should allow for a response time scale to account for unsteady effects as the flame structure adjusts to changes in the flame strain rates. These response timescales can potentially be incorporated with a similar formulation to the unsteady flamelet equation [70], which can also be accounted for in two-dimensional progress variable and mixture fraction manifold equation taken at the non-premixed limit [158]. The explicit evaluation and extension of pre-existing models against the results presented are reserved for future work.

6.3.8 Weighted PDFs

Figure 6.9 shows the mixture fraction PDFs in the entire domain along with the weighted PDFs by means and variances as calculated by equations 2.9 and 2.10 respectively. (Refer to Chapter 2, Section 2.2.1.2 for a summary of the notation convention and formulations of the probability calculations undertaken in the current chapter). Weighting by heat release rate and hydroxyl radical mass fractions helps focus the statistics on the reacting regions in the domain. The PDF results in Figure 6.9 show differing mixture distribution between the cases, consistent with the observations of Chapter 5. Cases C and D deviate the most from a flat ξ

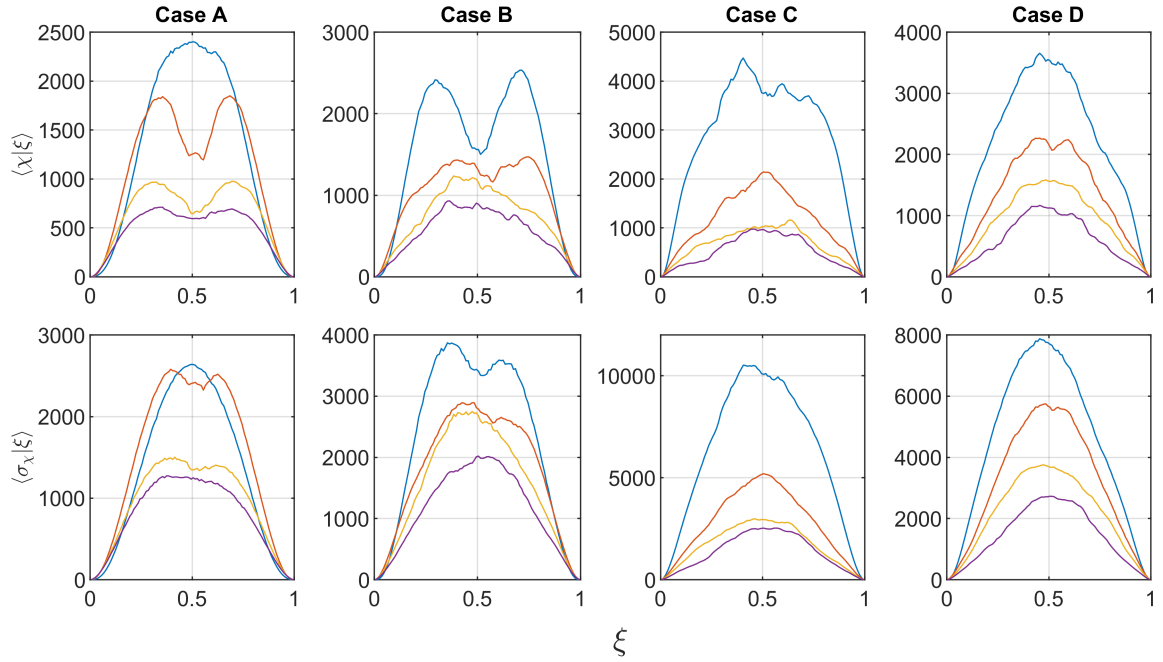


FIGURE 6.8. Scalar dissipation means and RMS in mixture fraction space. The same colour scheme in Figure 6.6 denotes different times.

PDF and instead follow a bimodal distribution at later times. Weighting the PDFs by mean heat release rate or Y_{OH} collapses the profiles for each case at different times, which indicates that over time, the proportion of mean heat release rate or Y_{OH} at every mixture fraction is stationary. However, the collapsed profiles are still distinct in shape and magnitude between the cases, although Cases A and B are closer as a pair, and so are Cases C and D, likely due to each of these pairs being confined to the same regions of a regime diagram as analysed in later sections. This same collapse between the profiles at different times is not observed when the weighting is done by the variances.

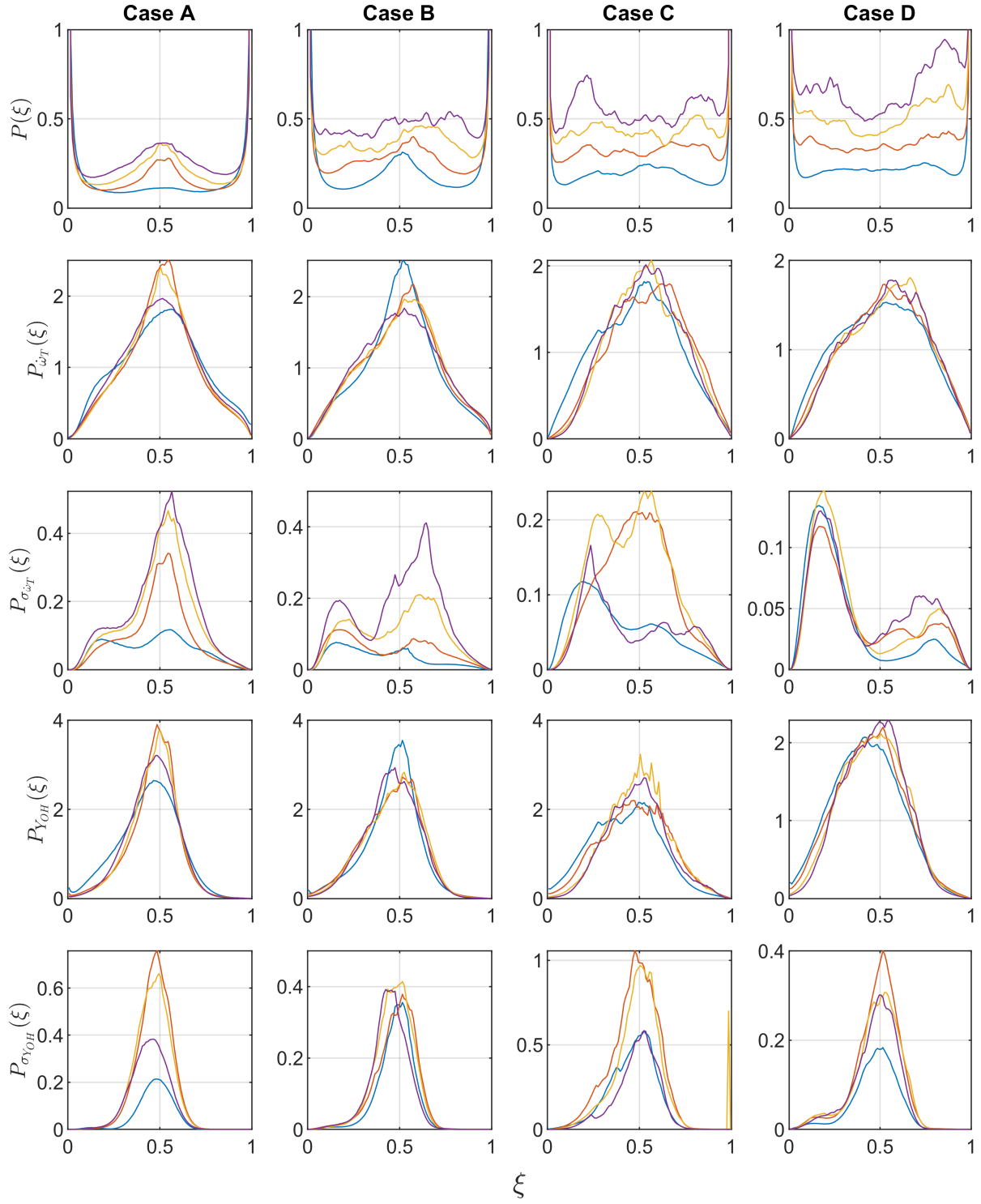


FIGURE 6.9. Mixture fraction PDFs in the entire domain at different times for all cases. The same colour scheme in Figure 6.6 denotes different times. The PDFs are weighted by heat release rate and OH mass fraction in the remaining rows first by their means and then by their variance for each quantity.

6.4 Combustion Regimes

6.4.1 Overview

The previous section highlighted a discrepancy in the flame behaviour between the cases, suggesting that the different initial perturbations lead to different combustion regimes. The classification of combustion regimes usually focuses on two aspects of the flame. The first is the level of premixedness, but since all the cases considered follow the same counter-flowing shear layer configuration, combustion is predominantly non-premixed, at least at earlier times. At later times, the varying levels and duration of extinction may produce premixed kernels in some cases, which then affect the re-ignition modes, as discussed further in Section 6.5. The second aspect of assessing the combustion regime considers the flow-chemistry interactions by directly comparing characteristic flow and chemical scales. This assessment is significantly more elusive for non-premixed combustion than premixed due to the additional mixing problem that is flow-dependent and complicates the depiction of universal non-premixed flame length scales [63]. Nevertheless, classifying non-premixed combustion regimes can help guide combustion modelling approaches as it can help depict trends and explore variable dependencies.

Relating the flame and flow scales in non-premixed combustion is commonly done by defining a Damköhler number. The choice of an appropriate chemical timescale poses a challenge, and different Damköhler number definitions exist in the literature depending on the physical scales considered, as with the Reynolds number earlier. With the current flow configuration being statistically one-dimensional (in the cross-stream direction), choosing a definition highlighting the diffusive scales is most convenient for analysing the cases presented. Moreover, since the unity Lewis number assumption is employed, and the overarching flammability is well described by heat release rate, the local Damköhler number is defined by:

$$Da = \frac{\tau_d}{\tau_c} = \frac{\dot{\omega}_T}{\left| -\frac{\partial}{\partial x_j} \left(\rho D \frac{\partial h}{\partial x_j} \right) \right|} \quad (6.1)$$

Here h denotes the sensible enthalpy, which relates to the total non-chemical energy in Chapter 3.2, Equation 3.5 by: $h = E + P/\rho - \frac{1}{2}u_i u_i$. Since Fickian diffusion is used in species and heat transport, this formulation correctly reflects the diffusive time scales in the simulations. Flame extinction occurs when the dissipation of heat flux by diffusive means overwhelms the heat generation from combustion. Therefore, this Damköhler number definition directly correlates with and tracks the local flammability in the shear layer. Furthermore, as a ratio that compares the relative magnitudes of these two mechanisms, it characterizes the flame stability throughout the mixing layer. This formulation is similar to others widely adopted in literature for mixing layer configurations [60], [160], [161].

6.4.2 Damköhler Number Dependent Statistics

To gain an appreciation of the varying combustion regimes between the cases, conditional statistics are explored in the Damköhler number space where the conditioning is done strictly over the Damköhler number. Figure 6.10 shows the conditional means and RMS of key quantities in Damköhler number space. Conditioning was done in log scale, similar to [60], to span the full range of Damköhler numbers in the flow and demonstrate overall trends. The means and RMS are shown in the same figure for each case for direct comparison. The number of samples in each bin decreases with increasing Da , and the results presented for each time are cut off at a threshold of 500 points to maintain good statistical fidelity. Each of the temperature, heat release rate, and OH mass fraction increases with Da , stabilising at the highest Da attained. The start of the plateau of these quantities appears at Da of order ten and marks highly ignited zones where the dependence of these quantities on Da ceases.

The temperature and OH mean peaks reflect the degree of extinction in each case and are consistent with previous observations. In these two quantities, discrepancies between the different time profiles for each case increase when $Da > 1$. The differences in OH mass fractions are significant and consistent with the trends observed in the PDFs in Figure 6.4. The fourth row's horizontal line marks the extinction profile's peak OH mass fraction. Case C profiles lie entirely beneath the line, supporting that it exhibits the most significant extinction but also shows reignition occurring after 0.1 ms, with a sharp rise between 0.15 and 0.2 ms.

