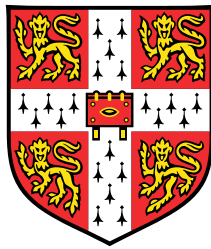


The bending effect in turbulent flame propagation



Girish Venkata Nivarti

Darwin College

University of Cambridge

A thesis submitted for the degree of

Doctor of Philosophy

6 June 2017

Declaration

This dissertation is the result of my own work and contains nothing which is the outcome of work done in collaboration except where specifically indicated in the text. It has not been submitted for another qualification to this or any other university. It contains nearly 33,300 words, 48 figures and 3 tables.

Girish Nivarti

1 June 2017

Abstract

In the present thesis, the sensitivity of flame propagation to the turbulent motion of burning gases is investigated. The long-standing issue of the ‘bending effect’ is focused upon, which refers to the experimentally-observed inhibition of flame propagation velocity at high intensities of turbulence. Plausible mechanisms for the bending effect are investigated by isolating systematically the effects of turbulence intensity. By providing a novel perspective on this topic, the thesis addresses the fundamental limits of turbulent burning.

The investigation employs Direct Numerical Simulation (DNS), which enables the basic conditions of burning to be controlled directly. A parametric DNS dataset is designed and generated by increasing turbulence intensity over five separate simulations. Effects of turbulent motion are isolated in this manner, such that the bending effect is reproduced in the variation of flame propagation velocity recorded. Subsequently, the validity of Damköhler’s hypotheses is investigated to ascertain the mechanism of bending.

Analysis of the DNS dataset highlights the significance of kinematic flame response in determining turbulent flame propagation. Damköhler’s first hypothesis is found to be valid throughout the dataset, suggesting that the bending effect may be a consequence of self-regulation of the flame surface. This contradicts the dominant belief that bending occurs as a result of flame surface disruption by the action of turbulence. Damköhler’s second hypothesis is found to be valid in a relatively limited regime within the dataset, its validity governed by flame-induced effects on the prescribed turbulent flow field. Therefore, this thesis presents turbulent flame propagation and the bending effect as emergent from the dynamics of a flame surface that retains its internal

thermo-chemical structure.

Finally, experimental validation is sought for the proposed mechanisms of bending. Comparisons have been initiated with measurements in the Leeds explosion vessel, based on which the widely accepted mechanism of bending was hypothesized twenty-five years ago. Modifications to the DNS framework warranted by this comparison have aided the development of novel computationally-efficient algorithms. The ongoing work may yield insights into the key mechanism of the bending effect in turbulent flame propagation.

Acknowledgements

I value all the love I have received these four years in a land so far from home. Foremost, I owe a deep debt of gratitude to my supervisor, Professor Stewart Cant, who created with arms wide open a space for me to learn. It is in this space that I was able to develop my ideas and find my personal brand of research, influenced by his style and backed by his courage. Still Stewart's portrayal of science as a dull and mechanistic procedure remains simply ironic, because science is just so much fun with him!

I am grateful to my teacher, Salil Srivastava, for imparting the foundations and *beauty* of science, Professor Kendal Bushe for the guidance up to Cambridge, and to Professor Epaminondas Mastorakos who conceived the basic idea on our very first meeting that culminated eventually into this thesis. My academic drive has benefited from the presence of Professor Simone Hochgreb, and I thank her for all the conversations we have shared. I am also grateful to Professor Andrei Lipatnikov for bridging the decades between us with passion and wine ever since Birmingham. Lastly, I am inspired deeply by Professor Derek Bradley and his incredible crew in Leeds. I am grateful to them, and to him for accommodating us in his academic life.

At Darwin, I have learned much in the shadows of fellows and friends. I thank sincerely Professor Andy Fabian for *stargazing* and conversations on turbulence, and Professor Sir Harry Bhadeshia for his kind mentorship and relentless humour. The content of this thesis has benefited significantly from the conversations with Dr. Giles Shaw, Dr. Matteo Corso and all members of *Gazebo Society*, and Dr. Richard Armstrong and the regulars at *DarBar*.

A special note of thanks goes to Eli-ran Bar-el and Stefanos Roimpas for the life-changing conversations over *fresh air* and the foundation of *Darwin Ring*,

to Loren Held for sharing the love for *turbulence*, to Dr. Stoyana Alexandrova – an ageless inspiration, to the residents of *Wordsworth Grove*, and to all the Porters at Darwin. Elsewhere in Cambridge, I found, to my great fortune, Erik Garrison over *magic flights* in chaos and aperiodic time crystals, Dr. András Bárány over linguistic coffees, Claudia Bedin at the *Scooter*, Christian Owusu whose love I will carry until the next flight to *Cambodia*, and *Space Cadets* who have been an artistic inspiration.

Credit is due to my seniors from early days Ryan Griffiths, Dr. Pranay Seshadri, and Dr. Ahmed Al-Shabab; I thank my colleagues and friends from Ashby Laboratory: Andrea Masi for *Brindisi*, Ashley Scillitoe for *Arsenal*, and Camille Bilger for *Camille*, *Marseille*, and the I♥Stewie group. Last but not at all the least, I am grateful to Peter Benie for sharing with me a piece of the wonder that he is, and to Katia Babayan for *Pushkin*.

The generous funding support of Cambridge International Trust has been vital to my life in Cambridge. I thank also the Cambridge Philosophical Society and the Cambridge Society for Applied Research (CSAR) for their kind donations and support.

My brothers in crime – Aamod Shanker and Ramkumar Ramachandra – are always with me no matter how distant their habitats. I cherish the good times with the *core team* members: Mikeshe and Shubha. Friendships from Vancouver have been inspirational throughout my time here; thank you Professor Artan Seshmani, Dr. Dan Brox, and Sneha Sheth for nourishing these bonds beyond Green College. My life with Annika Böddeling has been precious to me . . . she is simply my favourite!

The love of my family empowers me; thank you mummy, papa and deede.

to India:
the home of 0 and
the land of ∞

Contents

List of Figures	xv
List of Tables	xxi
Preface	xxiii
0 Introduction	1
1 Theoretical Background	5
1.1 Concepts of turbulent burning velocity	5
1.1.1 Damköhler: the hypotheses of 1940	7
1.1.2 Aerodynamic stretch and flame stretch	11
1.1.3 Regimes of premixed flame propagation	14
1.1.4 Bradley: the Leeds database	17
1.2 Simulations of turbulent burning velocity	20
1.2.1 Model equations for flame dynamics	20
1.2.2 Peters: the Thin Reaction Zones regime	25
1.2.3 What do Damköhler’s hypotheses mean today?	27
1.2.4 Thesis objectives and approach	29
2 The Direct Numerical Simulation method	31
2.1 Basic equations	32
2.2 Boundary Conditions	39
2.3 Numerical method	44
2.4 Benchmark solutions	47

3	Parametric Simulations of the Bending Effect	55
3.1	Design conditions for bending	55
3.1.1	Flame configuration and regime	58
3.2	Recorded effects of turbulence intensity	63
3.2.1	Images of the turbulent flame brush	63
3.2.2	Computation of turbulent burning velocity	73
3.3	Summary: on the bending effect recorded	74
4	Damköhler’s First Hypothesis	77
4.1	Flame Surface Density approach	77
4.1.1	Computation of flame surface area	83
4.2	Stretch rate components	87
4.2.1	Statistics of strain and propagation terms	88
4.2.2	Balance of strain and propagation	93
4.3	Summary: the role of DH1 in bending	96
5	Damköhler’s Second Hypothesis	97
5.1	Scalar flux transport in turbulence	98
5.1.1	Gradient transport hypothesis	99
5.2	Counter-gradient transport	101
5.2.1	Regime of counter-gradient transport	106
5.2.2	Computation of the diffusion coefficient	109
5.3	Summary: validity regime of DH2	112
6	Towards Validation with the Leeds Experiment	115
6.1	Leeds: expanding spherical explosions	115
6.1.1	Preliminary comparisons	117
6.2	Cambridge: freely propagating flames	118
6.2.1	Multi-step chemical kinetics	118
6.2.2	Fast adaptive timestep control	123
6.2.3	Linear turbulence forcing	127
6.2.4	Computational setup and regime	130
6.3	Summary: the ongoing comparative study	134

7 Conclusion	135
Appendix A	141
References	143

List of Figures

1.1	Photographs of turbulent Bunsen flames studied by Damköhler (1940). Contrasting regimes of turbulent flame propagation are observed upon increasing the Reynolds number (between top and bottom rows).	7
1.2	Illustration of a propagating flame surface interacting with a field of vorticity. At large-scales (red vortical regions), the interactions lead to wrinkling and aerodynamic stretch, whereas at relatively small scales, internal gradients (zoomed inset) may be modified leading to flame stretch.	12
1.3	Regime diagram proposed by Borghi (1985) to categorise topological and structural effects of turbulence on flame propagation.	15
1.4	The explosion vessel investigated by Abdel-Gayed and Bradley (1977) in Leeds to quantify effects of turbulence on flame propagation. Four fans generate nearly homogeneous isotropic turbulence in the reacting mixture filling the vessel volume. Turbulent flame propagation subsequent to successful ignition in the mixture can be observed through quartz windows.	17
1.5	Regime diagram as proposed by Peters (1999) demarcating the extent of the Thin Reaction Zones (TRZ) regime using $Ka = 1$ and $Ka_\delta = 1$ isolines.	26
1.6	Regimes proposed by Damköhler (1940) illustrated on the regime diagram proposed by Peters (1999). DH1 ($\ell_0 \gg \delta_L$) and DH2 ($\ell_0 \ll \delta_L$) correspond to the flamelet and Broken Reaction Zones (BRZ) regimes respectively.	28

List of Figures

2.1	Laminar propagating 1D flame solution modelled using single-step kinetics and unity Lewis number. A spatially-thin reaction zone (left) is simulated. The peak reaction rate occurs at $c = 0.8$ (right).	48
2.2	Grid resolution study to determine the bounds for flame chemistry resolution. Convergence fails for grids with resolution $\Delta x \gtrsim \delta_L/5$ where $\delta_L = 0.36 \times 10^{-3} m$ is obtained <i>a priori</i> on the finest grid.	49
2.3	Simulation snapshots of a counter-clockwise rotating vortex advected through a 2D inflow-outflow domain with inlet velocity $u_0 = 5 ms^{-1}$	51
2.4	Turbulent kinetic energy computed in a periodic $128 \times 128 \times 128$ HIT simulation. Panels show a) snapshot of energy spectrum in Fourier space and b) temporal decay of kinetic energy.	52
3.1	Inflow-outflow flame configuration used in the simulations. Left: 3D rendering of a propagating flame isosurface interacting with upstream turbulent eddies in the domain. Right: 2D axial slice showing the location of the flame and relative size of the domain.	58
3.2	Regime diagram showing the region of parameter space covered by the present simulations. The entire region between the flamelet regime and broken reaction zones regime is spanned by increasing u' successively across five simulations labelled I – V.	62
3.3	Contours of progress variable (colour) for each of the five simulations (columns, with u' value noted on top). Time evolution of the respective flame occurs down each column, with elapsed time noted on the left in each row.	64
3.4	Instantaneous snapshots of the turbulent flame leading edge $c = 0.01$ (coloured blue) and trailing edge $c = 0.99$ (coloured red) in cases with the lowest and highest u' , respectively. The arrow indicates the direction of flame propagation.	66

3.5	Distributions of the instantaneous mean curvature h_m and curvature shape factor S_h for the leading edge (solid lines) as well as trailing edge (dashed lines) surfaces in cases I and V (black and red lines, respectively).	67
3.6	Magnified view of the instantaneous leading edge (blue) and trailing edge (red) surfaces at $t = 4\tau_0$ as computed for case V with $u' = 30s_L$	69
3.7	Reaction rate contours $\dot{\omega}(x, z; y = 5L/6)$ in cropped axial slices of the domain (above) and reaction rate scatter $\dot{\omega}(c)$ across the entire domain (below) at $t = 4\tau_0$ for cases I and V.	71
3.8	Progress variable isosurface $c^* = 0.8$, corresponding to the peak reaction rate, in the lowest and highest intensity cases. Axial sections of the domain show the variation of reaction rate $\dot{\omega}$ across the domain.	72
3.9	Computed variation of the normalized turbulent burning velocity s_T/s_L with normalized turbulence intensity u'/s_L . The inset shows a typical variation of $s_T(t)$ and the corresponding value of s_T chosen from this variation.	74
4.1	Expectation of FSD Σ as a function of the axial coordinate x (left) and mean progress variable $\bar{c}$ (right) for three cases (I, III, and V) spanning the dataset. The laminar flamelet solution (red line) is shown for comparison.	79
4.2	Illustration of sampling methods (dashed lines). Left: sampling over spanwise sections of the domain across the mean turbulent flame brush ($\bar{c}_0^* < \bar{c} < \bar{c}_N^*$). Right: sampling over instantaneous progress variable c isosurfaces (solid lines) within the instantaneous turbulent flame brush ($c_0^* < c < c_N^*$).	80
4.3	Instantaneous normalized $\Sigma'(c)$ scatter (left column) at $t = 4\tau_0$ compared with the laminar flamelet profile (red line). Corresponding contours of $\Sigma'(\mathbf{x})$ (right column) are shown in an axial section overlaid with progress variable contours (black and white lines).	82