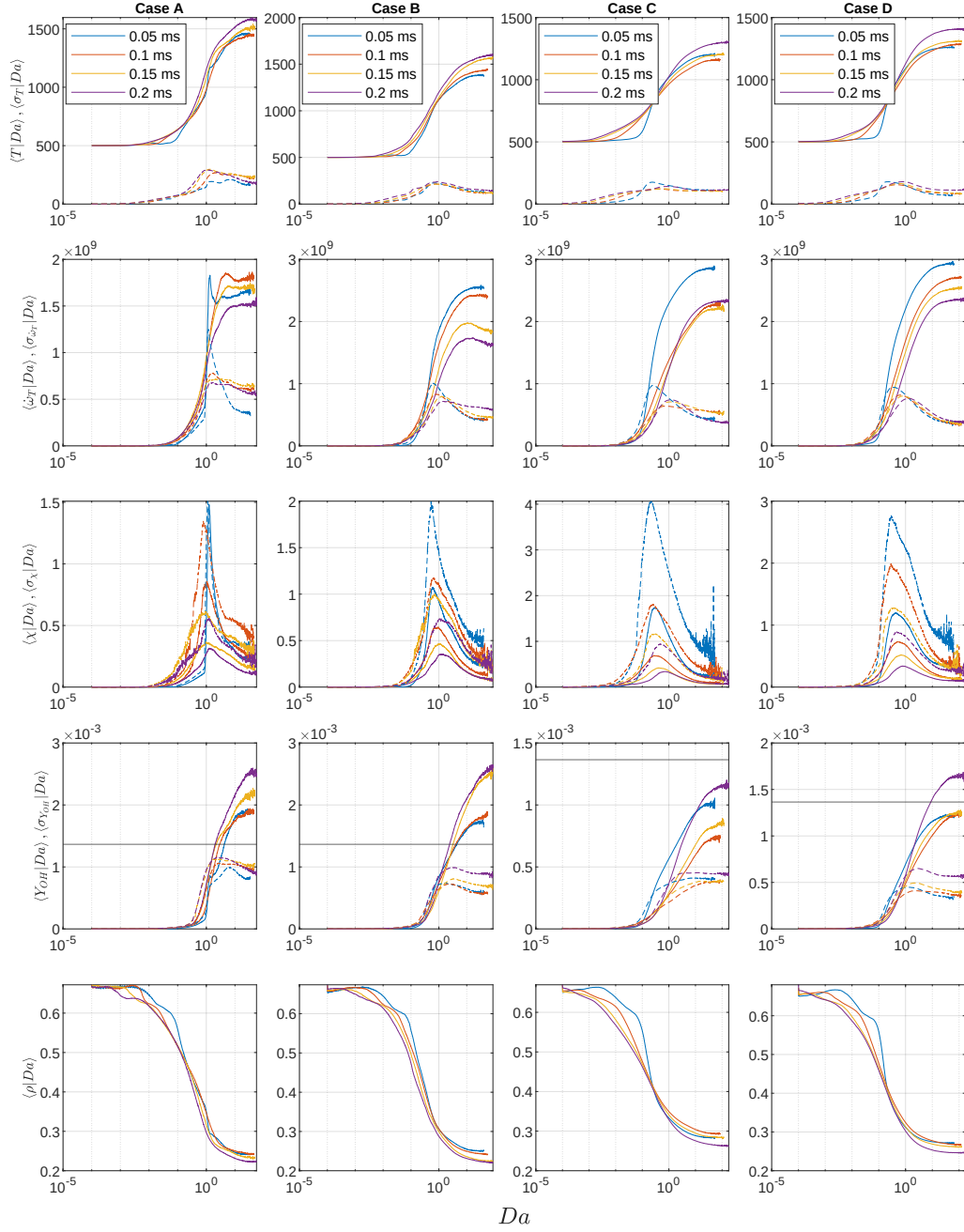


FIGURE 6.10. Means (solid lines) and RMS (dashed lines) of key quantities conditioned on Damköhler number (in log scale) at different absolute times (legend in first row). The scalar dissipation means and RMS in the third row are normalised by χ_q . The horizontal black line in the fourth row marks the peak of Y_{OH} near the quenching of a steady laminar flamelet. Only mean densities are presented in the last row.

The heat release rate profiles support this, showing Case C's most flammable regions (portions of higher Da) avoid flame blowout and maintain their reactions. For temperature, the RMS is at least an order of magnitude lower than the conditional means. For $\dot{\omega}_T$ and OH, the RMS is of comparable magnitude to the means up to $Da \approx 1$ after which it is overcome by the means which maintain more than double the RMS magnitude at the highest Da . This is due to the relatively more limited, highly flammable regions in each case and attests to the more definite statistics in these regions.

Unlike for the other quantities, the RMS for the scalar dissipation is up to twice the magnitude of the mean, indicating the presence of significant scalar dissipation fluctuation as expected. The mean values exhibit similar magnitudes to the ensemble averages discussed earlier in Figure 5.3, and both the RMS and means exhibit a similar trend to the previous Figure with decreasing dissipation with time. The peak dissipation values occur at Da , two orders of magnitude lower than the maximum Da each time. Since the conditional heat release rates maintain a similar order of magnitude for $1 \leq Da \leq 100$, then the diffusive strain must reduce significantly throughout this Da range, and the scalar dissipation results that peak at $Da \approx 1$ then plummet rapidly, confirm this. This indicates that the edges of flammable regions could be experiencing a diffusive strain, more than an order of magnitude larger than that endured by the most flammable cores in the shear layer.

Additionally, Case C results show a wider bandwidth of high scalar dissipation profile in Da range during extinction. So, in Da space, extinction is marked by the peak and the width of the χ profile in the high Da regions. This trend was not realised when statistics were observed in the heterogeneous direction as in Figure 5.3. The last row shows the mean densities, which reduce with increasing Da , consistent with how density decreases in the most reactive regions, as observed earlier at the centre of the shear layer.

To gain a deeper insight into the Damköhler number distribution throughout the domain and how that evolves for the different cases, Figure 6.11 outlines the Da PDFs, $P(Da)$ (first row). Initially, the PDF appears bimodal for all cases. For Cases A and B, this bimodal distribution is maintained to later times, indicating a more resilient low Da mode than in Cases C and D. The results demonstrate reduced resilience of this low Da mode with increasing perturbation

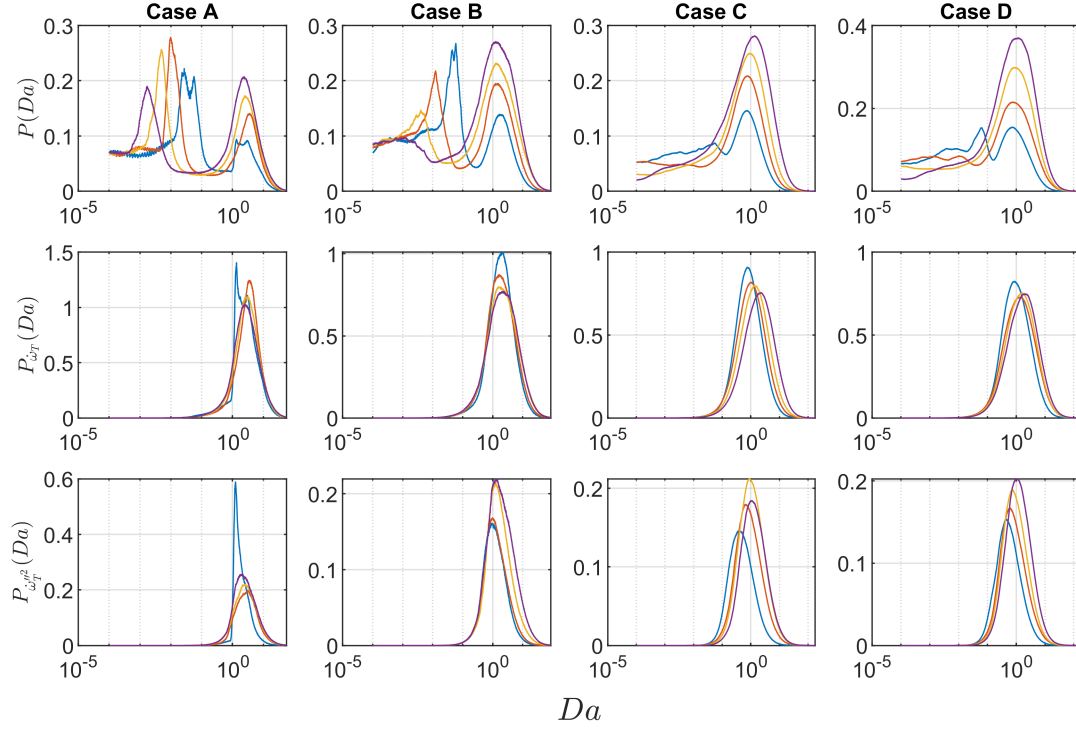


FIGURE 6.11. Damköhler number PDFs of the entire domain at different times (first row), heat release mean and variance weighted Damköhler number PDFs in second and third rows respectively. The coloured lines correspond to the same absolute times as in Figure 6.10.

eigenvalue. This Da mode indicates a prevalence of preserved non-reacting regions in the domain. The trend suggests that the cases with larger and more coherent eddies preserve these non-reacting regions for longer due to the lack of more widespread microscale mixing. So, although these cases manifest larger apparent mixing layer growth, as discussed earlier, these statistics indicate less profound mixing within the mixing zone in Cases A and B due to the lack of smaller eddies, as visually confirmed by the contours. The results also show the prevalence of regions of higher Damköhler number ranges. While the mean and RMS statistics in Figure 6.10 extended to high order Da , the PDFs show very little prevalence at Da greater than an order of unity.

The PDFs in the first row of Figure 6.11 indicate the prevalence of Da ranges across the domain. However, the results also include data from the free streams without mixing or reactions. To focus more on the mixing zone and further explore the relationship of Da with

reacting regions, the PDF is weighted by the mean heat release rate (second row) and its variance (third row).

The heat release weighted PDFs in the bottom two rows indicate that combustion occurs in all cases at Damkohler number of order unity. As time progresses, the PDFs march towards higher Da at different rates depending on the balance of their respective extinction and reignition events. The more the profiles displace towards higher Da , the greater the fraction of heat release contributed by re-ignition events ($Da \geq 10$). This displacement is considerably more prominent in Cases C and D, compared with A and B, whose mean-weighted profiles remain almost static in time, indicating more drastic re-ignition events in C and D. The results in the second and last rows of Figure 6.10 can also be used to estimate the extinction Damköhler number, Da_q for the cases, which remains relatively unchanged with time. Here, Da_q is the lower Damköhler number limit where $P_{\dot{\omega}_T}$ is less than 1% of the maximum heat release weighted PDF. The low heat release RMS at this Damköhler number region support this convention.

Since non-premixed combustion cannot occur without adequate mixing, observing the evolution of the Damköhler number in mixture fraction space is valuable. Figure 6.12 shows the mean and RMS of the Damköhler number conditioned on mixture fraction. The re-ignition of Case C is apparent by the sharp rise in the peak Da around stoichiometry between 0.1 ms and 0.2 ms to match the peak of Case D that rises more steadily with time due to its less extreme extinction. All cases have peaks centred around stoichiometry while slightly displaced to richer mixtures, as expected, since the flames in the shear layer are subjected to higher strains relative to the equilibrium flame. The profile peaks' magnitude and widths are consistent with previous observations. Higher peaks and thicker profiles correspond to less normal strain on the flammable ξ surfaces. So, cases with lower wavenumber perturbations maintain these, whereas cases with higher wavenumber perturbations and Reynolds number exhibit stronger flame-chemistry coupling and lower peaks. The higher Da values for Case B indicate fast chemistry relative to mixing, so the chemistry can keep up and more seamlessly adapt to flow perturbations and resulting strain rates. Case A's steady Da value is due to a lack of unsteady effects relative to the other cases, as the flow eddies are too large to distort the initial flamelet.

These cases may, therefore, more closely correspond to a laminar flamelet element behaviour. For Cases C and D, the mixing time scales are sped up and brought closer to the chemical ones. As a result, the chemistry is more obviously deterred by the flow and its higher strain rates. This increases the magnitude of the response timescale the chemistry needs to adjust to the flow condition changes, making unsteady effects more prominent. It is important to note that all cases are set up with the same fuel and oxidizer compositions, initial flamelet and mixture fraction profiles, and chemical mechanisms. Hence, the changes in Damköhler numbers are more directly attributed to changes in the mixing time scales. The RMS results in the last row of Figure 6.12 are large relative to the means, especially for Cases B and C, indicating large fluctuations in the flammability levels of mixture fraction iso-contours, particularly those close to stoichiometric mixtures.

It is well reported that increasing the flow Reynolds number increases flame quenching due to higher strain rates [93], where Reynolds number is commonly increased (at least partly) by increasing the velocities of the free streams. Here, the Reynolds number evolution is a function of both the initial free-stream velocities and the initial wavenumber range of the perturbations. Interestingly, the Damköhler number trends presented here are consistent specifically with the Taylor Reynolds number discussed earlier. The higher the Re_{λ_Y} the lower the Da . Therefore, at 0.2 ms, Case B, which has a lower Taylor Reynolds number than C and D, exhibits a higher Damköhler number. Moreover, at times before 0.2 ms, since Re_{λ_Y} is a lot higher for Case C than D, its Da is lower, whereas at 0.2 ms, when both Cases maintain the same Re_{λ_Y} , they also maintain very similar profiles of Da in ξ space. This emphasises the influence of the Taylor microscale on directing the mixing relevant to combustion.

Mixing can be due to both convective and diffusive effects, but in the shear layer configuration studied, the mixing is dominated by diffusive effects, as supported by the transport budgets in Figure 5.8 with the significance of the diffusion-based dissipation. A conservative assumption is that flow-chemistry effects are most noticeable when the Kolmogorov scales are comparable to the chemical scales. This may be true for unity Schmidt number flows, but in the cases considered, the Schmidt number averages between 0.6-0.7, which implies that molecular diffusive scales are larger than the viscous dissipation ones. This puts the Taylor microscale

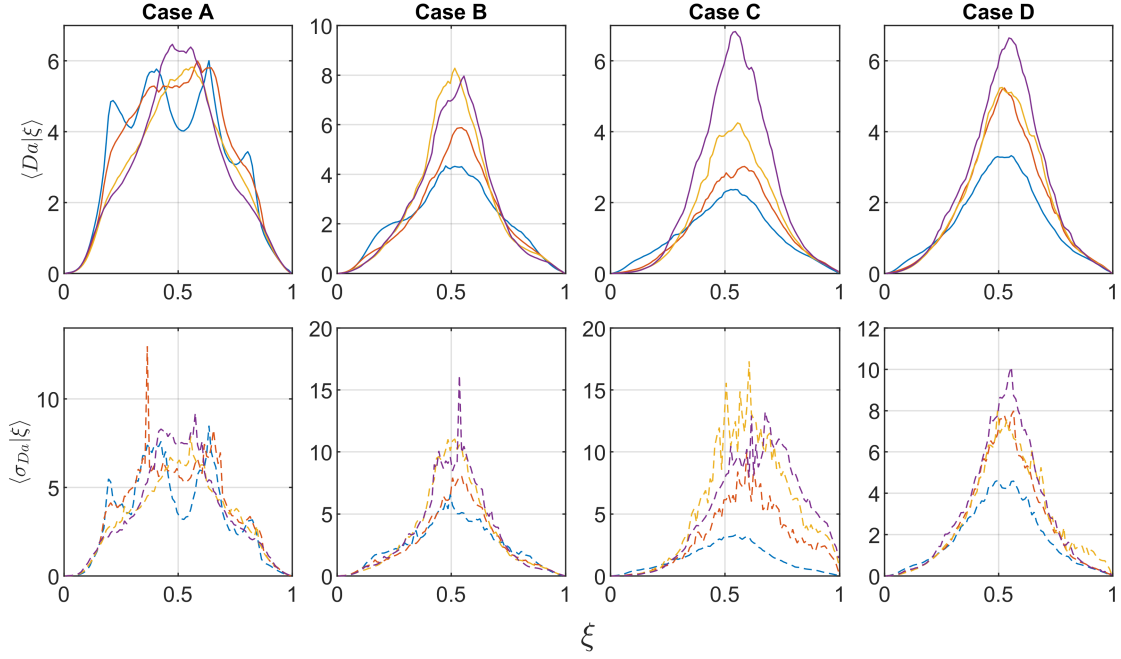


FIGURE 6.12. Damköhler number means (top) and RMS (bottom) conditioned on mixture fraction for all cases at different times. The coloured lines correspond to the same absolute times as in Figure 6.10.

closer to the relevant diffusive scales than Kolmogorov, which comes as no surprise; after all, Taylor-based Reynolds numbers (rather than Kolmogorov ones) have been historically used to track the power law of the inertial ranges of both velocity and passive scalar spectra [162]. Note that in Dimotakis’s work [9], a further refinement of the Taylor range is assumed, with an inner viscous Taylor scale defined at the lowest limit of the inertial range to correspond to 50 times the Kolmogorov scale. This is, however, assumed for fully developed turbulence that exhibits a broader separation of scales than what’s observed here during the transition. It also depends on the definition of the Taylor scale. Dimotakis estimates the Taylor scale using large-scale Reynolds number properties. Here, it is derived from the smallest length scales where the autocorrelation takes a maximum (Equation 2.27). So overall, the Taylor scale considered here is much closer to the Kolmogorov scale than the mid-range Taylor scale defined in [9]. Therefore, in this work, the Taylor scale is taken to represent the flow-dependent diffusive effects controlling combustion-relevant mixing and is assumed to more directly correlate to the Obukhov–Corrsin scale.

The second row of Figure 6.12 shows the RMS of the Damköhler number, which, compared with the previous RMS statistics, is high relative to the conditional means in the first row. This indicates a high degree of fluctuations of Da within a mixture fraction isocontour. Interestingly, a similar behaviour is shown for the scalar dissipation RMS in the third row of Figure 6.10. With the Damköhler number taken as a measure of flammability, this result indicates that within a surface of uniform flammability (constant Da), there is a large extent of fluctuations of mixture fraction gradients. These two results suggest that surfaces with a fixed flammability level do not coincide with a corresponding mixture state (constant ξ contour). This is not unexpected as surfaces of constant ξ are subjected to varying levels of normal strain. Even classical flamelet modelling approaches account for that by using both χ and ξ to close the flame structure. This can be confirmed visually by inspecting the stoichiometric mixture fraction contour in Figure 6.1. For Cases A-C, the stoichiometric surface can be seen to intermittently go in and out of regions of high scalar dissipation (marked in white). This is observed to a much lesser extent in Case D, where the stoichiometric surface maintains its presence in high χ regions, which is why its RMS is lower than all the other cases in Figure 6.12.

Nevertheless, the high RMS of scalar dissipation in the third row of Figure 6.10 indicate that other factors may be at play. This can be partly due to unsteady effects as a given mixture subjected to changing strain rates takes time to equilibrate its chemical state and, as a result, sways between different flammability levels, and so at a given Da value, a range of strain rates can coexist at least intermittently. So, these fluctuations are most evident during the transition and should even out with developing statistical self-similarity as the turbulence evolves consistent with the results. However, going back to the RMS results in Figure 6.12, the RMS maintains a closely similar profile for Cases A and B but increases with time for Cases C and D, which suggests additional factors than unsteady transitional effects. Inspection of the temperature contours shows a higher degree of curvature of the flame surface in these two cases due to the smaller ratio of the flow to the chemical scales as the perturbation eigenvalues are increased. This leads to scalar profile variations tangential to a flammability contour that is supported by the three-dimensional nature of turbulence and induces tangential diffusion effects that curve the flame surface and misalign the ξ and Da contours.

In summary, varying the perturbation eigenvalue may work to alter these three mechanisms: the normal strain across a ξ contour, the unsteady effects due to a variation of the response time to changes in the normal strain that is a function of the flow transition and should stabilise with self-similar evolution, and the variation of scalar gradients tangential to the flame surface which leads to tangential species and heat diffusion that in turn alters the normal scalar gradients and flame strain. These mechanisms are, therefore, not independent but intertwined and collectively explain how variations in the initial perturbation eigenvalues alter the resulting flame structure. However, further future analysis that isolates and explicitly calculates these strain components along with relevant multi-variate conditional PDFs is needed to test and confirm these hypotheses.

On top of these, there is also the feedback effect of the chemistry changes back on the mixing; for instance, high strains cause local extinction, which amplifies scalar dissipation even further [61]. The result is a heavily non-linear dependence of the flame structure on the initial perturbation that prevents a collapse of statistics on a temporal normalisation like the one applied to the mixing statistics.

6.4.3 Flow-Chemistry Scale Correspondence

Since non-premixed combustion involves heavy coupling between flow and chemistry effects, visualising combustion regimes while taking into account a measure of these two attributes can be valuable. This approach is widely adopted in premixed combustion but is not as popular in assessing non-premixed combustion regimes due to the lack of inherent chemical length scales that are universal to different flow configurations. In the present investigation, however, all cases are set up in the same configuration, so visualising and comparing these regimes between the cases is feasible. To produce a regime diagram, it is important to carefully consider the chemical and flow scales compared so that their choice encapsulates the aggregate of all the strong coupling mechanisms discussed above. For this, a large turbulent eddy Damköhler scale, Da_t , is defined and related to the local Da defined above by:

$$Da_t = \frac{\tau_t}{\tau_c} = \frac{\tau_t \tau_d}{\tau_d \tau_c} = \frac{\tau_t}{\tau_d} Da \quad (6.2)$$

Since the intention is to highlight regimes of flow-chemistry coupling, the above expression has to be related to the Reynolds number. The large turbulent energy-containing eddies correspond to the larger end of the spectra (i.e. energy-containing range) and are well captured by the integral length scales. These represent the accumulation and growth of the initial small perturbations during the transition process. To draw direct parallels to the Damköhler number definition, which is a scalar field with no direction, the turbulent Reynolds number is reconsidered over the mixing zone, such that:

$$Re_t = \left\langle \frac{\widetilde{\mathcal{K}^2}}{\widetilde{\epsilon V}} \right\rangle_{\delta_z} \quad (6.3)$$

With the turbulent scales defined in the above equation, these can then be related to the mechanical mixing timescale in Equation 6.2, where:

$$\tau_t = \frac{\widetilde{\mathcal{K}}}{\widetilde{\epsilon}} \quad (6.4)$$

What then remains to close the definition of Da_t is an appropriate choice for τ_d . In Equation 6.1, the choice for τ_d corresponded with heat diffusion for consistency with the heat release rate based on the chemical timescale. Here it is more appropriate to select a more overarching species diffusion time-scale to correspond more directly with turbulent scales used in τ_t definition. Moreover, since non-premixed combustion is conditioned on adequate mixing, an appropriate definition for τ_d here (similar to in [61], [63]) is:

$$\tau_d = \frac{1}{\langle \chi | \xi_{st} \rangle} \quad (6.5)$$

This closes the definition of Da_t . To draw insight into the flow-chemistry coupling dependence of the combustion regime, it is then helpful to relate Da_t with Re_t . With the large eddies well-represented by the integral scale and the diffusive scales by the Taylor scale, then:

$$\frac{\tau_t}{\tau_d} \sim \frac{I}{\lambda} \quad (6.6)$$

Here, λ refers to the transverse Taylor scale, the direction where the diffusive effects are prominent. Therefore, based on relations expressed in [2]:

$$\frac{I}{\lambda} = \frac{1}{\sqrt{10}} \sqrt{Re_t} \quad (6.7)$$

Relating this back to Da_t in Equation 6.2:

$$Da_t = \frac{1}{\sqrt{10}} \sqrt{Re_t} Da \quad (6.8)$$

6.4.4 Regime Diagram

Figure 6.13 shows the regime evolution of all cases with time, with different symbols used for each case, as explained in the figure caption. According to the expression above, lines with a constant slope of 1/2 correspond to constant Da , so Da_q based on the earlier definition with the heat-release weighted PDFs is marked in a solid black line. The higher the Damköhler number, the thinner the flame surface and the more instantaneous the ignition post-mixing, i.e. the more the flame behaves like a flamelet element. Therefore, defining a Da limit above which laminar flamelet assumptions produce a good approximation of the flame structure is sensible. Explicit testing the results against asymptotic flamelet theories is outside of the scope of the current study; however, [118] identified this limit to be $Da_{LFA} = 5Da_q$ through investigating flame-vortex interactions, and this limit is marked here through a dashed black line to help visualise trends.

Key Reynolds number values were also marked in Figure 6.13 based on previous observations. The goal was to define a region on the diagram that marks the transitional flow process from the beginning of self-similar evolution development to areas where turbulence appears fully developed. A vertical dashed blue line marks the start of this, corresponding to $Re_{\lambda_Y} = 50$, the value to which Cases A and B first saturate in Figure 5.5. Dimotakis [9] limit is used to mark the other end in a dashed red line, denoting fully developed turbulence.

Several observations can be derived from Figure 6.13 while noting that each point in the figure assesses the entire state of the mixing layer for each case and its evolution with time:

- (1) Through varying the initial perturbation, the same flow configuration exhibits different combustion regimes as the cases align themselves in separate areas in the diagram. Increasing the perturbation eigenvalue increases its state of turbulence and reduces its flammability due to a greater extent of flow-chemistry coupling.