List of Figures

4.4	Computed flame surface area ratio A_T/A_L compared with normalised turbulent burning velocity s_T/s_L in the recorded bending effect.	84
4.5	Comparisons of turbulent flame structure and propagation characteristics simulated using 1-step and 25-step reduced chemical kinetic models for case III with $u' = 10s_L$	86
4.6	Distribution of strain a_t and curvature h_m over the peak reaction rate isosurface $c^* = 0.8$ for three cases (lowest u' : solid line, highest u' : dotted line) spanning the entire dataset.	88
4.7	Joint probability distribution of strain rate a_t (scaled with Taylor scale strain rate u'/λ) and mean curvature h_m (scaled with Kolmogorov scale η) in the lowest and highest intensity cases. .	90
4.8	Distribution of displacement speed s_d over the peak reaction rate isosurface $c^* = 0.8$ in three cases spanning the dataset (solid line: lowest intensity and dotted line: high-intensity). . . .	91
4.9	Joint probability distribution of s_d (scaled with laminar flame speed s_L) and h_m (scaled with Kolmogorov scale η) in the lowest and highest intensity cases.	92
4.10	Variation of volume-integrated source-terms $\bar{a}$ and $\bar{h}$ of the transport equation for Σ' with increasing normalized turbulence intensity u'/s_L	94
5.1	Schematic showing gradient (G) transport of the progress variable flux. A disturbed flame surface (light dashed line) is wrinkled further (progressively darker solid curves) by vortical activity. The flame does not counteract this tendency, and is simply convoluted by turbulent fluctuations.	100

5.2	Schematic of the counter-gradient (CG) transport mechanism. At sufficiently high heat release factors $\tau = \rho_u/\rho_b$, the flame has a tendency to act against gradient transport. An initially wrinkled flame surface (dashed convoluted curve) may un-wrinkle as the lighter product peninsula is differentially accelerated in the direction of products (along red arrows, away from the direction of propagation).	101
5.3	Variation of mean scalar flux $\widetilde{u''c''}$ with the mean scalar gradient $\partial\tilde{c}/\partial x$. Colours denote corresponding values of the mean progress variable $\tilde{c}$ (blue: leading edge $\tilde{c} = 0.01$, red: trailing edge $\tilde{c} = 0.99$).	104
5.4	Instantaneous progress variable contours (black lines) and Favre velocity fluctuations u'' (background colours) in an axial cross-section $y = \frac{L}{2}; L < x < 2L, z$ of the domain.	105
5.5	Recorded correlations between u'' and c'' for case I (above) and case V (below). Colours indicate the progress variable value (blue: reactants, red: products) and size is proportional to the reaction rate magnitude. The transition from positive to negative correlation corresponds to the G/CG transition.	107
5.6	The Bray number N_B for each case simulated in the present dataset delineating the gradient/counter-gradient transport regimes at unity.	108
5.7	Computed normalized turbulent burning velocity s_T/s_L compared with predictions $\sqrt{D_T/D_L}$ of DH2 in the gradient diffusion regime $N_B < 1$. DH2 is invalidated in the CG transport regime denoted by $N_B > 1$ (shaded red).	111
6.1	Preliminary comparisons of methane-air flame propagation in experiments (Leeds) with $\phi = 0.6$, and DNS (Cambridge) with $\phi = 1.0$. The same turbulence intensity u'/s_L is prescribed (panel a) in both cases. Curvature distributions are normalized using the Taylor length scale λ	117

List of Figures

6.2	Profiles of thermo-chemical variables: temperature and chemical components (left) of the composition vector as well as radicals (right) computed using a 25-step chemical kinetic model.	121
6.3	Grid resolution study to determine the spatial resolution requirement for the 25-step methane-air chemical kinetic model. Convergence fails for grids with $\Delta x \gtrsim \delta_L/22.3$, where $\delta_L = 9.3\text{ mm}$ denotes the value obtained <i>a priori</i> using a fine grid. . .	122
6.4	Timestep history (panels a,b, and c) as well as timestep ratios (panel d) obtained using the PID controller $\alpha\beta\gamma$ and the modified PI4.2 controller $\alpha^*\beta^*$ due to Söderlind (2002) for various test problems.	125
6.5	Turbulent forcing strategy. Left: time evolution of mean turbulent kinetic energy $k(t)$ for an HIT simulation with $Q = 0$ and with $Q = \varepsilon/(2k_0)$. Right: region of turbulent forcing in the flame simulation.	129
6.6	Resolution constraints of chemistry (black dashed lines) and turbulence (red dashed line) as well as the corresponding computational expense (black and red solid lines, respectively) as a function of DNS domain size.	131
6.7	Combustion regimes corresponding to the Leeds experiment and the Cambridge DNS in the regime diagram with a modified definition of Ka.	133

List of Tables

3.1	Thermo-chemical input parameters.	57
3.2	Turbulence properties and dimensionless parameters.	60
6.1	Input parameters for the Leeds-Cambridge study.	133

Preface

Understanding combustion has been essential for sustaining progress this century. Be it our long-anticipated trip to Mars, or tomorrow's BA flight to Mumbai, human exploration hinges upon controlled turbulent combustion. At home, fire is necessary to cuisine, and far out in the cosmos, our very existence appears to be tied to turbulent flames. Indeed, today we are re-discovering our age-old relationship with combustion in its myriad forms. Using lasers, supercomputers and advanced mathematics, the complexity of these forms is being revealed once again. Unified conceptualisation of the turbulent flame is, therefore, being pursued with great optimism and curiosity.

A mode of intense and efficient burning is found to occur when fuel and oxidiser are mixed prior to ignition. The drawback, however, is that subsequent propagation of the 'premixed' flame is extremely sensitive to a variety of mixture properties. Turbulence is one such property; the chaotic dynamics that arise in a turbulent gaseous medium has manifold consequences in flame propagation. Damköhler (1940) conjectured in his foundational hypotheses that turbulence may only enhance burning. Yet over the 75 years since, evidence for inhibitive effects of turbulence has grown. So, it is believed increasingly that sufficiently-intense turbulence may extinguish a premixed flame. Bradley (1992) summarized these possibilities in a review entitled: 'How fast can we burn?'

The present thesis addresses this very question using supercomputers. The non-linear partial differential equations governing the motion of reacting gases are solved on thousands of processing cores. As a result, the complex interactions of the flame and turbulence are unveiled for scrutiny. By thereby re-investigating the foundational hypotheses of flame propagation, the thesis

Preface

contributes to a unified conception of the turbulent flame.

Chapter 0

Introduction

Scientific conceptions of the ‘flame’ seek to reconcile two distinct spatio-temporal perspectives. At large scales, the flame appears as a coherent surface with well-defined physical properties. At relatively small scales, the flame is described rather as a process that results in thermo-chemical transformation. Dynamics of the flame at these distinct scales govern in unison how fast a laminar gas mixture burns. In a turbulent burning mixture, the large- and small-scale perspectives of the flame are interlaced by the motion of gases at intermediate scales. As a result, difficulties arise in reconciling the ‘external’ surface and the ‘internal’ process perspectives of the flame. These difficulties are addressed in the present thesis by isolating and studying systematically the various scales of interactions between flame and turbulence.

Moments before the piston reaches top dead centre in an SI engine, a spark ignites the compressed fuel-air mixture. Subsequently, a thin ‘premixed’ flame propagates through the mixture, expanding it rapidly to restore the piston. Propagation of the flame surface, therefore, results in producing mechanical work. Mallard and le Chatelier (1883) pioneered a framework for calculating this ‘burning velocity’ of the propagating flame by linking it with various mixture properties. Interpreting this problem as being akin to heat conduction in thermal waves, Michelson (1889) formulated the burning velocity as a function of the temperature gradient across the flame surface. Hence, the perspective of the premixed flame as a coherent surface wedged between unburned and burned mixture states was born.

0. Introduction

Considered merely as a surface of thermal discontinuity, however, the flame lacks the properties ascribed to it otherwise by virtue of combustion chemistry. The activation energy required to spark-ignite a mixture, for instance, arises from a chemical requirement. During the subsequent flame propagation, this energy is sustained by exothermic chemical reactions. Indeed, under conditions in which this chemical energy is lost, the flame may even extinguish. Evidently, much of the sensitivity of the flame is linked to its chemical nature.

Lewis and von Elbe (1934) proposed, therefore, that the internal structure of the flame is determined not only by thermal but also by molecular gradients. Establishing this formally, Zel'dovich and Frank-Kamenetskii (1938) showed that a relatively-thin 'reaction zone' depletes molecules within the internal flame structure. This region releases heat whereas the preparatory 'pre-heat zone' sustains the balance between thermal and molecular diffusion. These studies provide a strong basis for the internal thermo-chemical structure that arises from the flame considered as a process.

The narrative so far addresses the burning velocity of laminar flames, where the motion of gases does not impart new scales to the problem of flame propagation. Mixtures of gases, however, are often turbulent. In fact, the very act of mixing itself is effected most commonly by the turbulent 'cascade' in the first place (Kolmogorov, 1941). The various cascading scales of turbulent motion blur the distinction between the large surface scales and the small process scales of the flame. This poses a severe challenge to the formulation of a consistent theory of burning velocity in turbulent flame propagation.

So in order to address turbulent flame propagation, Damköhler (1940) conceived of two extreme cases. In the first of his seminal hypotheses, all scales of turbulent motion are considered to be large, so that only the external surface attributes of the flame are affected. In the second hypothesis, all scales of turbulence are imagined to be small, so that only the internal process and the associated structure is affected. Therefore, Damköhler's conception divides turbulent flame propagation into manageable regimes that provide a basis for the prediction of turbulent burning velocity. In each of these regimes, turbulence is hypothesized to 'act' on the flame to 'enhance' the burning velocity.

This conception has underpinned the majority of investigations of turbulent flame propagation undertaken to date.

With the surge of aircraft technology in the 1940s, afterburners were invented. These help improve thrust, but may incur accidental flame blow-off at sufficiently high speeds. Karlovitz et al. (1953) theorizes that the latter may result from increased localized flame quenching due to steep velocity gradients in high-speed gaseous flow. Hence, the notion of ‘stretch’ was conceptualised so as to accommodate for the effects of gas motion inhibiting burning. This is generalized by Klimov (1963) – turbulent flame propagation was envisaged to be the consequence of interactions between ‘laminar flames in turbulence.’

Markstein (1964) and Williams (1985) improved upon this view, suggesting that components of the burning mixture may mediate the effects of turbulence on the flame. Furthermore, the possibilities that arise from increasing degrees of turbulence-flame interaction are illustrated by Borghi (1985) in a ‘regime’ diagram. Meanwhile, the integrity in turbulent flow of the internal flame structure – the so-called ‘flamelet’ – was questioned increasingly. The possibility of flame quenching in turbulence carries the implication that small-scale turbulent motion disrupts the structure of the flamelet, thereby dismantling the coherence of the flame surface. This challenges the entire conception, since Damköhler (1940), of a propagating turbulent flame as a laminar flame affected by turbulence. Hence, for decades to follow, the scientific community became pre-occupied with the search for conditions which might limit this hypothesis.

Abdel-Gayed and Bradley (1977) employed an explosion vessel in which the intensity of turbulence can be controlled in a manner similar to Damköhler’s theoretical conception. Correlating data from over a thousand experiments, it was suggested that though large-scale turbulent motion enhances flame propagation as per Damköhler’s first hypothesis, sufficiently small-scale turbulence may, in fact, inhibit flame propagation. The resulting variation of burning velocity over the entire range of turbulence regimes was termed ‘the bending effect’ as the graph tapered away from linearity in the small-scale regime.

Bradley (1992) conjectures that ‘bending’ occurs because velocity gradients

0. Introduction

of small-scale turbulence cause disruption of the internal thermo-chemical process of the flame. Yet Driscoll (2008) notes that in the twenty-five years since Bradley’s conjecture, little direct evidence of total flame structure disruption due to small-scale turbulence has emerged. So, the regime of ‘Thin Reaction Zones’ has been proposed by Peters (1999), suggesting mitigated damage to the flamelet hypothesis. This line of investigation continues to date, effects of turbulence and the degree of loss of flamelet structure being seen as the central problem of turbulent flame propagation.

The present investigation complements this dominant ongoing narrative. In the systematic simulations conducted here, it is evident that as the variety of turbulence scales become prominent, self-regulation of the flame follows suit. Hence, the role of flame-response appears to be significant in determining overall turbulent flame propagation. The bending effect emerges, therefore, as a competition between turbulent enhancement of the flame surface and the self-inhibition of the flame. In other words, it is not necessary for localized flame quenching to occur to observe the bending effect.

Furthermore, Damköhler’s forgotten second hypothesis is examined. A related theme is observed here as a limiting factor of burning, namely the effect of the flame on its surrounding turbulent flow. The resulting flame-induced acceleration of burned gases limits the enhancement of turbulent burning velocity in the small-scale turbulence regime. The present thesis highlights, therefore, that turbulent flame propagation and the bending effect are governed not only by the effects of turbulence on the flame, but equally by the effects of the flame on itself as well as on turbulence.

In Chapter 1, the theoretical background is discussed beginning with the foundational hypotheses laid out by Damköhler (1940). Furthermore, the bending effect and Bradley’s work is elaborated upon. The direct simulation approach employed to complement Bradley’s work is discussed in Chapter 2. The simulation dataset is designed and generated in Chapter 3, and is analysed for the validity of Damköhler’s hypotheses in Chapter 4 and Chapter 5. An outline of a collaborative investigation with Bradley and co-workers is presented in Chapter 6.

Chapter 1

Theoretical Background

1.1 Concepts of turbulent burning velocity

Beginning with Damköhler (1940), the turbulent burning velocity s_T has been seen as a conceptual extension of the laminar burning velocity, which may be measured or computed for laminar flames. Indeed, a theoretical solution for the burning velocity can be obtained analytically for only steady one-dimensional laminar premixed flames (Zel'dovich and Frank-Kamenetskii, 1938). For this idealised case, the steady-state equation for temperature can be solved to relate the laminar burning velocity with the thermal diffusivity α and the peak reaction rate $\dot{\omega}_{max}$ of the burning mixture as

$$s_L^0 \sim \sqrt{\alpha \dot{\omega}_{max} / E_a}, \quad (1.1)$$

provided the mixture has a large activation energy E_a and a unity Lewis number $Le \equiv \alpha/D$, i.e. equal thermal diffusivity α and molecular diffusivity D . These turn out to be reasonable simplifications in most contexts related to gaseous turbulent burning. Hence, the expression derived by Zel'dovich and Frank-Kamenetskii (1938) provides a foundational building block towards the formulation of expressions for the turbulent burning velocity s_T .

Libby et al. (1979) have noted, however, that s_T may have several conceptually different definitions to begin with. For instance, is s_T to reflect a local or a global measure of burning rate? Is it to imply a displacement speed of the

1. Theoretical Background

flame surface, or the consumption speed of the flame brush? One may derive a variety of formulations for s_T along each of these definitions. Furthermore, the sensitivities of the turbulent burning velocity to various factors, such as mixture thermo-chemical properties, may be vastly different than the laminar case. These sensitivities may vary considerably between different experimental configurations. As a result, difficulties arise in framing the problems of turbulent flame propagation in a unified manner. The conceptually-distinct burning velocity definitions have, in fact, been treated as the same in the past, resulting in graphs that contain a large amount of scatter (Driscoll, 2008).

To aggravate the problem, certain features of turbulent flows that render challenging the computation or measurement of turbulent burning velocity. Typical configurations for turbulent flames do not lend themselves in a straightforward manner to the computation of burning velocity as an eigenvalue, as is possible in the case of one-dimensional steady laminar flames (Peters, 2000). Furthermore, a variety of time and length scales are involved in turbulent flames, implying that the assumptions inherent to Equation 1.1 may not always be applicable to turbulent flames (Kerstein, 2002). Finally, the equations for turbulent flame propagation are evidently more complex to the extent that a direct solution approach is tedious (Poinsot, 1996). Due to these reasons, the problem of turbulent burning velocity remains to date without a consistent overarching formulation despite its significance to the field of combustion (Bray, 1990; Lipatnikov and Chomiak, 2002; Driscoll, 2008; Bradley et al., 2011).

Explanations of many phenomena related to turbulent flame propagation remain contested today because of the above-mentioned challenges. The focus of this thesis – the bending effect – presents such an example, bearing fundamental importance to the theory of turbulent burning. The bending effect refers to the variation of s_T with increasing turbulence intensity u' of the unburned mixture. Although a ‘bending’ of $s_T(u')$ has been witnessed and quantified in many investigations (Lipatnikov and Chomiak, 2002; Driscoll, 2008), it continues to be debated by several researchers to date. In the following, the conceptual background of this problem is presented, beginning and

ending with an evaluation of the seminal work of Damköhler (1940).

1.1.1 Damköhler: the hypotheses of 1940

A basic apparatus for investigating the turbulent burning velocity is the Bunsen burner (Lockermann, 1956). In this apparatus (shown in Figure 1.1), pre-mixed gaseous mixtures are issued from a vertical pipe such that a flame may be stabilised at the burner rim. As a result, the flame propagates constantly against the direction of reactants flowing out of the pipe. The turbulent burning velocity is, therefore, related directly to the global mass transformation rate of the unburned gas $\dot{m}$ in this context, so that

$$s_{L,T} = \frac{\dot{m}}{\rho_u Y_u A_0}, \quad (1.2)$$

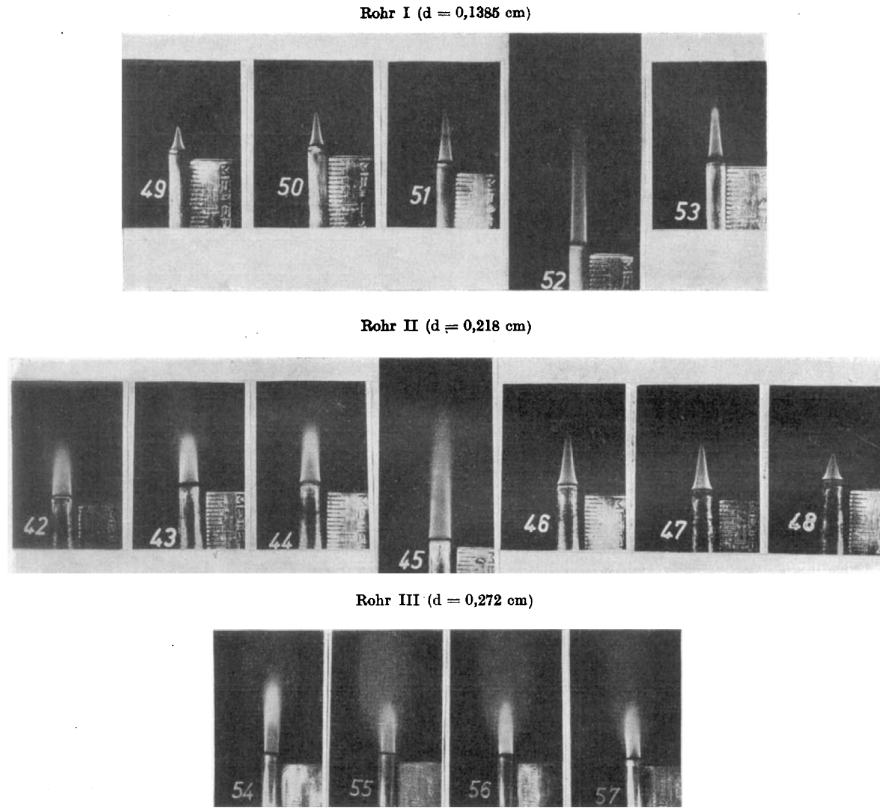


Fig. 4.
Die aufgenommenen Flammen.

Figure 1.1 Photographs of turbulent Bunsen flames studied by Damköhler (1940). Contrasting regimes of turbulent flame propagation are observed upon increasing the Reynolds number (between top and bottom rows).

1. Theoretical Background

for a known inlet mass flow rate $\rho_u Y_u A$. Here, ρ_u is the unburned gas density, Y_u is the mixture fuel mass fraction, and A_0 is the cross-sectional area of the pipe. Equation 1.2 holds for laminar L as well as turbulent T flames (note the subscripts in Equation 1.2). Damköhler (1940) exploited this equivalence, comparing the value obtained for turbulent flames with the laminar case.

In Figure 1.1, the laminar flame (top row) is seen as having a distinct surface whose area A_L can be measured to a fair degree of accuracy. If every point in the laminar Bunsen flame satisfies Equation 1.1, the overall burning velocity may be computed as

$$s_L \sim A_L \sqrt{D \dot{\omega}_{max}}, \quad (1.3)$$

upon substituting α with the molecular diffusivity D . Turbulent flames, characterised by a high Reynolds number $Re \equiv UL/\nu$, have a relatively ambiguous structure and shape in comparison (as seen in the bottom row of Figure 1.1). Damköhler (1940) proceeded, therefore, to relate these differences in terms of length scales expected in a turbulent flow relying on concepts proposed by Prandtl (1925). Measured values of s_T were compared with the computation of s_L based on Equation 1.3 in order to highlight differences which were then used to elaborate physical mechanisms of turbulent flame propagation. It was noted that $s_T > s_L$ in all cases, leading to the conclusion that ‘turbulence always increases the flame speed referred to the average flow cross section.’ Further, the effects of turbulence were separated into two regimes, hypothesizing the enhancement due to turbulence to occur ‘in a two-fold manner.’

Coarse-body turbulence

The first of these two ‘manners’ concerns a regime where the turbulence length scales ℓ are large compared to the laminar flame thickness $\delta_L^0 = \nu/s_L^0$, i.e. for $\ell \gg \delta_L^0$. Addressing this regime, Damköhler (1940) proposed that

Hypothesis 1 *‘for coarse-turbulence bodies exceeding the laminar flame thickness, the flame surface is effectively enlarged, which is, by roughening [the flame surface.] Thus the coarse-body turbulence effects a rise of the flame*

1.1. Concepts of turbulent burning velocity

velocity, . . . , even if the flame velocity in the individual surface elements is entirely the same as in laminar flow.'

wherein the flame velocity of individual surface elements refers to the local burning velocity s_L^0 or, equivalently, the local laminar flame speed. Damköhler (1940) argued further that the local velocity fluctuations u' which give rise to the 'roughening' balance the enhanced effective local burning velocity s_T , stabilizing the flame at the burner rim. This led to a linear relation $s_T \sim u'$. Hence, Damköhler's first hypothesis (hereby, DH1) may be summarised as follows

$$\frac{s_T}{s_L} = \frac{A_T}{A_L} \implies s_T \sim u' \quad (1.4)$$

where A_T is the enlarged turbulent surface area and A_L is the appropriate flow cross-section area. In this regime, it is the enhanced area ratio A_T/A_L that acts to magnify the laminar flame speed s_L to its equivalent s_T in turbulence. The statement of DH1 assumes, therefore, that the internal flame structure is preserved in a manner that leaves unchanged the thermo-chemical terms α and $\dot{\omega}_{max}$ in Equation 1.3. Framed in this manner, DH1 forms the basis of nearly all turbulent flame modelling to date.

Fine-body turbulence

The second 'manner' of s_T enhancement – Damköhler's second hypothesis (here called DH2) – concerns a limiting regime of high u' turbulence wherein the turbulence length scales $\ell \ll \delta_L^0$. Addressing this regime, which contrasts with DH1, Damköhler (1940) proposed that

Hypothesis 2 *'for fine-body turbulence, . . . , an amplification of every microscopic transport process in the flame surface must occur, especially between the reaction zone and the pre-heat zone. These transport processes [then] . . . govern the flame speed decisively.'*

wherein the microscopic transport processes referred to may be molecular diffusion or thermal conduction. Reasoning along these lines, Damköhler (1940) described the enhancement of s_T in 'fine-body' turbulence using the formula-

1. Theoretical Background

tion

$$\frac{s_T}{s_L} = \sqrt{\frac{D_T}{D_L}} \implies s_T \sim \sqrt{u'\ell_0} \sim \sqrt{Re}, \quad (1.5)$$

which is obtained by assuming that small-scales do not affect the area or reaction rate in Equation 1.3. The area A_L is not affected because the turbulence length scales are considered to be too small, whereas the reaction rate $\dot{\omega}$ does not change because the time scale of reaction is considered to be too small following Zel'dovich and Frank-Kamenetskii (1938). The statement of DH2 further applies the mixing length hypothesis of Prandtl (1925), by setting $D_T \sim u'\ell_0$ so that s_T in this regime may also be computed for a specified u' . It is implicit in this statement that the ratio D_T/D_L remains positive upon specifying the model for D_T . This ensures that the mathematical validity of DH2 is preserved.

The discussion above highlights that Damköhler (1940) not only conjectured the regimes of turbulent flame propagation, but also provided formulations for the burning velocity variation $s_T(u')$. By relating these regimes and the respective formulations to a few parameters such as u' and ℓ_0 , a platform for modelling flame propagation was pioneered. Soon after, Schelkin (1943) developed further the model of turbulent burning velocity s_T as a function of turbulence intensity u' . In an attempt to unify the two regimes, an expression was provided as

$$\frac{s_T}{s_L} = \sqrt{1 + \left(\frac{u'}{s_L}\right)^2}, \quad (1.6)$$

which heralded subsequently an era of seeking a unified model of $s_T(u')$ applicable to all regimes of combustion (Bray, 1990). These attempts continue to date as discussed by Lipatnikov and Chomiak (2002). The expectation is that scaling relationships satisfied by $s_T(u', \ell_0)$ reflect intimately the underpinning mechanisms that influence turbulent flame propagation. A primary focus has, therefore, been to find better fits to the experimental s_T variation so that the related propagation mechanisms may be revealed.