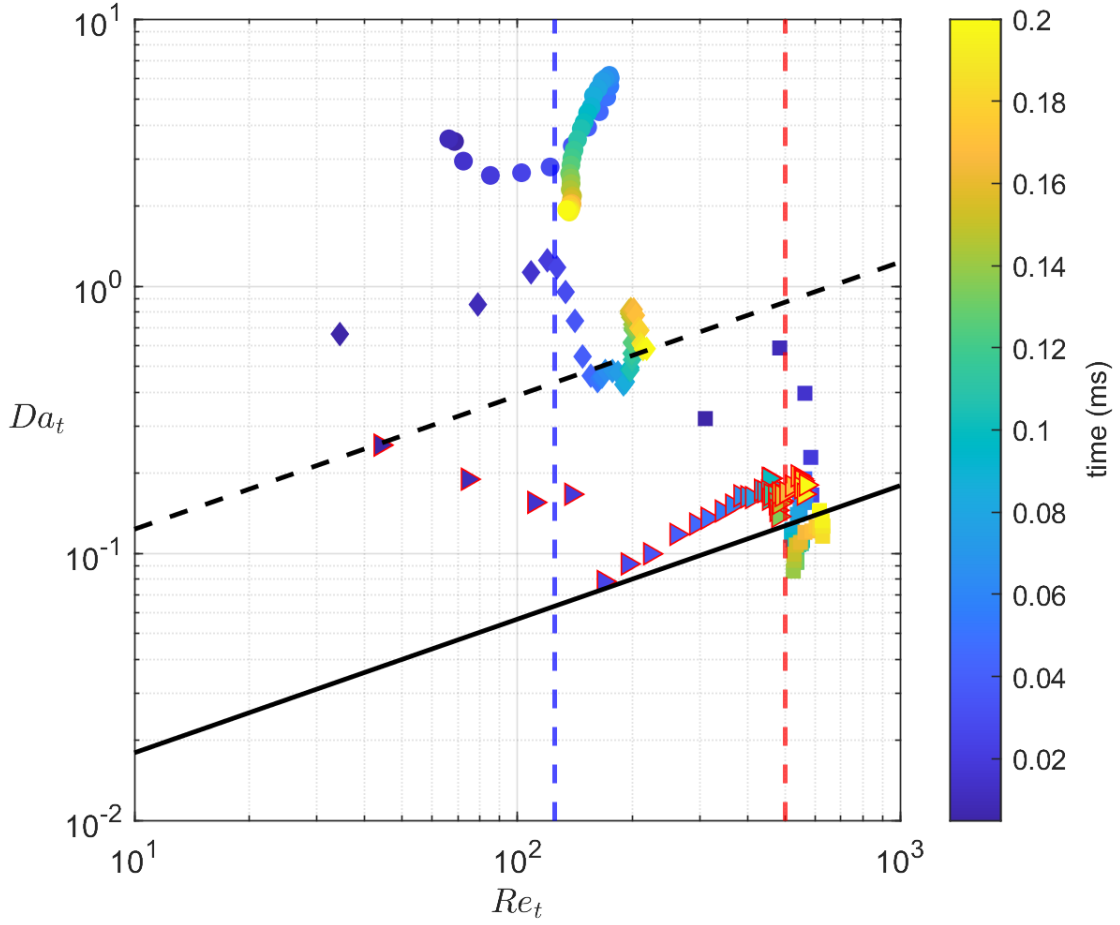


FIGURE 6.13. Regime diagram relating the large scale Damkhöler number (vertical) to the turbulence Reynolds number (horizontal) in log-log axes. The fill of the points corresponds to different absolute times, as shown in the colorbar. Different symbols correspond to different cases, with Case A (circles), Case B (diamonds), Case C (right-facing triangles with red outline), and Case D (squares). The solid black line corresponds to Da_q , and the dashed black line corresponds to the laminar flamelet assumption Damköhler number as defined in [118].

- (2) Maintaining the same perturbation wavenumber range and increasing ΔU maintains the same temporal evolution pattern but at higher Reynolds numbers and lower flammability conditions. This is derived by inspecting the results of Cases B and C and provides conclusive evidence that the small-scale mixing is sensitive to the initial perturbation wavelength bandwidth (relative to domain size or residence time).
- (3) Doubling the initial perturbation wavenumber reduces the average flammability by almost fivefold, judging by a sloping average Da line for each case. This can be attributed to the rising proximity of the flow scales to the chemical scales with

increasing wavenumber, which increases flame curvature effects and strain rates, as described earlier in this section.

- (4) After transition and intermittent fluctuations, the cases maintain a steady Da profile, indicative of self-similar evolution. The final steady state Da appears to be a function of the initial perturbation eigenvalue, as every case keeps a unique profile.
- (5) All cases exhibit a flammability transition characterized by a sharp drop in Da_t . Cases with the same normalised initial perturbation wavelength bandwidth endure this flammability transition at the same Re_t value. This is evident by looking at Cases A, B, and C profiles, which all transition just after the vertical blue line. Case D, however, which has a smaller perturbation wavelength, endures this flammability transition at a higher Reynolds number (the vertical red line).
- (6) The above point showcases that, like mixing and turbulence development, Reynolds number values are also non-universal for cases seeded from different perturbations under flammability transition. Therefore, deriving insights into the seeding flow perturbation and analysing flow regimes as dynamic systems with fundamental perturbation modes can yield valuable breakthroughs in turbulence and combustion control.
- (7) The flames endure resistance transitioning between flame regimes. Crossing these regimes implies crossing an equilibrium state between the chemical and flow scales, and the cases that approach the defined Da thresholds heavily fluctuate about it. This is observed with Case B results about Da_{LFA} , and Case D as it approaches Da_q following its transition before quickly reverting to a higher flammability state. Case C reaches high extinction levels intermittently before reigniting again and heading upwards past Da_q .

6.5 Re-ignition Modes

6.5.1 Overview

The previous section highlighted how variations in the initial perturbation can induce different combustion modes and varying degrees of flow-chemistry coupling. This discrepancy between the cases leads to varying levels of extinction, as shown in the regime diagram in Figure 6.13, where the cases stabilise at different Da levels before re-igniting. This is also evident from the conditional OH PDF statistics in Figure 6.4, where the PDFs and the conditional means approach the extinction profile to varying levels. Different extinction levels have been previously shown to play a significant role in mixing pre-existing combustion products and reactants ahead of re-ignition [61]. The cases investigated in [61] maintained the same flow scales but variable chemical scales due to different fuel and oxidizer compositions and demonstrated very different re-ignition mechanisms. This section investigates if similar behaviour manifests when the chemical scales are maintained, but the mixing scales are varied, and hence whether re-ignition mechanisms can be related to the flow-chemistry coupling and the seeding initial perturbation.

As reflected in previous analyses, variations in the initial perturbations lead to different extents of flow-chemistry coupling. The magnitude of the chemical feedback effects on the flow scales is non-negligible, as evidenced by the discussion of combustion regimes. Varying levels of flame extinction affect the flow composition, species diffusion, and hence mixing. The accumulation of these variations throughout the extinction process can heavily influence the reignition modes [61].

6.5.2 Flame Index

6.5.2.1 Definition

The flame index has been widely used to show the alignment of the fuel and oxidizer mixing throughout the flow to gain insight into the existing combustion regimes within a flame. This

is generally defined as:

$$FI = \frac{\nabla Y_F \cdot \nabla Y_O}{|\nabla Y_F| |\nabla Y_O|} \quad (6.9)$$

The flame index outlines the orientation of the direction of fuel flux relative to oxidizer flux. Since Fickian diffusion is adopted in this study, the species fluxes directly depend on the species gradients. Therefore, the above formulation represents cosine, the angle between the normal vectors of the fuel and oxidizer isosurfaces. Visualising this against the mixture fraction should elucidate the variation of this alignment across the range of fuel and oxidizer iso-contours. The fuel here is taken as the sum of CO and H₂ mass fractions, and the oxidizer is taken as O₂ mass fractions.

6.5.2.2 Conditional Means

The conditional means of a range of quantities on the flame index are presented in Figure 6.14. Four quantities that can be used to infer the flame behaviour and ignition are included: heat release rate, temperature, OH mass fractions, and Damköhler number. All four quantities present consistent trends with the flame index with initial peaks at the non-premixed limit, as expected from a counterflowing shear layer configuration. With time, these peaks increase, but a second peak appears at the premixed limit and grows with time. The temperature and Damköhler number conditional means for Case C increase steadily with time, like with the other cases, but the heat release rate and Y_{OH} stagnate until the latest time, where they rise to higher peaks. Therefore, these two quantities can better capture the flame behaviour. The temperature result for Case B is misleading as it implies a more premixed mode of reignition, as also shown in the late-time contours in Figure 6.1. However, temperature reflects the accumulation of heat, which appears to consolidate, for Case B, in regions of aligned gradients. This accumulation does not necessarily translate to ignition regions. It could be due to heat transport that might have been enhanced by the large-scale eddies in Case B that isolate large heat pockets without adequate small-scale mixing. The absence of prominent premixed peaks in heat release rate and Y_{OH} profiles at late time for Case B support this. The relative magnitudes of the peaks between the cases are consistent with previous observations made regarding the flammability of the different cases. The mean

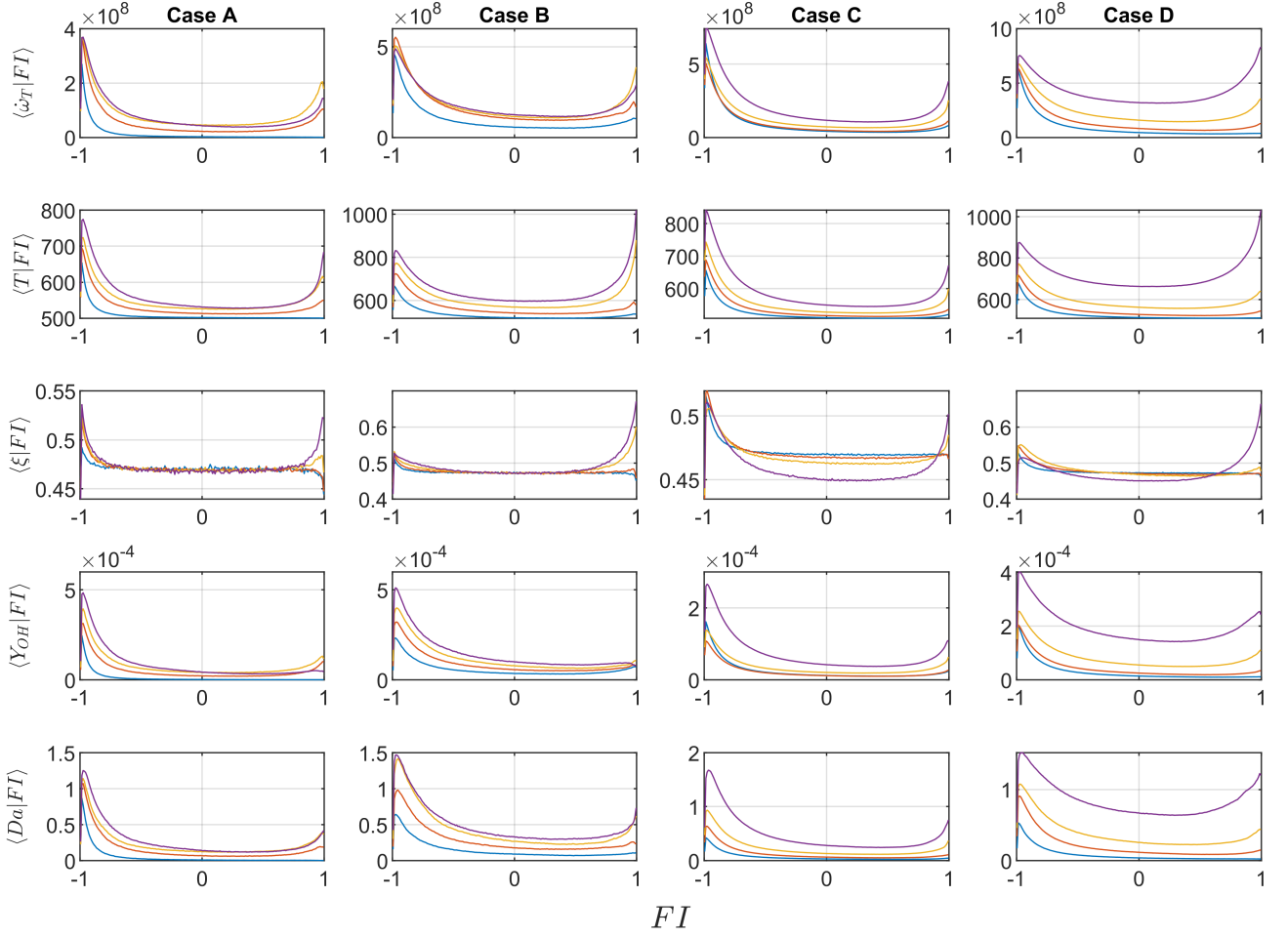


FIGURE 6.14. Key conditional statistics on flame index for all cases at different times. The last row corresponds to the mean Damköhler number weighted FI PDFs as defined in Equation 2.9. The coloured lines correspond to the same absolute times as in Figure 6.10.

mixture fraction is also shown, which maintains close to 0.5 average at intermediate FI and heads to richer mixtures at the limits of the flame index. This is important as the calculation of FI was undertaken as a scalar field in the entire domain, but these averages confirm that the predominant gradients were maintained in stoichiometric regions that are most susceptible to burning.