Damköhler's conception may be summarised as follows. Firstly, the turbulent burning velocity differs from the laminar burning velocity due to the effect of turbulence on the flame. Secondly, the burning velocity attained in

turbulence is always enhanced in comparison to the laminar burning velocity. Lastly, the level of enhancement is governed by flame surface area and turbulent diffusivity in two contrasting regimes of turbulence.

1.1.2 Aerodynamic stretch and flame stretch

A decade after Schelkin (1943), inhibitive effects of velocity gradients in the burning mixture were considered by Karlovitz et al. (1953). The notion of ‘stretch’ was developed and quantified in terms of

$$K = \frac{\delta_L^0}{U} \frac{\partial U}{\partial y}, \quad (1.7)$$

a function of velocity gradient $\partial U / \partial y$ modulated further by the flame thickness δ_L^0 and mean inflow velocity U . Attributing to stretch a negative effect on the laminar burning velocity, Karlovitz et al. (1953) were able to predict laminar flame extinction in a Bunsen burner. Klimov (1963) generalised this idea to obtain the stretch rate

$$\dot{s} = \frac{1}{A} \frac{dA}{dt}, \quad (1.8)$$

as the fractional rate of change of flame surface area A over time. Clearly, this expression relies on the notion of the flame surface area, so that the concept of stretch necessarily assumes DH1 to be valid in some sense. A persistent issue with stretch-based turbulence modelling has, therefore, been the difficulty in being able to address the invalidation of DH1 due to flame quenching from within the framework of DH1. Nevertheless, the work of Williams (1985) has provided a strong mathematical basis for stretch.

The stretch rate $\dot{s}$ defined in Equation 1.8 can be decomposed into the component prescribed by the flow and the component experienced as a consequence of the flame response (Williams, 1985). This decomposition is written as

$$\dot{s} = a_t + s_d h_m, \quad (1.9)$$

where the ‘prescribed’ component takes the form of tangential surface strain

$$a_t = \nabla \cdot \mathbf{u} - \hat{n} \hat{n} : \nabla \mathbf{u}, \quad (1.10)$$

1. Theoretical Background

and the component ‘experienced’ due to the flame response occurs as a result of normal propagation of the surface elements with mean curvature

$$h_m = \frac{1}{2} \nabla \cdot \hat{n}, \quad (1.11)$$

where $\hat{n}$ is the local flame surface normal vector (pointing in the direction of unburned reactants) and s_d is the surface displacement speed in this direction. Stretch rate thus obtained has been useful in describing a range of flame phenomena (Law, 1989). However, the effects of stretch, as well as the relationship between its components, are subtle and at times difficult to comprehend.

Extensive strain rate $a_t > 0$, for instance, increases the flame surface area by definition, but it may also reduce internal gradients causing the local displacement speed s_d to diminish. Strain has thereby proved vital in characterising extinction probabilities in flame propagation (Abdel-Gayed et al., 1984; Bradley et al., 1992). Figure 1.2 shows how both large-scale surface deformation (due to aerodynamic stretch) as well as small-scale process modification (due to flame stretch) may operate at the same time in a turbulent flame.

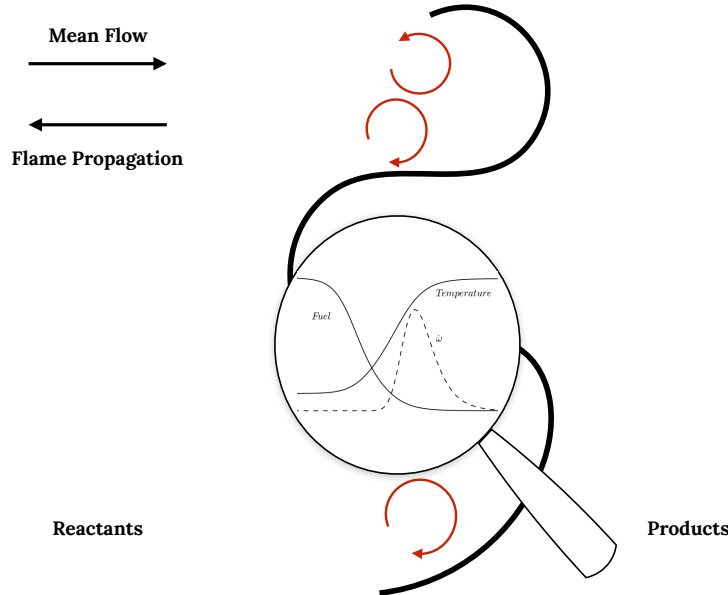


Figure 1.2 Illustration of a propagating flame surface interacting with a field of vorticity. At large-scales (red vortical regions), the interactions lead to wrinkling and aerodynamic stretch, whereas at relatively small scales, internal gradients (zoomed inset) may be modified leading to flame stretch.

1.1. Concepts of turbulent burning velocity

Further, strain may also effect part of the local flame surface curvature h_m (Pope, 1988), so that the two stretch components are not entirely independent of each other.

In a similar manner, the curvature component h_m can also play a supportive or inhibitive role on the local flame propagation velocity. Markstein (1964) characterised the role of mixture diffusive properties (through the Lewis number Le) in regulating flame surface curvature effects on flame propagation. Unifying these concepts, it was proposed (Clavin, 1985) that, for flame thickness δ_L^0 much smaller than the characteristic wrinkle size, the local normal displacement speed s_d varies according to

$$\frac{s_L^0 - s_d}{s_L^0} = \frac{1}{A} \frac{dA}{dt} \frac{\delta_L^0}{s_L^0} \text{Ma} \quad (1.12)$$

where the Markstein number Ma is related to the mixture Lewis number Le .

In turbulent flames, Clavin and Williams (1979) derived the large-scale behaviour of turbulent premixed flame propagation for mildly stretched flames. As a more general formulation, Bray and Cant (1991) proposed that flame stretch effects may be absorbed simply into DH1 using a factor $I_0 \lesssim 1$ under low levels of stretch, such that

$$\frac{s_T}{s_L} = I_0 \frac{A_T}{A_L}, \quad (1.13)$$

thereby modifying DH1 without invalidating its basic premise. Further, in order to address the difficulties in computing the exact area A_T of convoluted flame surfaces, a statistical approach was adopted. The mean Flame Surface Density (FSD, denoted by Σ) is defined, for example, as the mean flame surface area per unit volume allowing DH1 to be written (Bray and Cant, 1991) as

$$\frac{s_T}{s_L} = I_0 \frac{1}{A_L} \int_V \Sigma dv, \quad (1.14)$$

which is the same as Equation 1.4 with A_T replaced by the integral of FSD over the flame brush volume V . This description has helped account to some degree for the inhibitive turbulent stretch effects on the local chemical structure

1. Theoretical Background

(Driscoll, 2008). It remains unclear, however, what effects precisely lead to this variation of I_0 . The predominant role is believed to be the action of strain, which may quench flamelets locally (Abdel-Gayed et al., 1984). Curvature effects have been largely neglected, in comparison, and considered to ‘even out’ in the context of turbulence (Bradley et al., 1992).

Accounting for the increasingly disruptive effects of turbulence, a more general class of $s_T(u')$ models as that developed by Schelkin (1943) emerged. In an atmospheric pressure environment, a non-linear relationship

$$\frac{s_T}{s_L} \sim \left(1 + \left(\frac{u'}{s_L} \right)^n \right)^{(1/n)} \quad (1.15)$$

has been suggested to hold, proposing the exponent n as a parameter that may fit the scattered data. These models attempted to address the various bending curves of $s_T(u')$ observed in experimental measurements by Karpov and Severin (1980); Kido et al. (1989) as well as by Gülder (1991); Kobayashi et al. (1996); Shy et al. (2000b). The precise variations captured in these datasets have been reviewed in detail by Lipatnikov and Chomiak (2002). One such work is focused upon here: that of Bradley et al. (1992) and co-workers. A phenomenological conception of turbulent flame propagation developed at nearly the same time helped visualise subsequently the physical mechanisms responsible for such variations in $s_T(u')$.

1.1.3 Regimes of premixed flame propagation

Following Damköhler (1940), the classification of flame propagation regimes has been pursued based on the comparison of length scales involved in turbulent reacting flows (Borghi, 1985). Effects of turbulent stretch are considered in this framework as the result of an interaction between the various length scales ℓ of turbulence and those of flame chemistry (such as δ_L^0). The turbulence scales can be computed based on the k - ε model of turbulence (Jones and Launder, 1972). The flame speed s_L (referred to in DH1) is then expected to be ‘the same as in laminar flow’, i.e. correspond to s_L^0 , only if the Kolmogorov

1.1. Concepts of turbulent burning velocity

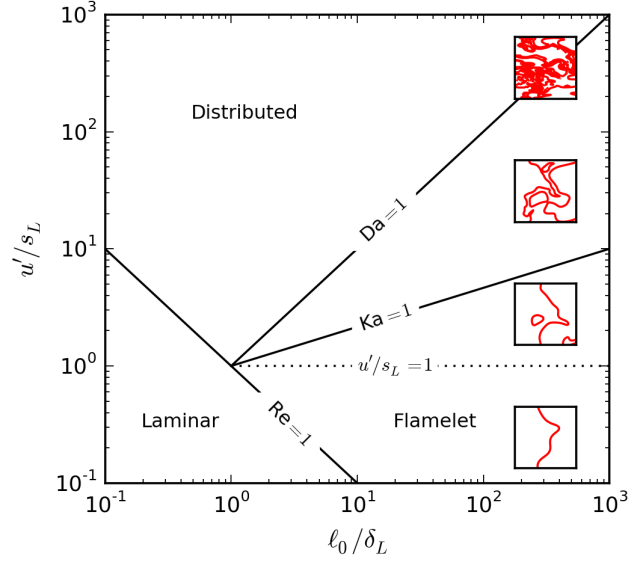


Figure 1.3 Regime diagram proposed by Borghi (1985) to categorise topological and structural effects of turbulence on flame propagation.

scale

$$\eta = \frac{\nu^3}{\varepsilon}, \quad (1.16)$$

and all scales larger than it, is larger than δ_L (where ε is the turbulent dissipation rate). The Karlovitz number

$$\text{Ka} \equiv \delta_L^2 / \eta^2 \quad (1.17)$$

is a dimensionless marker that delineates the regimes of turbulence-flame interaction by comparing the smallest turbulent microscale η with the flame length scale δ_L . In essence, the size of the Kolmogorov scales of turbulence is determined by the Reynolds number

$$\text{Re}_0 = u' \ell_0 / \nu \quad (1.18)$$

for a given integral length scale ℓ_0 and kinematic viscosity ν . Similarly, large-scale convective time scale may be compared with the flame time scale, using the Damköhler number

$$\text{Da} \equiv \frac{\tau_f}{\tau_c} = \frac{s_L \ell_0}{u' \delta_L} \quad (1.19)$$

1. Theoretical Background

where $\tau_f = \ell_0/u'$ and $\tau_c = \delta_L/s_L$. Many different diagrams have been proposed all loosely based on the variety of turbulence flame interactions possible for different ranges of these dimensionless groups (Borghi, 1985; Abdel-Gayed et al., 1989). A classical diagram is shown in Figure 1.3 with various visualizations of the flame structure associated with the respective regimes.

In the Borghi diagram as Figure 1.3 is called, isolines of unity Ka , Da and Re are used to demarcate the regimes of turbulence-flame interaction (Borghi, 1985). The ‘flamelet’ regime satisfies the Klimov-Williams criterion $Ka < 1$ and, hence, DH1 is expected to be valid in this regime based on the phenomenological description. With increasing disruption of the local internal flame structure, different regimes of flame propagation are evident until at the highest intensities of turbulence, ‘distributed’ combustion prevails. Many experiments have reported a significant departure from the linear relation $s_T \sim u'$ implied by DH1 in turbulent premixed flames with $Ka > 1$. This so-called ‘bending effect’ of the $s_T(u')$ curve has been isolated to occur when all parameters but u' are maintained constant within the parameter space consisting of u' , ℓ_0 , s_L , and δ_L (Bradley, 1992; Lipatnikov and Chomiak, 2002; Driscoll, 2008). It was inferred that stretch effects begin to play an important role at high intensities, where the deviation from linearity is observed in $s_T(u')$.

Renormalisation group theories attempted to use such disparities in time scales to find the scaling behaviour of s_T in various regimes of combustion. A rigorous approach pursued by Yakhot (1988) led to a relatively complex relationship of the form

$$\left(\frac{s_T}{s_L}\right)^2 \log\left(\frac{s_T}{s_L}\right) = \left(\frac{u'}{s_L}\right)^2, \quad (1.20)$$

that has also been derived heuristically (Kerstein et al., 1988) without considering the detailed internal structure. However, with the development of detailed internal chemical structure (Williams, 2000) of the premixed flame, the renormalisation group theories are faced with the challenge of accounting for various other scales in the problem, so that these have not been able to account successfully for the bending effect.