6.5.2.3 Integrated Weighted PDF

Looking at conditional means alone can be misleading, as shown in [60], as mean data does not provide insight into the distribution and weighting of values at each flame index. To better

appreciate this, the PDF of the flame index is considered and weighted by the mean heat release rate, as defined by Equation 2.9, to focus on the ignited samples. Furthermore, this weighted PDF is integrated across three areas of the flame index to gain an appreciation of the proportion of cumulative heat release within different regions of fuel-oxidiser gradient alignment. Aligned gradients region was defined to span angles between 0 and $\frac{\pi}{4}$ between the fuel and oxidizer iso-surface normals, whereas opposed gradients were defined with angles $\geq \frac{3\pi}{4}$. Intermediate gradients spanned all angles in between and were taken to correspond to mixed-mode combustion. Figure 6.15 shows the cumulative heat release distribution across the different regions for all cases and at various times (bottom row), along with the proportion of heat release at high Da (top row) to correlate the burning modes with extinction and reignition. $Da \geq 5$ were taken as the high Da threshold as inspection of Figure 6.10 show that it is the value after which heat release rate becomes independent of Da .

All cases are predominantly burning in non-premixed mode (opposed gradients) with less than 20% of all heat release due to premixed (aligned gradients) or mixed-mode (intermediate gradient) combustion. However, the proportion of premixed and mixed-mode combustion increases with time due to the enhanced mixing brought about by extinction. This is consistent with increased heat release at high Da , indicating increased ignition. In fact, the proportion of heat release at high Da correlates well, both in magnitude and trend, with the proportion of heat release in mixed-mode and premixed regions.

There are differences in the growing trends of premixed and mixed-mode combustion between the Cases. Cases C and D show a monotonic increase in ignition within aligned and intermediate gradient regions. In contrast, Case B almost maintains the same proportion of non-premixed to premixed combustion throughout, although the flammability of this case varies with time. Case A exhibits similar behaviour to B: there is no continuous steady increase in the flammable region of the aligned gradient. However, it differs from B by having 99% of the heat release confined to opposed gradients up to 0.05 ms, followed by a sudden increase of heat release in aligned gradients by 0.1 ms. This can be explained by the less effective small-scale mixing for Cases A and B due to their predominantly large eddies (small wavenumber initial perturbations), making the mixing process more sensitive to extinction.

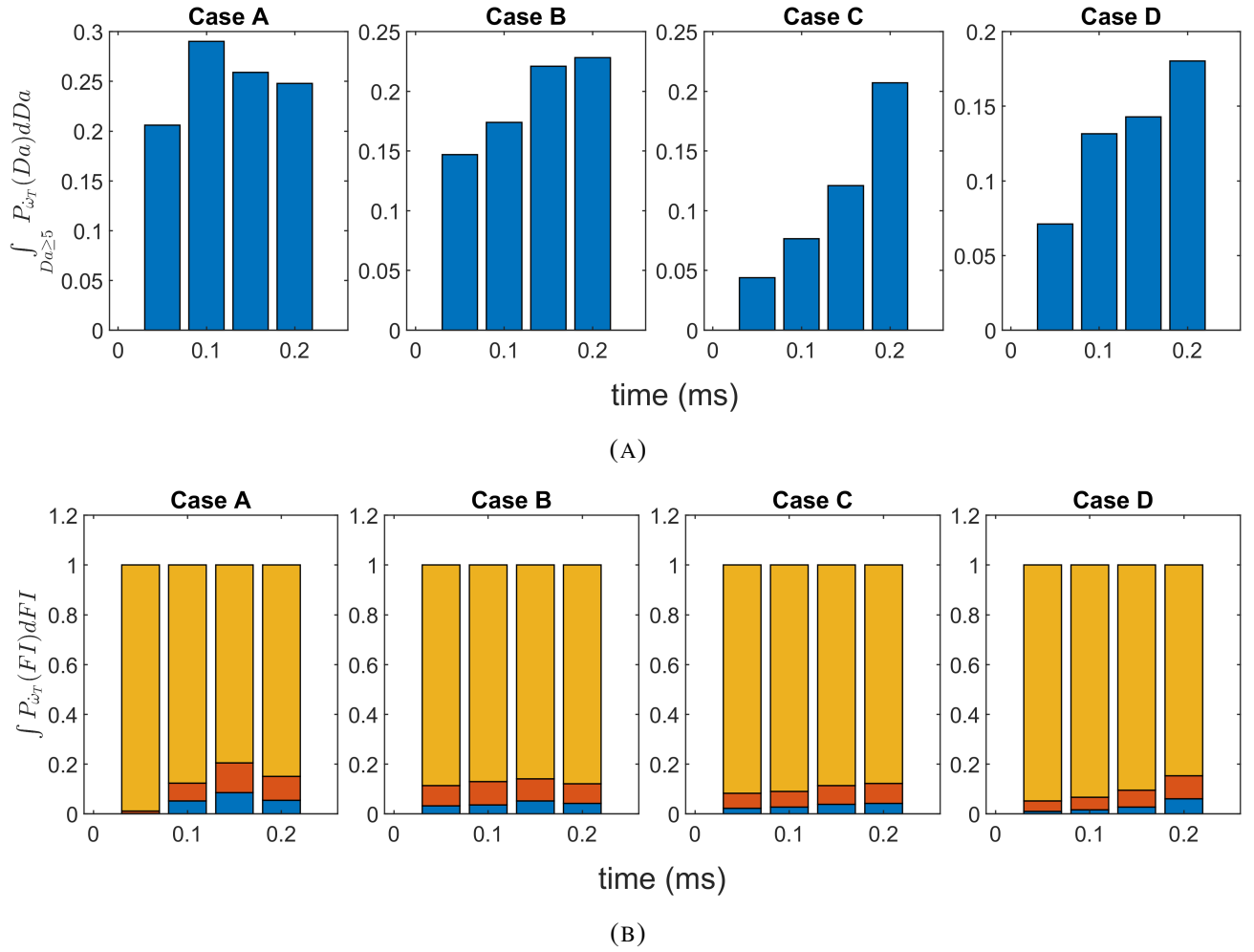


FIGURE 6.15. (A) The proportion of heat release at high Damköhler numbers for each Case at four different times (0.05, 0.1, 0.15, and 0.2 ms). (B) The heat release mode breakdown between premixed (blue), mixed-mode (orange), and non-premixed (yellow) at the same four different times, based on the flame index. These modes are based on the flame index alignment such that yellow corresponds to the total proportion of heat release produced at opposed fuel-oxidiser gradients, whereas blue and orange correspond to the proportion at aligned and intermediate gradients, respectively.

As a result, the premixed modes increase rapidly at early times and decrease slightly later as the non-premixed flames spread to locally extinguished regions. Moreover, the ignition trend for Case A is different from all the other cases as it increases at 0.1 ms and then decreases, whereas ignition is monotonically increasing at varying levels for all the other cases.

In contrast, Cases C and D have more effective local mixing and a more prolonged extinction process that maintains a steady trend. This is confirmed by the delayed further ignition in these Cases as suggested by the first row of Figure 6.15, where a more sizeable increase in heat

release rate occurs at high Da after 0.15 ms compared to Cases A and B. Relating these results to the regime diagram, it is possible that more prominent ignition (or re-ignition) occurs after the Case stabilises following it crossing a critical Reynolds number and transitioning into a flow regime with more enhanced mixing. The results for Case D support this as it is the only case that crosses both Reynolds number thresholds and exhibits two distinct and sizeable increases in heat release rates at high Da at times that align well with the regime diagram explanation. Case D only crosses the second threshold Re_t as it starts at an already high Re_t and spends most of the time overcoming extinction, so the more sizeable jump in ignition is realised at the final time.

In all cases, the increase in mixed-mode combustion, which can grow to 10% heat release contribution, significantly outweighs that of premixed combustion. This emphasizes that unlike in [61], neither of the cases here exhibit entire flame blowout despite their different mixing scales and how especially Cases C and D approach and even surpass extinction thresholds as shown with Damköhler number and scalar dissipation earlier. The lack of more eminent extinction prevents a total shift in combustion mode during re-ignition to allow for premixed flame propagation phenomena. The monotonic trends of Cases C and D may indicate that changes may occur if the cases were allowed to run for later times. However, the prominent re-ignition indicators for Case C in the previous statistics suggest this is unlikely. Instead, it is more likely that the steady transfer between the non-premixed and mixed modes over time is due to the fully developed turbulence in these cases, resulting in enhanced mixing.

Note that the integral-based statistical framework above only attributes less than 25% (except for Case A) of the total heat release to re-ignition events, with most heat release from pre-existing flame elements. Inspection of the flame index means conditioned on Da revealed a predominant non-premixed state at $Da \geq 5$ with an increasing tendency of premixedness (albeit still in negative FI , just less negative) towards ignition for Cases C and D, as discussed. Similarly, flame index PDFs weighted by Da (calculated as in Equation 2.9) confirm the discussions and conclusions above. Ultimately, joint PDFs of Da and FI will reveal more specific insight, but these were not calculated and are reserved for future extensions of this work.

6.5.3 Product Alignment Index

6.5.3.1 Definition

While the above analysis provides some insight into the level of fuel-oxidiser mixedness in burning regions, it doesn't necessarily elaborate on the mechanisms of ignition/re-ignition. Non-premixed combustion can propagate through edge flames and/or turbulent flame folding through a shear layer. If flame extinction is more eminent, enhanced mixing of the reactants can lead to re-ignition in a premixed/partially premixed mode, but the results above indicate this is unlikely in the cases considered. Auto-ignition is another possible mechanism, but that doesn't apply here as the fuel and flow conditions are not favourable [163], [164].

Edge flames propagate when there is a lack of alignment between the stoichiometric mixture surface and iso-surfaces of high flammability (usually marked by prominent combustion species like OH), which has been reported in cases discussed here, as explained in the earlier section. This misalignment results in flames propagating through the edges of the surfaces along the points of intersection of these iso-contours, re-igniting extinguished regions along the stoichiometric surface if the strain conditions are favourable [159], [165]. As a result, edge flames propagate at their own speed along (or in the vicinity of) the stoichiometric iso-surface and so do not necessarily align with either of the counterflows. The locally extinguished regions provide favourable reactant mixing and gradient alignment conditions. Therefore, edge-flame ignition in mixing layers can manifest as premixed/partially premixed under flame indicators, which aligns with the results above.

Turbulent flame folding occurs when three-dimensional turbulent eddies contort the flame surface and, in the process, bring together ignited and extinguished regions, which promotes heat and species diffusion across areas of varying levels of flammability and brings about ignition [61], [115]. These same eddy motions can also increase flame strain and distort the flame, reducing its stability [166]. Therefore, whether this results in ignition or extinction depends on the coupled flow-thermochemical conditions, which are complex and difficult to predict. Ignition through this mechanism is non-premixed and manifests as opposed to fuel-oxidiser gradients.

To help better delineate the prevalence of edge flame propagation and turbulent flame folding, a product alignment index PA is introduced. This is defined similarly to FI but instead measures the degree of alignment between a mixture fraction isosurface and a flame marker iso-surface, taken here as the hydroxyl radical mass fraction:

$$PA = \frac{\nabla \xi \cdot \nabla Y_{OH}}{|\nabla \xi| |\nabla Y_{OH}|} \quad (6.10)$$

Aligned gradients between mixture fractions and product mass fractions iso-contours are, in general, indicative of non-premixed mode combustion [158] and under ignition conditions would therefore correlate more with turbulent-flame folding mechanisms. Opposed and intermediate gradients, on the other hand, better correspond to edge-flame propagation.

6.5.3.2 Conditional Means

Figure 6.16 outlines key mean quantities conditioned on the product alignment index. While the distribution of ignition-marking quantities overwhelmingly peaked at non-premixed conditions, the PA statistics are bi-modal, indicating the potential prevalence of both ignition mechanisms. This is particularly obvious in Y_{OH} means that were almost exclusively uni-modal in FI space. The two indexes are related in the fourth row of Figure 6.16, which shows the conditional mean of the flame index in PA space. This confirms how aligned ξ and Y_{OH} gradients correspond to a non-premixed state with a direct correlation between increasing PA and negative FI . As PA goes to negative values, FI becomes less negative, indicating increasing premixedness while maintaining an overwhelmingly non-premixed regime. The sharp drop in mean FI is due to the ignition as PA tends towards -1 and highlights edge-flame prevalence at this product alignment limit. Overall, the results here confirm the presence of both ignition mechanisms.

While most of the results above demonstrate a balance between the two ignition mechanisms, there are some differences. Looking at Y_{OH} conditional means, A and B show a higher peak at $PA = 1$ than C and D, which maintain balanced peaks. This may indicate more prevalent flame-folding ignition in A and B. Flame-folding is more due to the larger turbulent eddies that can bring together different regions of the stoichiometric surface than the smaller eddies

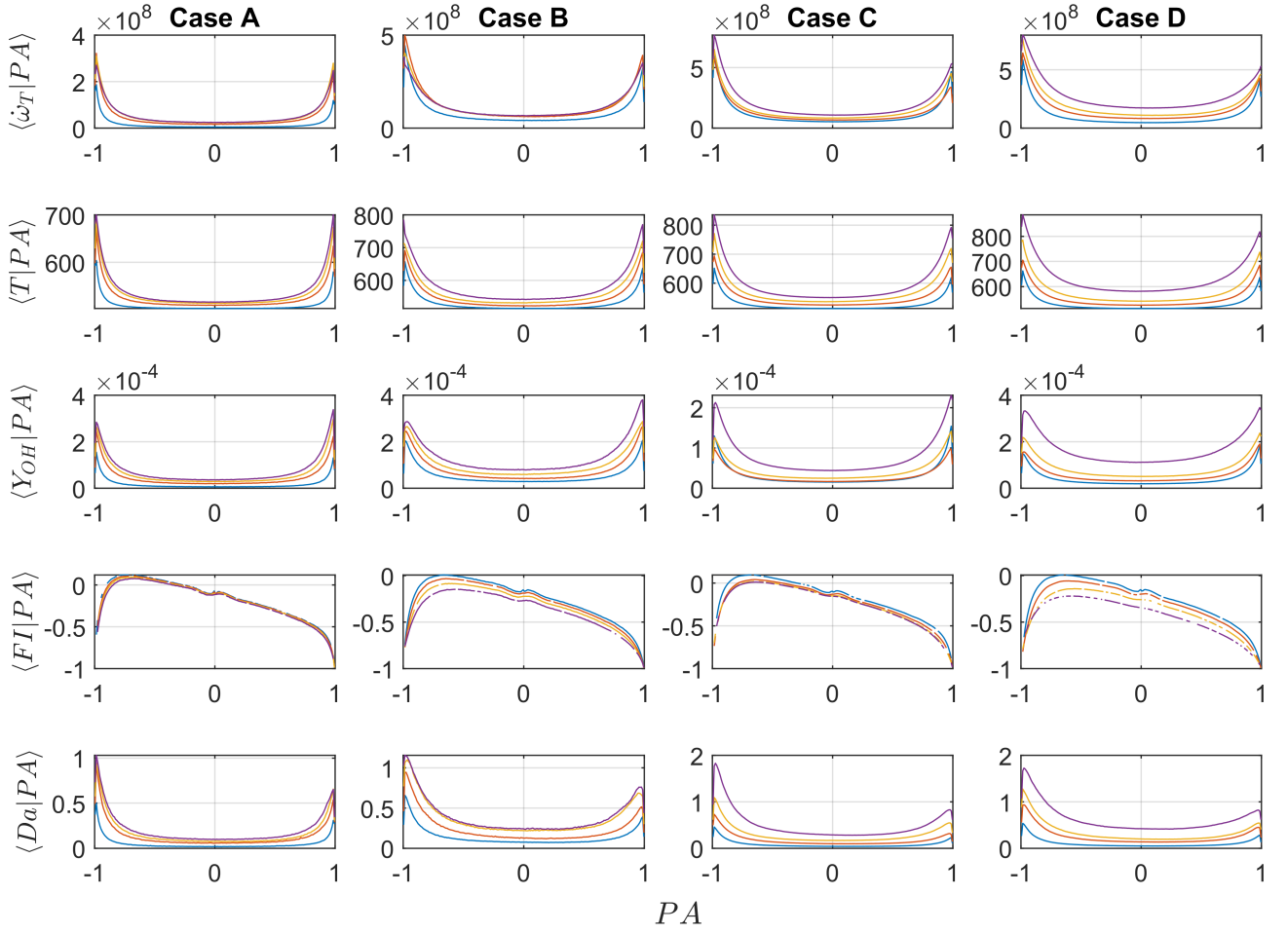


FIGURE 6.16. Key conditional statistics on product alignment for all cases at different times. The last row corresponds to mean Damköhler number weighted PA PDFs as defined in Equation 2.9. The coloured lines correspond to the same absolute times as in Figure 6.10.

that can de-stabilise the chemical scales [166]. Cases A and B, with their smaller wavenumber perturbations, maintain a higher presence of larger eddies than smaller ones, especially relative to C and D, which explains this observation. Interestingly, while the Damköhler number means in mixture fraction space for C and D are lower than B as shown in Figure 6.12, the mean Damköhler numbers in PA space for C and D, firstly have markedly higher peaks at opposed gradients than at aligned, secondly peak at higher Damköhler numbers at $PA = -1$ than any of the peaks of Cases A and B. This indicates a strong prevalence of edge flame propagation in C and D, which can be visually confirmed by inspecting the contours in Figure 6.1, where an edge flame can be clearly seen for C along the stoichiometric surface.

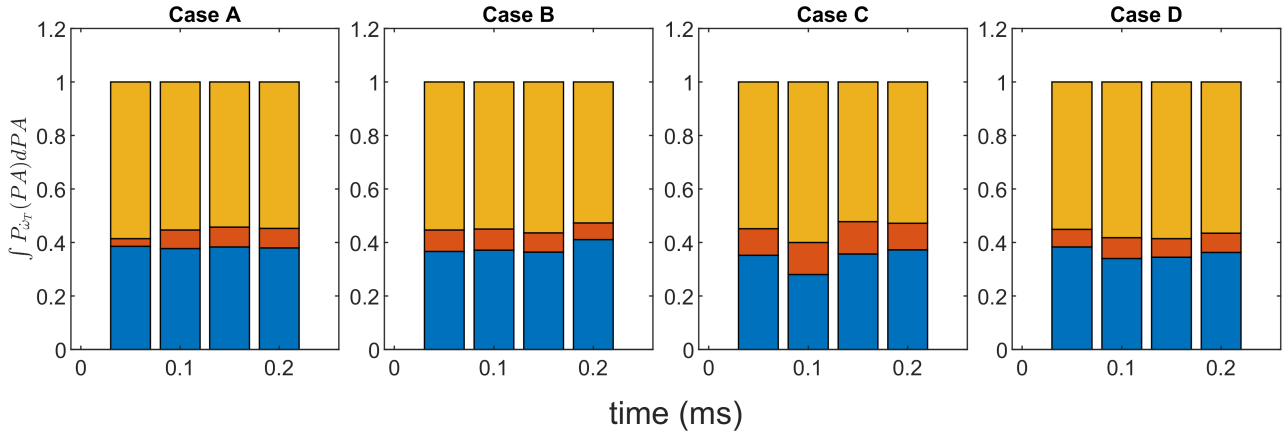


FIGURE 6.17. The heat release mode breakdown between $PA \geq \cos(\frac{\pi}{4})$ (blue), $\cos(\frac{3\pi}{4}) < PA < \cos(\frac{\pi}{4})$ (orange), and $PA \leq \cos(\frac{3\pi}{4})$ (yellow) at four different times (0.05, 0.1, 0.15, and 0.2 ms). Yellow corresponds to the total proportion of heat release produced at opposed mixture fraction and hydroxyl radical mass fraction gradients, whereas blue and orange correspond to the proportion at aligned and intermediate gradients, respectively.

6.5.3.3 Integrated Weighted PDF

To obtain a more direct measure of the relative prevalence of these ignition mechanisms, the cumulative heat release weighted PDF of the product alignment index is outlined in Figure 6.17. Similar to FI , it is important to note that these statistics haven't been explicitly extracted from reacting regions. For that, joint PDFs of the heat release rate or Damköhler number and product alignment must be calculated, which is not done here. Instead, the approach here provides an integral view that can be used to approximate the proportion of burning under either mechanism.

In [115], Hawkes concluded flame folding was the predominant ignition mechanism in a burning Syngas slot jet configuration. The results here suggest that flame folding in transitional flows is secondary to edge flame propagation as an ignition mechanism, though not by a significantly large margin. Moreover, the choice of initial perturbation affects the proportion of both mechanisms in ignition. For instance, Case C has the highest proportion of intermediate and opposed gradients and was visually shown to employ edge flames. This is followed by Case D, which maintains the second-highest prevalence of edge-flame favourable statistics. Although previous studies have shown that edge flame propagation speed is weakly negatively correlated with scalar dissipation rate [159], [167], the dependency is with χ on

a logarithmic scale; hence, the differences in strain rates between the cases are not significant enough to realise a measurable variation in edge flame propagation due to the increased strain.

Therefore, cases with more small-scale eddies and higher Reynolds number conditions maintain more favourable conditions for edge flames than flame-folding despite the higher strain rates indicated by the earlier scalar dissipation rate statistics for these cases. All cases highlight a weakly increasing trend in flame-folding conditions, which may explain why flame-folding dominated in [115] as the flows were initialised with a turbulent jet and the slot jet configuration results in double shear layer effects that expedite the turbulent transition. So the results in [115] are later in the turbulence development than the ones here. This emphasizes the importance of more accurately defining the beginning of turbulent flow regimes and delineating between transitional and turbulent flow regimes when accounting for model closures, as the physics of transition and the resulting burning mechanisms and flame structures can vary greatly.

6.6 Conclusion

While the previous chapters established a clear dependence of both the turbulence and the mixing development on the fundamental primary shear instabilities, this chapter was dedicated to exploring the full extent of the mixing variabilities that result from the perturbation variations. The focus was on thoroughly assessing the flame structure across various diagnostics and interrogating the underlying physics that led to the observable differences between the cases. This thorough and consistent account of the flame structure of cases naturally transitioning from a fundamental instability provides a valuable dataset for assessing and informing future combustion and mixing model developments for flames in transitional flow regimes.

Regarding the dependency on the initial perturbation parameters, distinct trends were demonstrated depending on the nature of the initial perturbation variation. Exploring mixture fraction-dependent statistics revealed different flame structures between each of the cases. Increasing the free-stream velocities increased the strain rate and scalar dissipation, resulting in reduced flame stability (i.e., flame intermittency) and prominence of unsteady effects. At

the same time, reducing the perturbation wavelength mitigates this flame intermittency by improving the small-scale mixing, although leading to increased curvature effects as evidenced by the vorticity contour observations. A higher wavelength perturbation at the same free-stream velocities grows more rapidly with downstream distance and amplifies the strain rate from the free-stream flows.

Assessing the flame structure in Damköhler number space revealed more intricate details about the flame structure variations resulting from the different initial perturbations and confirmed the observations derived from the mixture fraction statistics.

Relating the flow and chemical scales while taking into account the insights from the explored Damköhler number and mixture fraction statistics, a combustion regime diagram was outlined, showcasing distinct separation in the evolution of the combustion regimes between the flows seeded from different perturbations. This separation confirmed the sensitivity of both the mixing and flame structure to the seeding perturbation wavelength and demonstrated the lack of a universal instability-independent turbulent Reynolds number value that characterizes a clear flammability transition.

Finally, variability in re-ignition mechanisms between the cases was assessed by analysing the alignment of chemical species gradient profiles. The results revealed some discrepancies between current observations and those obtained in turbulent counterflowing jet flames. Moreover, there was some variability in the predisposition towards the re-ignition mechanism between the cases of different initial perturbation eigenvalues, where cases with smaller perturbation wavelengths and higher free-stream velocities were more predisposed towards edge-flame propagation ignition. Direct contour visualisation and joint PDF calculations of gradient alignments with heat release rate are needed to validate this observation further.

Conclusion

7.1 Summary

This thesis investigated the dependence of turbulent mixing on fundamental, primary shear instabilities. Turbulent mixing is essential in a wide range of energy and propulsion applications, and the increase in complexity of desirable applications like hypersonic propulsion and nuclear fusion motivates a deeper understanding of how varying states of mixing unfold. Assessing the dependence of turbulent mixing on well-defined parameters holds the prospect of enabling a degree of control over process output, stability, and efficiency. Shear instabilities are prevalent in all turbulent mixing applications. They dominate the turbulence generation process based on both practical observations and theoretical studies and, therefore, were a natural choice for this investigation. The parameters investigated in this thesis appear directly in the eigenvalue representation of primary shear instabilities- Kelvin-Helmholtz Instabilities (KHI)- directly affecting the instability that drives turbulence generation. These parameters are the initial perturbation wavelength bandwidth and the free-stream velocities of the flows between which shear effects exist.