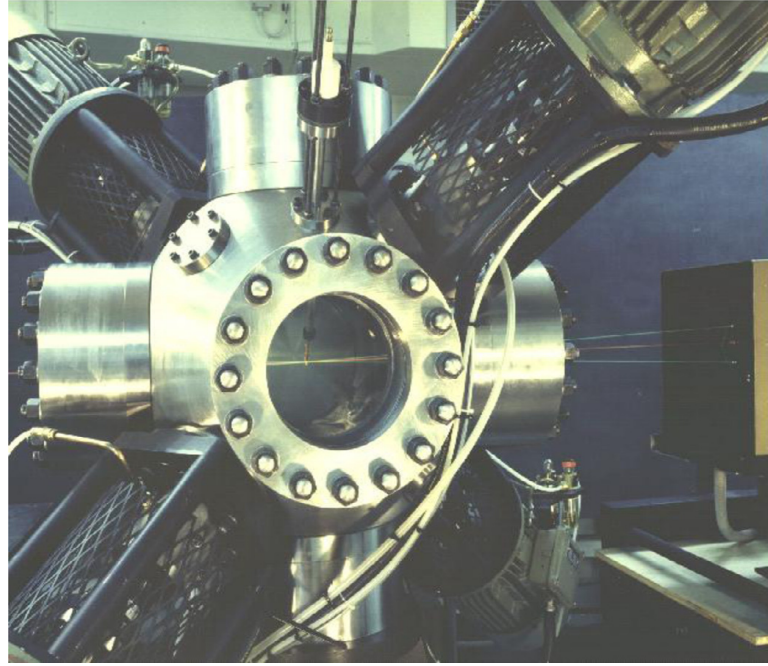


Figure 1.4 The explosion vessel investigated by Abdel-Gayed and Bradley (1977) in Leeds to quantify effects of turbulence on flame propagation. Four fans generate nearly homogeneous isotropic turbulence in the reacting mixture filling the vessel volume. Turbulent flame propagation subsequent to successful ignition in the mixture can be observed through quartz windows.

1.1.4 Bradley: the Leeds database

In England, motivated by the need to verify the inhibitive effects of small-scale turbulence, Andrews et al. (1975) devised an explosion vessel. The principal advantage of the vessel is the ability to generate homogenous isotropic turbulence using four fans located along the vertices of a tetrahedron as shown in Figure 1.4. Flame kernels initiated using a spark in the centre would propagate spherically in the field of turbulence, and by varying the speed of the fans, turbulence intensity u' may be regulated. By avoiding direct contact with walls and indirect interaction through wall shear generated turbulence, the experiment was able to reduce anisotropies in turbulence. Abdel-Gayed and Bradley (1977) followed with experiments of turbulent flame propagation under increasing turbulence intensity in this vessel.

Summarising the sensitivity of turbulent burning velocity s_T to various

1. Theoretical Background

mixture properties, Abdel-Gayed et al. (1985) presented the relation

$$\frac{s_T}{s_L} = f\left(\frac{u'}{s_L}, \text{Re}_0, \text{Le}, \beta\right) \quad (1.21)$$

where u'/s_L is the normalised turbulence intensity used in the Borghi diagram in Figure 1.3, Re_0 is the Reynolds number defined in Equation 1.18, Le is the mixture Lewis number and β , the Zeldovich number, is a function of the activation energy E_a . Abdel-Gayed et al. (1987) conducted the same experiments under a wide range of equivalence ratios and turbulence intensities; a bending effect in $s_T(u'/s_L)$ was evident. Further still, at high enough intensities, the premixed flame would fail to grow. This supported the hypothesis that the bending effect occurs due to local flame quenching.

Bradley et al. (1992) sought to characterise this flame quenching due to the contribution of tangential strain rate to the overall stretch rate. Hence, a strain rate scale was assumed to be related to the Taylor scale λ as provided by Batchelor (1952). The Karlovitz number based on this scale $Ka = \delta_L^0/\lambda$ is derived as

$$\text{Ka} = 0.157 \text{Re}_0^{-\frac{1}{2}} \left(\frac{u'}{s_L}\right)^2. \quad (1.22)$$

Further, along the early work of Wohl et al. (1953), Abdel-Gayed et al. (1989) pointed out the role of Lewis number in accentuating the effect of hydrodynamic strain on turbulent premixed flames. Hence, quenching criteria were developed based on correlations with 1650 experiments as follows

$$\text{KaLe} \geq 6.0 \quad (1.23)$$

for which flames quench globally. Here, the Karlovitz number Ka is meant to denote the role of strain and the Lewis number Le that of the thermo-chemical mixture properties. Curvature and flame propagation effects are neglected. Indeed, in the expression of Equation 1.9 in terms of flame kernel radius R

$$\dot{s} = \left(\frac{U}{R} + \nabla_t U\right) + \frac{s_d}{R}, \quad (1.24)$$

where the first term includes the strain rate term computed using the tan-

1.1. Concepts of turbulent burning velocity

gential derivative operator ∇_t and the second is the curvature term. Bradley et al. (1992) hypothesised that ‘as flow and turbulence velocities increase, the bracketed terms will increase relative to [the second term].’ The bracketed terms representing prescribed flow field effects such as tangential strain were hypothesised to dominate in comparison to the flame curvature term. Based on this, it suggested that bending marks the onset of a departure from the locally flamelet structure – the foundational basis of DH1 – leading to quenching of the flamelet due to excessive straining (Abdel-Gayed et al., 1985).

Two aspects of the work in explosion vessels have been explored since. First, a relationship of turbulent burning velocity with the flame configuration appears to be inevitable (Bedat and Cheng, 1995; Filatyev et al., 2005). Hence, it is believed increasingly that a general explanation of the bending effect without considering turbulence generation mechanisms may be infeasible (Driscoll, 2008). Further, the relationships between strain and flame propagation have been investigated, primarily to determine the degree to which transient strain determines the overall flame propagation. Recent work of Steinberg and Driscoll (2009) has revealed through cinema stereography, for instance, aspects of the non-linear relationship between strain and curvature, which are found to be tightly coupled.

Further, while the work of Bradley and co-workers has had significant impact in terms of the explanation of bending, a consistent general correlation of $s_T(u')$ was never provided. Recently, Shy et al. (2000b) considered radiation losses in methane-air premixed flames when mixed with diluents and found that a correlation using Damköhler number better approximates methane-air s_T/s_L data across different values of equivalence ratio (ϕ). The relation is as follows

$$\frac{s_T - s_L}{u'} \sim \text{Da}^{0.59} \quad (1.25)$$

where the constants were obtained through correlations across many experiments. Shy et al. (2000a) observe a similar bending effect in $s_T(u')$ with two distinct slopes in low and high u' regimes. The mechanism and physical ramifications of this scaling remain to be understood. In this regard, simulations provide a window to access detailed information of the flow field and flame

1. Theoretical Background

process.

1.2 Simulations of turbulent burning velocity

1.2.1 Model equations for flame dynamics

Direct Numerical Simulations

With advances in computing, an important approach has emerged that allows turbulent premixed flames to be simulated exactly under prescribed conditions (McMurtry et al., 1986). Emerging dynamics of flame propagation can then be inspected to ascribe physical mechanisms to the phenomena of interest. This provides a significant amount of information accessible for analysis as opposed to experimental techniques.

In Direct Numerical Simulation, or DNS, the governing equations for turbulent gaseous reactive flow are prescribed first. Under certain initial and boundary conditions, these equations may be solved to a high degree of numerical accuracy. The equations include the Navier-Stokes equations as well as the transport equations for the various chemical species involved in the combustion reactions. Local mass-fractions Y_α of an arbitrary number of active chemical species may be computed according to the transport equation

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_\alpha) = -\nabla \cdot \mathcal{J}_\alpha + \dot{\omega}_\alpha \quad (1.26)$$

where $\alpha = 1, \dots, N$ is the species index, $\mathcal{J}_\alpha$ is the molecular diffusion flux of the species α . Hydrocarbon combustion may involve $N > 50$ such chemical species. In order to accurately model the transport of these species, a corresponding reaction mechanism must be evaluated that provides the local reaction rates $\dot{\omega}_\alpha$. The solution of these additional chemical transport equations poses a severe computational challenge over and above the expensive direct numerical integration of the Navier-Stokes equations. Nevertheless, simplified 2D simulations have been feasible when employed in conjunction with reduced chemical kinetic models (Poinso et al., 1995). These reduced kinetic models consider the transport and chemistry of $N \leq 25$ chemical species thereby re-

1.2. Simulations of turbulent burning velocity

ducing computational expense. Such simulations have provided insight into the mechanisms that underpin the observed dynamics of flame propagation.

In premixed flames, a further simplification may be adopted assuming that the overall reaction relies on just a few key chemical species (Peters, 1988). It is assumed often that the reaction progress variable

$$c = \frac{Y_\alpha - Y_{\alpha,b}}{Y_{\alpha,u} - Y_{\alpha,b}} \quad (1.27)$$

may denote sufficiently the progress of the overall combustion reaction locally from an unburned u to burned b state provided α corresponds to a chemical species that ensures monotonicity of c . Hence, the problem of simulating premixed turbulent combustion may be reduced faithfully (Bray and Cant, 1991) to a single tractable equation

$$\frac{\partial \rho c}{\partial t} + \nabla \cdot (\rho \mathbf{u} c) = -\nabla \cdot (\rho D \nabla c) + \dot{\omega}_c \quad (1.28)$$

alongside equations that describe the flow. Here, Fick's law has been used to model the diffusive mass flux in terms of the gradient ∇c of reaction progress variable. Such a framework forms the basis for turbulent premixed combustion modelling and, despite its simplicity, has provided much insight into the dynamics of premixed flame propagation as discussed by Bray (1990); Lipatnikov and Chomiak (2002).

For instance, 2D flame propagation in a laminar flow with a single vortex has been simulated by Poinso et al. (1991a). Dynamics of vortex-flame interactions were investigated for a range of vortex intensities in order to gain insight into the regime of validity for DH1. Hence, as Poinso (1996) notes, the effects of excessive strain on flame quenching may be studied without having to consider a turbulent flow. Interestingly, the area enhancement mechanism of DH1 was shown to remain valid despite local flamelet quenching because quenching was found to be intermittent in nature. This reinforced the conclusions of Meneveau and Poinso (1991) who, through DNS of vortex-pair premixed flame interactions, also observed that Kolmogorov scales did not have any effect on the flame front barring short-lived high strain rates imposed by

1. Theoretical Background

these scales.

The flamelet regime $Ka \leq 1$ corresponds to $\eta \geq \delta_L^0$, so it is argued that turbulence can not disrupt the local laminar flamelet structure in this regime Peters (1999). Experimental evidence by Bedat and Cheng (1995); Shepherd et al. (2002) as well as DNS evidence from Poinso et al. (1995) not only supports this argument but emphasises further that local flamelet structure persists even for $Ka > 1$. At the same time, some experimental works (Gilder and Smallwood, 2007) question the persistence of flamelet structure in similar or even milder conditions. Models have been developed (Cant et al., 1991; Duclos et al., 1993) on the assumption that DH1 persists (in fact, up to $Ka \approx 16$) so long as quenching ‘does not inhibit the growth of the active flame surface’ (Meneveau and Poinso, 1991). Experimental studies have since correlated s_T data within the extended DH1 framework (1.13 and 1.14), reformulating the stretch factor I_0 as a ‘burning factor’ $P_b \sim I_0^2$ instead (Bradley et al., 2011).

Further to computing exactly the solutions under prescribed hypothetical conditions, as noted by Kerstein (2002), DNS also allows for investigation of exact but unclosed equations of flamelet evolution. Diagnostic tests of these equations which are arrived at using various assumptions provide further insights into phenomena such as flame quenching (Poinso et al., 1991b). Moreover, such unclosed equations have been developed to be applied for turbulent combustion modelling in other frameworks (Veynante and Vervisch, 2002). Three common examples (Bilger et al., 2005) are provided below.

Bray-Moss-Libby model

Proposed over several joint investigations (Bray and Moss, 1977; Bray, 1980), the BML model presents turbulent flame propagation in terms of the Favre-averaged form of Equation 1.28 in steady state

$$\nabla \cdot \tilde{\rho} \tilde{\mathbf{u}} \tilde{c} = -\nabla \cdot \tilde{\rho} \widetilde{\mathbf{u}'' c''} + \tilde{\dot{\omega}}, \quad (1.29)$$

which is valid for $Re \gg Da \gg 1$ so that the diffusive term may be ignored. Favre mean quantities $\tilde{q} = \overline{\rho q} / \bar{\rho}$ represent density-weighted averages whereas q'' denotes the respective fluctuations, i.e. $q = \tilde{q} + q''$. In this framework,

1.2. Simulations of turbulent burning velocity

propagation of the mean flame surface $\tilde{c}$ emerges as a consequence of convection (l.h.s.) and the two terms on the r.h.s. which denote respectively the turbulent scalar flux $-\nabla \cdot \widetilde{\rho \mathbf{u}'' c}$ and the chemical source-term $\bar{\omega}$.

Analysis of DNS datasets using the BML framework has led to insights related to the various terms that play a role in flame propagation. One example is provided by the manifestation of counter-gradient turbulent transport (discussed in Chapter 5) proposed originally by Bray (1980). Evidence for counter-gradient transport has since been found in various DNS datasets (Rutland and Cant, 1994; Veynante et al., 1997; Chakraborty and Cant, 2009), and this has allowed further analysis of the mechanisms responsible for it (Bray, 1995; Veynante and Poinso, 1997; Veynante and Vervisch, 2002).

Counter-gradient transport relates to the effect of the flame motion and heat release on the turbulence. Still further, this relates to the concept of flame generated turbulence initiated long ago by Karlovitz et al. (1951). Again, DNS provides a framework for investigating the underlying mechanisms of such effects (Louch and Bray, 2001). The BML model therefore provides a valuable tool for investigating key mechanisms involved in turbulent flame propagation. In the present work, this framework is employed to understand the ramifications on DH2 by elaborating on its validity limit in Chapter 5.

Flame Surface Density

Another exact but unclosed formulation has been provided in terms of the transport of Flame Surface Density (Pope, 1988; Cant et al., 1991; Candel and Poinso, 1990). This formulation provides an evolution equation of the average local flame surface-to-volume ratio

$$\frac{\partial \Sigma}{\partial t} + \nabla \cdot (\langle \dot{\mathbf{X}} \rangle_s \Sigma) = \langle \dot{s} \rangle_s \Sigma, \quad (1.30)$$

in terms of the mean stretch rate $\langle \dot{s} \rangle_s$, which acts as the source-term. The quantity $\dot{\mathbf{X}} = \mathbf{u} + s_d \hat{n}$ is the local velocity of the surface under consideration such that s_d is the displacement speed along the normal direction $\hat{n}$. In contrast to the BML formulation, the FSD framework provides a perspective in terms of the evolution of an isosurface. DNS datasets may be investigated for budgets

1. Theoretical Background

of the FSD equation in a Favre-averaged formulation (Trouvé and Poinso, 1994). As a result, the FSD framework allows for investigation of stretch rate influences on particular isosurfaces. Unsteady investigations have also been conducted allowing the possibility of understanding concepts such as negative flame speed (Gran et al., 1996; Peters et al., 1998).

Furthermore relationships between individual stretch rate components (introduced in Section 1.1.2) can be investigated based on this framework. For instance, Echekki and Chen (1996) concluded that negative curvature reduces the rate of stretch, and its contribution is further enhanced by the nonlinear behaviour of s_d as a function of curvature. Further, the structure and the effects on flame topology and resulting flame propagation rates were inferred (Echekki and Chen, 1996).

While Lewis number effects have been observed in turbulent flame curvatures (Haworth and Poinso, 1992), significant evidence has also been gathered supporting purely kinematic effects of curvature (Cant, 1999). These possibilities have been investigated further in 3D by Chakraborty and Cant (2004, 2009) within the same framework. Thus, this allows verification of earlier claims made by Bradley et al. (1992) regarding flame propagations in regions where stretch rate may dominate a predictable quenching stretch rate $\dot{s}_q$. These concepts are, therefore, further investigated in the present work by linking the concept of stretch rate source-terms with the bending effect behaviour.

Level set approach

Instead of computing locally the mean progress of reaction, the flame surface itself may be tracked using a level-set approach (Kerstein et al., 1988). Assuming the flame surface to be thin compared to the flow scales, the convective transport of a passive scalar G provides

$$\frac{\partial G}{\partial t} + \dot{\mathbf{X}} \cdot \nabla G = 0 \quad (1.31)$$

where the local velocity $\dot{\mathbf{X}} = \mathbf{u} + s_d \hat{n}$ as before is the vector sum of local flow velocity $\mathbf{u}$ and the local displacement velocity $s_d \hat{n}$ of the flame surface along its normal $\hat{n} = \nabla G / |\nabla G|$. By analysing the dynamics of this interface it

1.2. Simulations of turbulent burning velocity

is, as with FSD, possible to inspect local surface behaviour, but here changes to the local velocity of the isosurface. Indeed, the FSD can be shown to be proportional to the mean of the gradient modulus $|\nabla G|$ (Cant and Mastorakos, 2008).

Indeed, it is interesting to note that the experimentally observed bending effect can be reproduced by tuning long-established models such as the Coherent Flame Model (Duclos et al., 1993) and the G -equation model (Wenzel and Peters, 2000). Despite these apparent successes, a mechanism of bending expressed using physically-intuitive terms remains elusive. DNS offers a useful tool to investigate such mechanisms.

1.2.2 Peters: the Thin Reaction Zones regime

The level-set approach formed a key part of an investigation conducted by Peters (1999). A scaling analysis was adopted to differentiate the Thin Reaction Zones (TRZ) regime from the corrugated and distributed regimes identified earlier (see Section 1.1.4). The overall flame time scale was identified as $\tau_F \sim D/s_L^2$ in relation to diffusion, whereas the inner reaction time scale was associated with the reaction zone thickness $\ell_\delta \sim 0.1\delta_L$. This divide between the flame time scale and the reaction time scale was exploited to formulate two closely related Karlovitz number expressions. A Karlovitz number defined as

$$\text{Ka} \equiv \frac{\tau_F}{\tau_\eta} = \frac{\delta_L^2}{\eta^2}, \quad (1.32)$$

the ratio of a chemical scale (τ_F or δ_L) to the Kolmogorov scale (τ_η or η) determines the overall flame related stretch. In contrast, the ratio

$$\text{Ka}_\delta \equiv \frac{\tau_\delta}{\tau_\eta} \sim \frac{\ell_\delta^2}{\eta^2} \sim 0.01 \frac{\delta_L^2}{\eta^2}, \quad (1.33)$$

denotes a comparison of the Kolmogorov time scale with the reaction zone time scale ℓ_δ . According to Peters (1999), the TRZ regime lies between $Ka = 1$ and $Ka_\delta = 1$. Figure 1.5 shows the Borghi diagram of Figure 1.3 as conceptualized in terms of the regimes proposed by Peters (1999).

The Broken Reaction Zones (BRZ) regime $Ka \geq 100$ corresponds to $\eta \leq$

1. Theoretical Background

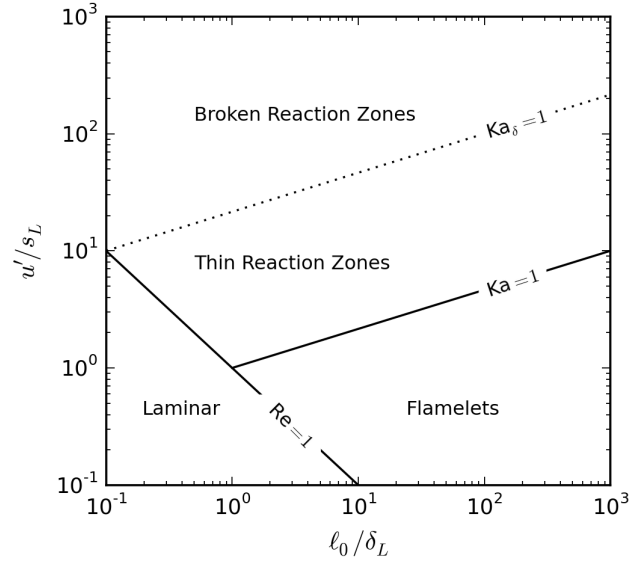


Figure 1.5 Regime diagram as proposed by Peters (1999) demarcating the extent of the Thin Reaction Zones (TRZ) regime using $Ka = 1$ and $Ka_\delta = 1$ isolines.

$\delta_L/10$ and, hence, turbulence microscales may be expected to affect the local internal flame structure. Recent DNS evidence (Poludnenko and Oran, 2011) shows that close to $Ka \approx 100$, the effects of turbulence are limited to disruption of the preheat zone. The reaction zone remains largely unaffected and retains flamelet structure locally.

Investigating the scaling proposed in Damköhler's hypotheses, Peters (1999) further employed the notion of TRZ to understand the bending effect in terms of the level-set approach. This was related, thereby, to the difference in effects of kinematic restoration and scalar dissipation in the corrugated and TRZ regimes, respectively. There is reason however to re-investigate these results because the level-set approach limits the description of the simulated flames to a surface with no internal structure. In another study, Wenzel and Peters (2000) arrived at a dataset that captured bending across the same regime boundary. However, instead of using the G equation as a diagnostic tool, it was used as the equation for simulation, thereby requiring a model input of local burning velocity. Hence, it remains to be settled that bending indeed occurs across this boundary of regimes. Other diagnostic frameworks outlined above may be expected to shed light on this problem. Hence in Chapter 4, the

bending effect is investigated in the framework of the FSD approach.

Several recent DNS studies have resolved to investigate flames at high turbulence intensity. These have included DNS of laboratory-scale flames (Bell et al., 2005, 2007; Day et al., 2012) as well as canonical configurations including spherical flame kernels (Jenkins and Cant, 1999; Fru et al., 2011) and statistically planar flames (Poludnenko and Oran, 2011; Aspden et al., 2011; Savre et al., 2013; Lapointe et al., 2015). More realistic configurations are also being addressed under similar levels of turbulence (Sankaran et al., 2007; Hawkes et al., 2012). These efforts have paved a way for systematic studies which attempt to isolate the parameters critical to the bending effect (Hamlington et al., 2011; Poludnenko, 2015; Lapointe and Blanquart, 2016). As yet, however, a consolidated framework for addressing the bending effect is lacking.

Furthermore, several computational investigations have corroborated the resilience of the flamelet structure (especially, the reaction zone) to intense turbulence (Wenzel and Peters, 2000; Lipatnikov and Chomiak, 2002; Bell et al., 2007; Poludnenko and Oran, 2011; Wang et al., 2016a). As a result, a description of bending in the absence of flamelet quenching may be sought (Filatyev et al., 2005). More recent DNS simulations and their comparison with experiments at high u' (Wang et al., 2016b,a) support the plausibility of such an explanation. Some experiments, however, have provided contrary evidence and disputed the persistence of flamelet structure as well as the validity of DH1 in moderate to intense turbulence (Gülder and Smallwood, 2007; Yuen and Gülder, 2013). Subsequent DNS studies have, therefore, focused on illuminating further the role of quenching at high u' (Aspden et al., 2011; Savard and Blanquart, 2015; Lapointe et al., 2015). To shed light on this problem, Damköhler's foundational hypotheses (Damköhler, 1940) are reframed with regard to these investigations.

1.2.3 What do Damköhler's hypotheses mean today?

Damköhler's regimes, DH1 as well as DH2, correspond to regions in the Peters regime diagram with contrasting values of length scales ($\ell_0 \gg \delta_L$ and $\ell_0 \ll \delta_L$) along a constant Re isoline (as discussed in §5 of Damköhler (1940)). As seen

1. Theoretical Background

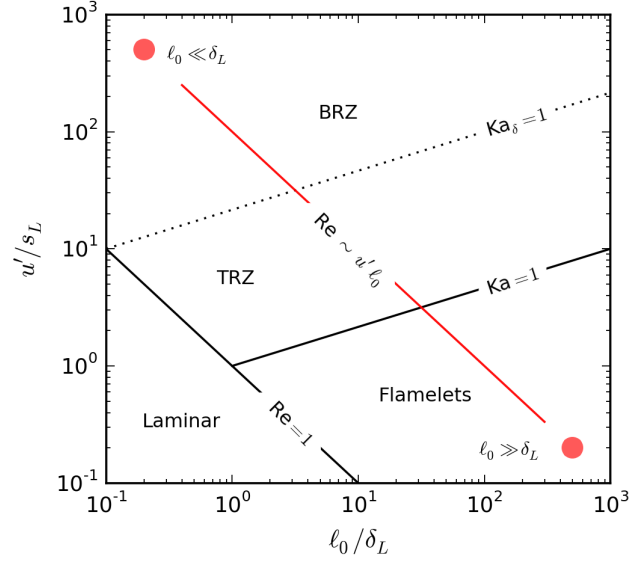


Figure 1.6 Regimes proposed by Damköhler (1940) illustrated on the regime diagram proposed by Peters (1999). DH1 ($\ell_0 \gg \delta_L$) and DH2 ($\ell_0 \ll \delta_L$) correspond to the flamelet and Broken Reaction Zones (BRZ) regimes respectively.

in Figure 1.6, these belong to two extremities of the regime diagram, such that DH1 corresponds to the flamelet regime and DH2 to the BRZ regime.

The size of these turbulent microscales is inversely related to the intensity u' of a homogeneous isotropic turbulent flow field through the relation $\eta \propto \text{Re}^{-3/4}$ for a given integral scale ℓ_0 (Frisch, 2004). Hence, DH1 is expected to be strictly valid for a turbulent flow with a specified ℓ_0 if u' is low enough that $\eta > \delta_L$. It is unclear, however, how far into the TRZ regime the first hypothesis continues to be valid. Furthermore, Damköhler proposed each of the two hypotheses to elucidate the primary mechanism of s_T enhancement in their respective regimes of turbulence. While a primary mechanism operates, the secondary mechanism was expected to ‘recede in the background’ contributing alongside albeit to a lesser degree. Over the years, the range and upper u' limit of validity for DH1 has received significant attention. The lower u' limit of validity for DH2, however, remains unknown still.