Turbulent mixing is a complex phenomenon that involves a high degree of interdependence of different physical processes and scales of fluid motion. The complexity is further exacerbated when the mixing process is assessed within an application such as combustion or nuclear fusion, which can add rapid compositional and fluid property changes or hypersonics that add elements of compressibility and acoustic effects (known as secondary instabilities). Prominent historic advancements in understanding turbulent mixing and its dependencies were mostly conducted through experimental investigations. However, with the highly chaotic

nature of turbulence and limited diagnostics available to collect comprehensive data sets from experiments, additional significant advancements in the field stagnated. This changed with the continuous improvement of computing and storage facilities that enable high-fidelity numerical simulations, which provide access to comprehensive flow field information and the opportunity to artificially isolate elements of interdependent physics to test hypotheses and develop deeper understanding.

The present study leverages advancements in HPC and undertakes high-fidelity DNS to curate a comprehensive dataset of developing flows from fundamental shear instabilities to derive a deeper understanding of the different dependencies of turbulent mixing on the initial conditions and support future modelling efforts for transitional reacting flows.

The initial perturbations were derived and implemented in accordance with the linear theory that well-describes the initial stages of the natural laminar to turbulent transition process [24], instead of the more common fully turbulent initialisation approaches that lead to unnatural turbulence evolution and misleading transition process. The KHI implementation in the initial condition is modelled in an eigenvalue-eigenvector framework to assess the evolution of turbulent mixing as a dynamic system. The simulation results are systematically assessed for quality through mesh convergence of key relevant quantities, gradients, and statistics in Chapter 3. Additionally, the results and analysis are heavily interrogated for consistency throughout the thesis without revealing any discrepancies. Furthermore, comparisons are constantly drawn between the present results and previously published experimental and numerical work without yielding significant unexplained or inconsistent deviations.

The analysis in this thesis is undertaken within three main paradigms to systematically assess the dependence of turbulent mixing on the seeding shear instability.

The first is presented in Chapter 4 and assesses the evolution of the different flow and turbulence scales without chemical reactions to avoid the added variability of flow-chemistry interactions and establish a reference that reacting cases can be compared against. The main findings of this assessment were:

- (1) The flow and turbulence evolution are dependent, in their transition, on both the initial shear instability wavelength and the mean velocities of the free streams. Furthermore, it is the relative dimensions of the instability to the domain size (or residence time if comparing time scales) that are important rather than the absolute value of the perturbation wavelength bandwidth.
- (2) The growth rate of all large-scale flow thickness measures agree in their dependence on the initial perturbation. If assessed in time, the trends are consistent with the results from linear theory and the eigenvalue definition, which confirms the robustness of linear theory in assessing the evolution of the large flow scales. If the growth is assessed against downstream distance, initial perturbations with lower free-stream velocities and higher perturbation wavelengths grow the shear layer more rapidly. The results also show that unlike the chemical product thickness [11], or the mixture fraction threshold thickness, the streamwise velocity threshold thickness is well correlated with the vorticity thickness and should, therefore, not be used to assess an outer-scale Reynolds number without a doubling factor to avoid misleading turbulence assessments.
- (3) Under a Strouhal number-like normalisation (t^*) of the independent evolution coordinate that incorporates the most unstable forcing wavelength of the initial perturbation in addition to magnitude normalisation of the thickness measure by the same wavelength, a self-similar collapse between the different thickness measures is observed during both the transitional stage of flow development and the asymptotic steady state.
- (4) The onset of asymptotic self-similar evolution of large-scale flow and turbulence measures (integrated dissipation and Reynolds stresses) is consistent between different large-scale parameters and for all Cases seeded from different initial perturbations. The onset is consistently marked by $t^* = 20$, which shows a direct dependence of turbulence development on both the seeding perturbation wavelength (relative to domain size) and free-stream velocity. This t^* value aligns with three major vortex amalgamation events.

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- (5) Assessing the spectral distribution of turbulent energy and Reynolds stress profile demonstrates that a t^* value of 20 cannot realise universal turbulent behaviour at the finer scales. Instead, an excess of three vortex pairings and an outer-thickness Reynolds number above 2×10^4 are collectively needed to realise universal behaviour. Moreover, the effects of the initial perturbation still manifest late in the flow evolution, as evidenced by the different wavenumber functional dependence of the turbulent energy spectra between cases seeded from different perturbations.
 - (6) The results explain that characterization of fully developed turbulence based on the Reynolds number alone is insufficient and is likely the cause of the wide disagreement in the literature on a Reynolds number threshold to mark the turbulence transition. Instead, for turbulence to fully develop, the seeding perturbation is required to provide a capacity for an energy-transferring mechanism to occur an adequate number of times within the confines of the physical system. A high Reynolds number is still required to allow a wide range of scales to weather viscous effects and allow scale separation, but only if the perturbation and mechanism occurrence capacity requirements are met. If these conditions are collectively satisfied, then the results support the universal behaviour of various turbulence quantities while still showcasing the information of the seeding perturbation, which is not fully forgotten even in this asymptotic state of developed turbulence.

The second analysis framework, presented in Chapter 5, directly assesses the mixing behaviour but shifts the focus to the reacting cases to draw a direct correlation with the resulting flame behaviour in subsequent analyses. The main findings of this chapter were:

- (1) Unlike the flow and turbulence scales, the large mixing scales are more sensitive to the free-stream velocities than the perturbation wavelength. The trends in the growth of the mixing thickness are, however, the same against t^* , with increasing growth observed with a larger perturbation eigenvalue.
- (2) The finer mixing scales extend the dependency on the perturbation wavelength, where larger wavelength perturbations lead to more rapid onset of asymptotic mixing

state as characterized by scalar dissipation rates, mixture fraction variance transport budgets, and mechanical-to-scalar mixing time scale ratio.

- (3) Even beyond the mixing transition, the effects of varying the perturbation wavelength manifest and affect the scalar PDF behaviour, where smaller initial perturbation wavelengths lead to a greater extent of marching PDF behaviour at the mixing transition owing to different morphology of the turbulent eddies when the flows become stationary. This discrepancy is observed even in cases that manifest the same steady-state Taylor Reynolds number but with a different initial perturbation wavelength. More interestingly, if the outer-scale Reynolds number is considered, the case with the smaller initial wavelength demonstrates scalar PDF behaviour that is more representative of the mixing transition than the case with a larger outer-scale Reynolds number (at the same downstream location) but a larger initial perturbation wavelength. This reinforces that Reynolds numbers alone are insufficient to characterize the onset of the mixing transition and its asymptotic behaviour, as explained in Chapter 4.
- (4) Lastly, although correlations manifest between the downstream location where an asymptotic mixing state is achieved (i.e. t^*) and the choice of initial perturbation parameters, the significance of $t^* = 20$ to denote elements of this transition (as highlighted in Chapter 4), even at the large scales, is diluted in reacting cases due to varying levels of flow-chemistry interactions between the cases.

The third and final analysis framework, presented in Chapter 6, assessed the flame structure variations and their evolution in the dependence on seeding perturbation. This assessment validates the mixing dependence on the initial perturbation to a wider extent than has been explored in any earlier work. The flame structures were thoroughly examined under various diagnostics, revealing significant differences driven by initial perturbation variations. This comprehensive analysis provides a valuable self-consistent dataset for future developments in combustion and mixing models, particularly for flames in transitional flow regimes.

Key trends emerged regarding the dependence on initial perturbation parameters. Specifically, increasing free-stream velocities led to higher strain rates and scalar dissipation, reducing

flame stability and amplifying unsteady effects. In contrast, shorter perturbation wavelengths mitigated flame intermittency by enhancing small-scale mixing, though at the cost of increased curvature effects. On the other hand, higher wavelength perturbations grew more rapidly downstream, further amplifying strain rates.

Analysis of flame structure in Damköhler number space offered deeper insights into how different initial perturbations affect flame dynamics, confirming the findings from mixture fraction statistics. A combustion regime diagram was constructed by correlating flow and chemical scales to highlight distinct evolutions of combustion regimes based on the initial perturbation characteristics. This analysis underscored the sensitivity of both mixing and flame structure to the seeding perturbation wavelength.

Finally, re-ignition mechanisms were examined across different cases, identifying variability influenced by initial perturbation eigenvalues. Cases with smaller perturbation wavelengths and higher free-stream velocities were more prone to edge-flame propagation ignition. Further validation through contour visualization and joint PDF calculations of gradient alignments with heat release rate is recommended to solidify these findings.

7.2 Practical Implications

The results of this thesis support that varying system design attributes that influence the turbulence seeding instabilities can provide tractable means of controlling mixing and, hence, combustion output and stability. This impinges on additional design considerations in propulsion applications that leverage transitional flow regimes. Another important implication is that practical turbulent states observed in these applications retain some information about the seeding instability in their statistics, specifically if they are not fully developed but likely even if the Reynolds number is above the transition threshold. Therefore, the transition is not restricted from laminar to developed turbulence, but even one turbulent state can transition to another with a new unique footprint of the seeding instability, resulting in different mixing evolution throughout the transition process. Consequently, design methodologies of new propulsion systems need to leverage this element of process control, and the implications of

this are vast! For instance, gas turbines could utilize variations in surface roughness to manage heat dissipation and reduce thermal loads, nozzle geometries could be carefully designed to ensure desirable instability scales relative to combustion chamber dimensions, and activated plasma could be utilized to actively modulate turbulence leading up to ignition/detonation in hypersonic propulsion systems.

7.3 Future Outlook

While shear instabilities are key drivers of turbulent transition and mixing, they rarely occur in isolation from buoyant effects. Additionally, shock waves and acoustic phenomena often accompany scenarios where precise control of turbulence and mixing is crucial. The interactions between these primary instabilities remain poorly understood, particularly in terms of their contributions to mixing development. This gap in knowledge largely stems from the challenges of creating experimental setups capable of systematically investigating the complex, nonlinear physics involved.

However, the increasing accessibility to exascale computing and advancements in data analysis techniques, such as machine learning and artificial intelligence, present new opportunities to explore these intricate interdependencies. As we enter a new technological era with growing demands for cutting-edge energy and propulsion technologies, uncovering the complexities of turbulent mixing and finding ways to harness its evolution could be key to overcoming several critical technological bottlenecks.

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Appendices

Appendix A: Derivation of the KHI Initialisation and its Implementation

An important motivation for this study is to investigate the transition to turbulence, so it is important to accurately model the turbulence-inducing initial condition to adequately represent the underlying physical shear instability. The KHI is initialised as a velocity perturbation superimposed on the mean velocity profiles throughout the initial domain. The use of the velocity field to initialise the instability is a natural choice as it directly drives the instability growth and turbulence and has been commonly used in a large number of studies [11], [32], [37], [38], [97], [109]. In his study of different turbulence generating initial conditions, Fathali [97] referenced using linear stability theory to derive the initial disturbance to be a valid method, but one that lacks the broad-spectrum energy profile that is characteristic to turbulent fields. Since the initial disturbance here aims to simulate a fundamental instability and observe its development into turbulence rather than directly simulate a fully turbulent boundary layer inflow condition, this approach is suitable for this study's focus.

As shown in Section 2.3.2, the start of a KHI is an amplitude perturbation, which is more conveniently expressed as a velocity perturbation in the initialisation. Therefore, the KHI initialisation adopted here starts with an amplitude perturbation that is derived very similarly to the material interface perturbation in Richtmyer-Meshkov instability (RMI) studies [12], [25], [26], [78]. This initial condition has been originally formulated by D. Youngs and builds on the multimode perturbed interface initialisation outlined in [168].

The initial two-dimensional amplitude perturbation is initialised at the centre plane of the cross-stream direction, with variations along the streamwise (y) and spanwise (z) directions. The amplitude perturbation is defined in two-dimensional spectral space over narrowband wavenumber ranges in both directions. These narrowband ranges vary between the different

simulations, but all maintain the same perturbation bandwidth $R = \frac{\lambda_{max}}{\lambda_{min}} = 2$. The term narrow is used here, consistent with the convention, to emphasize that $R \leq 2$ is adopted in all cases considered in this study. Choosing a narrowband perturbation to initiate the transition to turbulence is intentional. Initialising the flow with a broadband spectrum is commonly adopted in studies [14], [37], [53], [55] and results in rapid turbulence generation without allowing for a physically realistic transition process to transpire as the initial perturbation broadband spectrum is usually representative of boundary layer turbulence from the start. At the same time, choosing an initial perturbation to be a single or a handful of modes as in [11], [44], [97], is too simplistic and also not physically representative of turbulence generating flow perturbations. This choice of perturbation usually results in dominant and ordered coherent structures overwhelming the flow, which are not representative of turbulence and hence usually require additional artificial distortion, as done in these studies, to develop turbulence. The choice of implementing a narrowband perturbation, therefore, lies in between those two extremes, such that it acknowledges that physical perturbations rarely manifest as distinct and isolated modes. A narrowband perturbation is, therefore, able to adequately capture a perturbation of a well-defined length scale without being too wide that it is either already turbulent or leads to unrealistically rapid turbulence development. Examples of physical narrowband perturbation can include a narrow range of initial surface perturbation induced due to a surface roughness profile in a nozzle, a narrow mixing layer with a dominant eddy length scale, or tip vortices and swirls induced by a nozzle or rotor blade tip. There is still an element of randomness in these flow perturbations that needs to be accounted for in the initialisation, as demonstrated below.