Recent investigations in intense (Poludnenko and Oran, 2011; Savard and Blanquart, 2015) and extreme u' turbulence (Wabel et al., 2016) have highlighted the significance of diffusive transport processes in determining s_T under such conditions. Appropriate modifications of DH2 are being proposed so as to

fit the s_T data acquired. One may ask, if the transition between Damköhler's two proposed regimes lies within the TRZ regime, then what is the appropriate marker for recording such a transition? Third, does such a transition mark an onset of validity for DH2? How far down into the TRZ does DH2 remain valid? The aim of the present work is to gain some insight by studying the relationship between s_T and underlying mechanisms.

1.2.4 Thesis objectives and approach

Evidently, several important questions regarding turbulent burning velocity remain open. The present thesis investigates specifically the bending effect in turbulent burning velocity. The following questions are addressed

1. *Is bending real?* Firstly, a DNS dataset is designed carefully to capture systematically the variation of turbulent burning velocity s_T with turbulence intensity u' . As a consequence, the very possibility of recording a bending effect in $s_T(u')$ is explored. The range of u' considered span the entire Thin Reaction Zones regime conceptualised by Peters (1999). The DNS method employed is discussed in the following chapter, and the simulation dataset is designed and generated in Chapter 3.
2. *Is bending kinematic or chemical?* Secondly, upon registering a bending effect, the mechanism governing this variation of $s_T(u')$ is investigated. The validity of Damköhler's first hypothesis is verified within the dataset, providing an insight into whether the bending phenomenon retains the thermo-chemical structure of the flame. The plausibility of a kinematic mechanism of bending is explored within the framework of the Flame Surface Density approach in Chapter 4. Due consideration is given to the possible role of flame surface curvature.
3. *Is Damköhler's second hypothesis valid?* Finally, the validity of the neglected hypothesis of Damköhler (1940) is investigated in the DNS dataset. The objective is to shed further light on the mechanisms underpinning the recorded bending effect. The associated role of flame-induced self-acceleration in limiting the validity of DH2 is studied within

1. Theoretical Background

the framework of the Bray-Moss-Libby model in Chapter 5.

The thesis concludes with an ongoing work that aims to validate the proposed explanations with experiment. The Leeds explosion vessel is considered for this comparison in Chapter 6. By probing the possible mechanisms of the bending effect, this thesis therefore aims to provide an insight into the long-standing problem of turbulent flame propagation.

Chapter 2

The Direct Numerical Simulation method

As discussed in the previous chapter, Direct Numerical Simulation (DNS) provides the ability to capture and analyse flame dynamics in detail by resolving the various scales of gas motion in space and time. Until recently, DNS has yielded significant insights into turbulent flame propagation (Chakraborty and Cant, 2004; Poludnenko and Oran, 2011). Yet its application to the bending effect remains to be addressed (Lipatnikov and Chomiak, 2002; Driscoll, 2008). Hence, in the present work, the bending effect is investigated using the methodological framework of DNS as follows.

The basic equations governing combustion chemistry and species transport are written in a 3D form. In order to close the basic equations, a set of well-posed boundary conditions (BCs) is supplied as appropriate for the flame configuration. Further, an initial condition (IC) is applied to the variables of the basic equations. This is done in such a manner that the computational effort required to reach a statistically significant solution is minimised. Upon the imposition of an IC and appropriate BCs, the system of equations are converted to a high-order discretised form in space and time. This enables a numerical approach to obtaining the solution. The numerical algorithm is implemented in a `FORTRAN77` computer code called `SENGA2` developed by Cant (2013). Time-dependent solutions of the desired problem are obtained by running the code (also called solver) on supercomputing clusters.

2. The Direct Numerical Simulation method

Each of these aspects specific to the presently used DNS framework are elaborated below. The presentation of the basic equations follows the style of Buckmaster and Ludford (1982). Following the presentation of the framework, a set of benchmark solutions conducted to verify the computational method is discussed. These benchmarks are presented in a manner leading progressively up to the primary DNS investigations of the current work.

2.1 Basic equations

Consider first the temporal evolution of a homogeneous gaseous mixture undergoing chemical reaction. At any time t during the reaction process, the mixture is described by its composition vector $\mathbf{Y}(t) = \{Y_\alpha(t) : \alpha = 1, \dots, N\}^T$ which comprises mass-fractions of each component (chemical species) denoted by the index α . At any such time,

$$\sum_{\alpha=1}^N Y_\alpha(t) = 1, \quad (2.1)$$

providing a constraint to the temporal evolution of the N mixture components. Hence, any $N - 1$ components of the gaseous mixture determine the composition vector $\mathbf{Y}(t)$ completely. The density $\rho(t)$ of the gaseous mixture is computed as

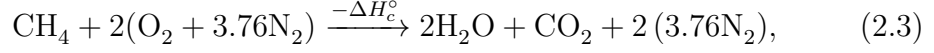
$$\rho(t) = \sum_{\alpha=1}^N \rho_\alpha(t) Y_\alpha(t), \quad (2.2)$$

the mass-weighted-average of component densities $\rho_\alpha(t)$. The temperature $T(t)$ may be assumed to be the same for all components and is obtained using the caloric equation of state. Together, the local fields $\mathbf{Y}(t)$, $\rho(t)$, and $T(t)$ form a basis for the time-evolving thermo-chemical state-space of a homogeneous reacting gaseous fuel-air mixture.

Kinetic models pertinent to hydrocarbon combustion chemistry are presented in the sections below. By providing a model for the reaction rate $\dot{\omega}$, these descriptions address the time-evolution of the thermo-chemical state space.

Combustion Chemistry

The overall chemical reaction for the combustion of a stoichiometric mixture, i.e. with equivalence ratio $\phi = 1$, of methane and air may be expressed as



where it is assumed that air is composed of O_2 and N_2 in a molar proportion of 1:3.76, and that N_2 remains inert throughout the reaction.

The overall reaction given by Equation 2.3 proceeds exothermically, releasing ΔH_c° as the heat of combustion for methane. The rate of the overall reaction $\dot{\omega}$ denotes the rate of consumption of reactants or, equivalently, the rate of formation of products. However, the overall reaction is composed of many elementary reactions where intermediate chemical species are formed and consumed. The ‘full’ chemical mechanism has been elaborated for methane-air combustion, for example in the **GRI-MECH 3.0** (Smith et al., 2017) and it consists of $M > 300$ elementary reactions and $N > 50$ species. A reduced kinetic model (with $M < 50$) is computationally tractable while at the same time it can describe some of the primary underlying physics of flame propagation. Two such reduced chemical kinetic models are considered in the present thesis.

One-step Kinetics

The most basic description of the overall combustion reaction is



which models the chemical mechanism of combustion as a one-step irreversible transformation from unburned reactants R to burned products P . The rate $\dot{\omega}$ of a one-step reaction is expressed simply in the Arrhenius form

$$\dot{\omega}_\alpha = A\rho Y_\alpha e^{-E_a/(R^\circ T)}, \quad (2.5)$$

based on the overall activation energy E_a and overall collision factor A . The index α may correspond to R or P , which can be assigned the thermo-chemical

2. The Direct Numerical Simulation method

properties (such as enthalpy of formation ΔH_f°) of the reactants and products of the overall reaction given by Equation 2.3. This allows the overall heat release ΔH_c° and its rate to be accounted for by this kinetic model.

Upon the specification of an appropriate Lewis number Le and activation energy E_a , the flamelet structure and propagation speed may be also computed with reasonable accuracy (this is discussed in Section 2.4). By accounting for these salient aspects of combustion processes (Le , E_a , and ΔH_c°), this seemingly simple kinetic model has provided satisfactory explanations of many combustion phenomena related to laminar as well as turbulent flame propagation. These are presented in the review by Lipatnikov and Chomiak (2002). As a further bonus, computational expense is minimal because the model requires only one species to be transported, with the other determined as $Y_P = 1 - Y_R$.

Due to these merits, the one-step kinetic model is chosen in the parametric simulations of the bending effect in Chapter 3. This has allowed further investigation of the Damköhler's hypotheses in the recorded bending effect (Chapter 4 and Chapter 5). Nevertheless, the role of intermediate chemical species in the bending effect can be elaborated only by considering multi-step kinetics.

Multi-step Reduced Kinetics

An improvement upon the one-step kinetic model is to use multi-step kinetic models. These are obtained by reducing systematically the 'full' chemical mechanism of combustion using steady-state assumptions for elementary reactions and fast chemistry approximations for intermediate species. In this manner it may sometimes, but not always, provide a more realistic description.

A 25-step kinetic model due to Smooke and Giovangigli (1991) is used in Chapter 6. The consideration of various reaction pathways helps model the role of intermediate species transport in the bending effect. Furthermore, two other kinetic models were investigated: the 4-step kinetic model due to Peters and Williams (1987), and the 68-step model due to Sandia National Laboratories (Kee et al., 1986). These models were not adopted because the

former was found to be computationally stiff and the latter computationally prohibitive. The single-step model is the one used primarily in the present investigation. Initial comparisons using such the 25-step kinetic model have been considered in Chapter 4, but the description of multi-step kinetics is deferred until Chapter 6 where it is used for experimental validation.

In a volume that exhibits flame propagation, the state $\{\rho, \mathbf{Y}, T\}$ changes spatially as well, so that the local state is affected by species transport. This spatio-temporal evolution is addressed in the following sections. Adiabatic systems are considered so that volumetric heat transfer may be neglected.

Continuum Description of Species Transport

In turbulent flame propagation, spatial variations of the composition vector $\mathbf{Y}(\mathbf{x}, t)$ may be described using its transport equation. This is determined by the equation of mass-balance for each species α

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho \mathbf{v}_\alpha Y_\alpha) = \dot{\omega}_\alpha, \quad (2.6)$$

where $\mathbf{v}_\alpha$ is the local species velocity and $\dot{\omega}_\alpha$ is its rate of formation source-term. The variable $\dot{\omega}_\alpha$ is modelled using one of the chemical kinetic models discussed above. A further relation is needed, however, for the species velocity $\mathbf{v}_\alpha$. The precise molecular contribution in $\mathbf{v}_\alpha$ can be made explicit by defining the local bulk velocity as the mass-averaged velocity of the mixture components

$$\mathbf{v} \equiv \sum_{\alpha}^N Y_\alpha \mathbf{v}_\alpha, \quad (2.7)$$

in similar fashion to Equation 2.2 for the local bulk gas density. The molecular diffusion velocity $\mathbf{V}_\alpha = \mathbf{v}_\alpha - \mathbf{v}$ is introduced subsequently so that the species mass-transport equation may be re-written as

$$\frac{\partial \rho Y_\alpha}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_\alpha) = \dot{\omega}_\alpha - \nabla \cdot (\rho \mathbf{V}_\alpha Y_\alpha), \quad (2.8)$$

where the unclosed term (the second term on the r.h.s.) is explicitly a molecular diffusion term. In non-reacting mixtures, the diffusive flux $\rho \mathbf{V}_\alpha Y_\alpha$ is ex-

2. The Direct Numerical Simulation method

pressed as a consequence of the local concentration gradient of the component α . This formulation (Bird et al., 1960) is due to Fick, and is applied to reacting mixtures as is for the sake of simplicity. Hence, in the present work

$$\mathbf{V}_{\alpha,j}Y_{\alpha} = -D_{\alpha}\frac{\partial Y_{\alpha}}{\partial x_j}, \quad (2.9)$$

neglecting the Soret effect (molecular diffusion due to temperature gradient). The species diffusion coefficient

$$D_{\alpha} = \frac{\lambda}{\rho C_p \text{Le}_{\alpha}} \quad (2.10)$$

is related to its thermal conductivity λ and heat capacity C_p via the Lewis number Le_{α} . The ratio λ/C_p expressed as a function of temperature

$$\frac{\lambda}{C_p} = A_{\lambda} \left(\frac{T}{T^{\circ}} \right)^r, \quad (2.11)$$

holds for the local mixture with constants A_{λ} and r specified *a priori*. Due to its relative simplicity, this approach is adopted in the present work from Chapter 3 through Chapter 5 assuming a unity mixture Lewis number. In Chapter 6, this framework is changed. The Fick's law of Equation 2.9 is modified so that a dependence on the local composition vector is reflected. Similarly, the values of D_{α} and λ are obtained based on the local properties of the mixture.

Mass, Momentum and Energy Transport

The sum of mass balances for each species in Equation 2.8 yields the continuity equation for the bulk fluid written as

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad (2.12)$$

under the compatibility conditions $\sum_{\alpha=1}^N \dot{\omega}_{\alpha} = 0$ and $\sum_{\alpha=1}^N \mathbf{V}_{\alpha} Y_{\alpha} = 0$. Similarly, the local momentum balance equation for the mixture can be obtained by adding individual momentum-balance equations for each component species.