The power spectrum of the narrowband amplitude surface perturbation, ζ , is defined as:

$$P_1(\underline{\kappa}) = \begin{cases} C & \underline{\kappa}_{min} \leq \underline{\kappa} \leq \underline{\kappa}_{max} \\ 0 & otherwise \end{cases} \quad (A.1)$$

$$\begin{aligned}
P(\underline{\kappa}) &= \int_0^\infty P_1(\underline{\kappa}) d\underline{\kappa} \\
&= \int_0^{\omega_{ymax}} \int_0^{\omega_{zmax}} \frac{C}{2\pi \underline{\kappa}} d\omega_y d\omega_z \\
&= \int_0^{\omega_{ymax}} \int_0^{\omega_{zmax}} \frac{C}{[\zeta(\omega_y, \omega_z)]^2} d\omega_y d\omega_z
\end{aligned} \tag{A.2}$$

The rationale behind choosing a constant power spectrum is due to the narrow nature of the perturbation, where a functional form of the initial spectrum is unlikely to produce different behaviour. This is not the case if a broadband spectrum is used, however, as shown for RMIs in [78], but broadband initialisations are beyond the scope of this study due to the strenuous resolution requirements that render their DNS impractical. C is set to be $\propto \sigma^2$ where σ is the standard deviation of the perturbation. In RMI studies, care is taken to set σ sufficiently small so that the initial behaviour can be adequately predicted through linear analysis. Since the focus is on KHI, where the perturbations grow initially exponentially and are, therefore, quickly beyond the limits of linear theory approximations, such a choice is not needed. Baltzer [37] used a 10% rms fluctuation amplitude in his initialisation of shear layer disturbance, so did Pantano [14] and Almagro [55]. Similarly, here σ is taken to be $0.1\lambda_{min}$. The mean fluctuation amplitude in wave number space is denoted by $\overline{\zeta(\omega)}$.

The spatial formulation of the amplitude perturbation can be determined by taking the inverse discrete Fourier transform of $\sqrt{\frac{C}{2\pi \underline{\kappa}}}$. Recognizing that $\zeta(y, z)$ is a real-valued expression, it would take the general functional form of:

$$\zeta(y, z) = \sum_{j=-n_{ymax}}^{n_{ymax}} \sum_{k=-n_{zmax}}^{n_{zmax}} \mathbb{Re} [\hat{q} e^{i(\omega_j y + \omega_k z)}] \tag{A.3}$$

where $\hat{q}$ denotes the complex coefficients of the discrete Fourier transform and the wave-numbers are expressed as $\omega_j = \frac{2\pi j}{L_y}$ and $\omega_k = \frac{2\pi k}{L_z}$. $n_{ymax} = \frac{L_y}{\lambda_{min}}$ and $n_{zmax} = \frac{L_z}{\lambda_{min}}$, both rounded to the nearest integer. The minimum perturbation wavelength is $\lambda_{min} = \frac{L_y}{\bar{n}}$ and $\bar{n}$ can be either 8 or 16 depending on the case considered, as shown in the following section 3.5. The $\mathbb{Re}$ is to denote the real component of the complex number.

To improve computational efficiency through better leveraging of array operations, Euler's formula and trigonometric identities are used to expand Equation A.3 and sum over the

positive and real quadrant, such that:

$$\begin{aligned}\zeta(y, z) = \sum_{j=0}^{n_{ymax}} \sum_{k=0}^{n_{zmax}} & [a_{jk} \cos(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & + b_{jk} \cos(\omega_y(y - y_0)) \sin(\omega_z(z - z_0)) \\ & + c_{jk} \sin(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\ & + d_{jk} \sin(\omega_y(y - y_0)) \sin(\omega_z(z - z_0))] \end{aligned} \quad (\text{A.4})$$

where y_0 and z_0 denote the initial centre of the shear layer in the streamwise and spanwise directions, respectively. In all single shear layer cases considered, this lies at the geometric centre of the domain.

To define the Fourier coefficients, we require that the mean of their contribution squared to be related to the power spectrum such that:

$$[\overline{\zeta(\omega)}]^2 = \frac{1}{4} \left[\overline{a_{jk}^2 + b_{jk}^2 + c_{jk}^2 + d_{jk}^2} \right] = \frac{C}{2\pi \underline{\kappa}} \quad (\text{A.5})$$

where the $1/4$ factor comes from the fact that each of the Fourier coefficients is multiplied by a pair of sines and/or cosines and $\overline{\cos^2} = \overline{\sin^2} = \overline{\cos \times \sin} = \frac{1}{4}$, this means that to satisfy the form of the power spectrum prescribed in Equation A.2, each of the Fourier coefficients needs to be defined such that they're $\propto \frac{C}{2\pi \underline{\kappa}}$.

Furthermore, to simulate the randomness of the initial perturbation, the coefficients for each mode are formed from a random number picked from a Gaussian distribution. This process uses a deterministic Mersenne Twister algorithm to allow for simulation repeatability, provided the same seed is chosen in the algorithm.

Since Equation A.4 only considers positive wavenumbers, the modal amplitudes correspond to the single-sided spectrum; hence, compensation must be made for doubling the zeroth wave numbers. This renders the general expression of the Fourier coefficients with a_{jk} as an example:

$$a_{jk} = \sqrt{f(\omega_y, \omega_z) \Re S(j) S(k)} \sqrt{\frac{C}{2\pi \underline{\kappa}}} \quad (\text{A.6})$$

with $\Re$ the random number assigned for each of the coefficients and $S(j)$ is $1/\sqrt{2}$ for $j=0$, and 1 for $j>0$ (similarly $S(k)$ $1/\sqrt{2}$ for $k=0$, and 1 for $k>0$). The first coefficient on the right-hand side, $f(\omega_y, \omega_z)$, above, is a fraction calculated at each streamwise and spanwise wavenumber combination to ensure that the contribution added by this two-dimensional increment is within the bounds of the radial (κ) wavenumber limits. The standard deviation of all the modal amplitudes is then rescaled linearly to σ for consistency.

With the amplitude perturbation spatial term fully defined, this then needs to be converted into an equivalent velocity perturbation to be implemented in the initial conditions while still representing fundamental KHI. To ensure a divergence-free initial velocity field, the velocity field is initialised from a vector potential:

$$\mathbf{u} = \nabla \times \phi \quad (\text{A.7})$$

Relating ϕ in Equation A.7 with Φ defined in Section 2.3.2:

$$\nabla \times \phi = \nabla \Phi \quad (\text{A.8})$$

Since ϕ is the representative vector potential of the amplitude perturbation ξ , it only has vector components in the y and z directions. Therefore, with partial derivatives denoted following the comma such that i,j, and k are the cross-stream(x), streamwise(j), and spanwise (z) directions, respectively:

$$u_i = \Phi_{,i} = \phi_{k,j} - \phi_{j,k}, \quad u_j = \Phi_{,j} = -\phi_{k,i}, \quad u_k = \Phi_{,k} = \phi_{j,i} \quad (\text{A.9})$$

Therefore all three velocity components can be defined if ϕ_j and ϕ_k are known and these can be calculated from Φ by rearranging and integrating the expression for u_j and u_k in Equation A.9:

$$\phi_j = - \int \Phi_{,k} dx = - \frac{\partial [\int \Phi dx]}{\partial z}, \quad \phi_k = \int \Phi_{,j} dx = \frac{\partial [\int \Phi dx]}{\partial y} \quad (\text{A.10})$$

Let $\varphi = \int \Phi dx$. Relating Φ to the amplitude perturbation ζ from Equations 2.37-2.39 and taking the real component of A (the eigenfunction from Equation 2.41) while noting that this is a non-buoyant simulation setup so the RTI term in the eigenvalue expression (Equation

2.40) is zero:

$$\begin{aligned}
\Phi &= \zeta(y, z) \frac{A e^{-\underline{\kappa}|x-x_0|}}{\zeta^*} \\
&= \zeta(y, z) S(x - x_0) \frac{\frac{\omega_y \sqrt{\rho_1 \rho_2} |U_1 - U_2| \zeta^*}{\underline{\kappa}(\rho_1 + \rho_2)} e^{-\underline{\kappa}|x-x_0|}}{\zeta^*} \\
&= \frac{\omega_y \sqrt{\rho_1 \rho_2} \Delta U}{\underline{\kappa}(\rho_1 + \rho_2)} e^{-\underline{\kappa}|x-x_0|} S(x - x_0) \zeta(y, z) \\
&= \Phi_0 S(x - x_0) \zeta(y, z) e^{-\underline{\kappa}|x-x_0|}
\end{aligned} \tag{A.11}$$

with $\zeta(y, z)$ defined in Equation A.4 and $S(x - x_0)$ is 1 for $x > x_0$ and -1 for $x < x_0$. The fuel and oxidizer free-stream densities are ρ_1 and ρ_2 , respectively. As Φ is now fully defined, φ is:

$$\varphi = \int \Phi dx = -\frac{\Phi_0}{\underline{\kappa}} \zeta(y, z) e^{-\underline{\kappa}|x-x_0|} \tag{A.12}$$

Hence, expanding:

$$\begin{aligned}
\phi_j &= \Phi_0 \frac{\omega_z}{\underline{\kappa}} [b_{jk} \cos(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\
&\quad - a_{jk} \cos(\omega_y(y - y_0)) \sin(\omega_z(z - z_0)) \\
&\quad + d_{jk} \sin(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\
&\quad - c_{jk} \sin(\omega_y(y - y_0)) \sin(\omega_z(z - z_0))] e^{-\underline{\kappa}|x-x_0|}
\end{aligned} \tag{A.13}$$

and:

$$\begin{aligned}
\phi_k &= \Phi_0 \frac{\omega_y}{\underline{\kappa}} [-c_{jk} \cos(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\
&\quad - d_{jk} \cos(\omega_y(y - y_0)) \sin(\omega_z(z - z_0)) \\
&\quad + a_{jk} \sin(\omega_y(y - y_0)) \cos(\omega_z(z - z_0)) \\
&\quad + b_{jk} \sin(\omega_y(y - y_0)) \sin(\omega_z(z - z_0))] e^{-\underline{\kappa}|x-x_0|}
\end{aligned} \tag{A.14}$$

With ϕ_j and ϕ_k fully defined above, the initial velocity perturbation components can now be determined from Equation A.9 by differentiation of the above expressions and summing up components as needed. The final form above constitutes an eigenvalue, $\Phi_0 = \frac{\omega_y \sqrt{\rho_1 \rho_2} \Delta U}{\underline{\kappa}(\rho_1 + \rho_2)}$ that follows directly from linear theory as shown in Equation 2.40, and an eigenfunction that still complies with the general form of Equation 2.41, whilst satisfying all the aforementioned

requirements. This study considers the effect of varying elements of the eigenvalue on the flow development and combustion. Since σ scales with the wavenumber range, the total energy of the initial perturbation is kept the same between the cases by scaling the number of modes with the wavenumber magnitude.

Moreover, since KHIs are inherently exponential in their growth, and the aim of the collated DNS library is to look at both the transitional and fully developed regimes, Equations A.13, A.14 are multiplied by an additional attenuation factor of $\frac{\omega_z}{\kappa}, \frac{\omega_y}{\kappa}$ respectively. The advantage of choosing this for attenuating the initial perturbation over an arbitrary constant (as used, for example, for amplifying the two test cases in [11]) is that it scales with the narrowband range chosen for the perturbation and thus allows for easier comparison across the cases studied. Lastly, each of the ϕ components in Equations A.13 and A.14 are multiplied by a correction factor, $h(x)$, to allow for the finite domain length in the cross-stream direction, so that there are no fluctuations at the cross-stream boundaries:

$$h(x) = \frac{1 - e^{-2\kappa(h_0 - |x - x_0|)}}{1 - e^{-2\kappa h_0}} \quad (\text{A.15})$$

where h_0 is the width of the fluids on either side of the shear layer (equal to x_0 in all the single shear layer simulations). This completes the vector potential definition, and the corresponding velocity perturbations are calculated using Equation A.9. These perturbations are then superimposed on the mean velocity profile outlined in Equation 3.6, which completes the velocity field initialisation.

From the formulation of the vector potential mode amplitudes, looking at the eigenvalue, Φ_0 , the modes most oriented in the direction of the flow (streamwise) are the ones that dominate the instability as the mixing layer grows. This is consistent with the physical observation of the instability and linear theory results reported in [24].