This is given by the Navier-Stokes equations in compressible form

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \quad (2.13)$$

upon neglecting gravitational and other body forces. The variable p introduced here is the local hydrodynamic pressure, whereas $\boldsymbol{\tau}$ is the viscous stress-tensor of the bulk fluid. Both variables must be modelled in order to close the system. The local pressure p emerges, as a consequence of Dalton's Law for single-phase systems (Buckmaster and Ludford, 1982), as the sum

$$p = \sum_{\alpha=1}^N p_{\alpha}, \quad (2.14)$$

of partial pressures given by the ideal gas law for a perfect gas

$$p_{\alpha} = \rho R^{\circ} T Y_{\alpha} / W_{\alpha}, \quad (2.15)$$

for each individual component α with molar mass W_{α} . Assuming the mixture to be a Newtonian fluid, the viscous stress tensor $\boldsymbol{\tau}$ is computed as

$$\tau_{ji} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ji} \right), \quad (2.16)$$

where the viscosity

$$\mu = \frac{\lambda}{C_p} \text{Pr}, \quad (2.17)$$

is expressed as a linear function of λ/C_p using the Prandtl number Pr , which is assumed constant.

Lastly, the equation of energy-balance is derived for the chemically reacting flow system. The local internal energy for a compressible flow is defined as

$$e \equiv \frac{1}{2} u_j u_j - \frac{p}{\rho} + \sum_{\alpha=1}^N Y_{\alpha} h_{\alpha}, \quad (2.18)$$

where h_{α} is the local enthalpy of species α given by the integral

$$h_{\alpha} = \int_{T_0}^T C_{P,\alpha} dT + h_{\alpha}^0 \quad (2.19)$$

2. The Direct Numerical Simulation method

for a specified value of formation enthalpy h_α° . The mass-specific heat capacity $C_{p,\alpha}$ is approximated using a polynomial in temperature tabulated *a priori* for each species (McBride and Gordon, 1967). The transport equation for e is also obtained in a similar manner as for the mass and momentum balance, and can be written as

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho \mathbf{v} e) = -\nabla \cdot p \mathbf{v} + \nabla \mathbf{q} + \boldsymbol{\tau} : \nabla \mathbf{v} \quad (2.20)$$

assuming the work done by molecular interaction forces is negligible (Buckmaster and Ludford, 1982). The heat flux vector $\mathbf{q}$ is introduced here as new unclosed variable. Neglecting radiative transfer and the Dufour effect (heat flux due to concentration gradient), the components of $\mathbf{q}$ are expressed in terms of the variables ρ , T , V_α , Y_α and h_α as follows

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \sum_{\alpha=1}^N \rho V_{\alpha,j} Y_\alpha h_\alpha, \quad (2.21)$$

using Fourier's conduction law (first term on r.h.s.) and the sum of diffusion enthalpies (second term). Hence, a closed system of equations is obtained.

Summary of equations in closed form

Conservative variables ρ , ρu_i , ρe , and ρY_α are described as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) = 0, \quad (2.22)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j u_i) = -\frac{\partial}{\partial x_i} (p) + \frac{\partial}{\partial x_j} (\tau_{ji}), \quad (2.23)$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e) = -\frac{\partial}{\partial x_j} (p u_j) + \frac{\partial}{\partial x_j} (q_j) + \frac{\partial}{\partial x_j} (\tau_{ji} u_i), \quad \text{and} \quad (2.24)$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j Y_\alpha) = \dot{\omega}_\alpha + \frac{\partial}{\partial x_j} (\rho V_{\alpha,j} Y_\alpha), \quad (2.25)$$

where $e \equiv \frac{1}{2}u_j u_j - p/\rho + \sum_{\alpha=1}^N Y_\alpha h_\alpha$ and the variables p , τ_{ji} and q_j are modelled as

$$p = \rho R^\circ T \sum_{\alpha=1}^N Y_\alpha / W_\alpha \quad (2.26)$$

$$\tau_{ji} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ji} \right), \quad \text{and} \quad (2.27)$$

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \sum_{\alpha=1}^N \rho V_{\alpha,j} Y_\alpha h_\alpha \quad (2.28)$$

and, finally, the variables $V_{\alpha,j}$ and $\dot{\omega}_\alpha$ are expressed as

$$V_{\alpha,j} Y_\alpha = -\mathcal{D}_\alpha \frac{\partial Y_\alpha}{\partial x_j}, \text{ and} \quad (2.29)$$

$$\dot{\omega}_\alpha = A \rho Y_\alpha e^{-E_\alpha/(R^\circ T)}, \quad (2.30)$$

where λ , C_p , $\mathcal{D}_\alpha$ and μ are functions of temperature. All other constants are known *a priori* from the mixture components and chemical kinetic models.

2.2 Boundary Conditions

Equations of transport – Equation 2.22 through Equation 2.25 – follow the general conservative form

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{C} = \mathbf{D} + \mathbf{S}, \quad (2.31)$$

in which $\mathbf{U} = \{\rho, \rho u_i, \rho e, \rho Y_\alpha\}^T$ are the conserved variables, $\mathbf{C}$ and $\mathbf{D}$ are the convective and diffusive fluxes, and $\mathbf{S}$ is the vector of source-terms. These equations do not require any further information in an unbounded domain with infinite extents in all dimensions; however, such a problem is not amenable to numerical solution in a finite time. Hence, unbounded domains of infinite extent must be truncated to lend computationally-tractable domains. This is done by exploiting various symmetries in the solution expected. For instance, the periodic BC exploits translational symmetry in the specified direction. Such BCs are used routinely to render computationally feasible 3D simulations

2. The Direct Numerical Simulation method

of homogeneous isotropic turbulence (Pope, 2001).

Basic Concepts and Flame Configuration

In directional flows such as vortex advection and flame propagation, the translational symmetries are broken in at least one dimension. Hence, periodic BCs cannot be applied for the simulation of such problems. In such circumstances, because the domain must nevertheless be truncated, a different kind of BC must be specified at the artificial boundaries.

The most basic configuration for modelling a propagating flame is a 1D domain with inflow and outflow boundaries on either end (discussed in Section 2.4). In this configuration, laminar inflow balances the propagating flamelet between the boundaries. This problem can be extended to two dimensions by considering a planar flame where the added span-wise dimension is assigned periodic BCs. Extending the 2D configuration to three dimensions, a 3D inflow-outflow configuration is obtained. Such a domain is necessary for modelling realistically the turbulent energy spectrum. A statistically planar flame may propagate in the longitudinal or x direction (inflow-outflow) and the remaining directions are assigned periodic BCs. This configuration is used for the flame simulations conducted in the present work (see Section 3.1.1).

Primitive Variables

At the inflow and outflow boundaries, the solution is specified in terms of primitive variables $\mathbf{U} = \{\rho, u_i, p, Y_\alpha\}^T$ rather than conservative variables $\mathbf{U}$. This is because the imposed values are generally known in primitive rather than conservative form. The primitive variables $\mathbf{U}$ follow a transport equation that may be obtained by transforming the conservative equations 2.31 using the Jacobian matrix $\mathbb{P} = \partial\mathbf{U}/\partial\mathbf{U}$

$$\text{Conservative Form} \xrightleftharpoons[\mathbb{P}]{\mathbb{P}^{-1}} \text{Primitive Form}, \quad (2.32)$$

to arrive at an equivalent system of equations

$$\frac{\partial\mathbf{U}}{\partial t} + \mathbf{A} \cdot (\nabla\mathbf{U}) = \mathbf{D} + \mathbf{S}, \quad (2.33)$$

written using primitive variables, where $A = \mathbb{P}^{-1} \partial \mathbf{C} / \partial \mathbf{U}$ is the corresponding flux-transformation matrix. Since the two forms are equivalent, closure of one system of equations is informed by the other.

The primitive system consists of hyperbolic (unsteady diffusive terms) as well as non-linear terms (reaction rate source-terms). The corresponding equations require an appropriate number of constraints for closure (Poinsot and Lele, 1992). The imposition of these constraints at the boundaries, however, introduces unwanted waves in the domain of solution that may contaminate the numerical solution over time. A challenge in flame simulations, therefore, is to suppress all such unwanted effects of the artificial boundary (Sutherland and Kennedy, 2003).

Navier-Stokes Characteristic Boundary Conditions

One approach to reduce spurious boundary-effects is to use the characteristic wave form of the primitive equations. The idea is to be able to specify the amplitudes of the known waves while diminishing the amplitudes of the unknown or unwanted waves. In an inflow-outflow configuration, waves travel in the longitudinal x direction, so that the primitive form of equations can be written in the boundary-normal form as

$$\frac{\partial \mathbf{U}}{\partial t} + A_{(n)} \cdot (\nabla^{(n)} \mathbf{U}) + A_{(t)} \cdot (\nabla^{(t)} \mathbf{U}) = \mathbf{S}, \quad (2.34)$$

upon neglecting the diffusive terms $\mathbf{D}$ in Equation 2.33. Subscripts n and t indicate normal and transverse components to the boundaries. The characteristic decomposition of this equation is written as

$$\frac{\partial \mathbf{U}}{\partial t} + \begin{bmatrix} \frac{1}{\rho a} (\mathcal{L}_5^{(x)} - \mathcal{L}_1^{(x)}) \\ \mathcal{L}_3^{(x)} \\ \mathcal{L}_4^{(x)} \\ \mathcal{L}_2^{(x)} + \frac{1}{a^2} (\mathcal{L}_5^{(x)} + \mathcal{L}_1^{(x)}) \\ \mathcal{L}_5^{(x)} + \mathcal{L}_1^{(x)} \\ \mathcal{L}_{5+\alpha}^{(x)} \end{bmatrix} = \mathbf{S} \quad (2.35)$$

2. The Direct Numerical Simulation method

in the locally one-dimensional inviscid (LODI) formulation. Each of the terms $\mathcal{L}_i^{(x)}$ denote here the characteristic wave-amplitude variations in the axial direction; transverse terms as well as diffusive terms are neglected in the LODI formulation. The terms $\mathcal{L}_i^{(x)}$

$$\mathcal{L}^{(n)} = \begin{bmatrix} \mathcal{L}_1^{(x)} \\ \mathcal{L}_2^{(x)} \\ \mathcal{L}_3^{(x)} \\ \mathcal{L}_4^{(x)} \\ \mathcal{L}_5^{(x)} \\ \mathcal{L}_{5+\alpha}^{(x)} \end{bmatrix} = \begin{bmatrix} \lambda_1^{(x)} \cdot \frac{1}{2} \left(\frac{\partial p}{\partial x} - \rho a \frac{\partial u}{\partial x} \right) \\ \lambda_2^{(x)} \cdot \frac{1}{2} \left(\frac{\partial \rho}{\partial x} - \frac{1}{a^2} \frac{\partial p}{\partial x} \right) \\ \frac{\lambda_3^{(x)}}{2} \cdot \left(\frac{\partial v}{\partial x} \right) \\ \frac{\lambda_4^{(x)}}{2} \cdot \left(\frac{\partial w}{\partial x} \right) \\ \lambda_5^{(x)} \cdot \frac{1}{2} \left(\frac{\partial p}{\partial x} + \rho a \frac{\partial u}{\partial x} \right) \\ \frac{\lambda_{5+\alpha}^{(x)}}{2} \cdot \left(\frac{\partial Y_\alpha}{\partial x} \right) \end{bmatrix} \quad (2.36)$$

are characteristic wave-amplitudes with characteristic velocities $\lambda_k^{(x)}$

$$\lambda_1^{(x)} = u - a, \lambda_2^{(x)} = \lambda_3^{(x)} = \lambda_4^{(x)} = \lambda_{5+\alpha}^{(x)} = u, \lambda_5^{(x)} = u + a. \quad (2.37)$$

in the boundary-normal direction n , which refers to the longitudinal/ x direction here. Given the sound speed a , the incoming and outgoing waves at a given boundary may be distinguished based on the sign of the characteristic velocities $\lambda_i^{(x)}$. In subsonic flow $u < a$, all waves except $\mathcal{L}_5^{(x)}$ are incoming at the left inflow boundary, whereas all waves except $\mathcal{L}_1^{(x)}$ are outgoing at the right outflow boundary. In order to specify the BCs for Equation 2.35, only the incoming characteristic wave-amplitudes need to be specified, while the outgoing waves can be computed using the solution in the domain. These characteristic wave-amplitudes arise in the characteristic form

$$\frac{\partial \mathcal{U}}{\partial t} + \mathcal{L}^{(n)} = \mathcal{S}, \quad (2.38)$$

of Equation 2.33 obtained by transforming the inviscid primitive form as

$$\text{Primitive Form} \xrightleftharpoons[\mathbb{S}^n]{(\mathbb{S}^n)^{-1}} \text{Characteristic Form} \quad (2.39)$$

using the matrix of right eigenvectors $\mathbb{S}^n$ of the flux transformation matrix A . The characteristic variables $\mathcal{U} = \mathbb{S}^{n-1}U$ have source-terms $\mathcal{S}$ (Sutherland and Kennedy, 2003). Knowing the characteristic variables and the source-terms, the wave-amplitudes $\mathcal{L}_i$ can be estimated. These may then be specified at the appropriate domain boundaries. Once the characteristic wave-amplitudes are computed, these are supplied in the primitive equation which is transformed back to the conservative form and solved numerically at the boundary.

Subsonic constant-density inflow

At the inlet, the characteristic wave-amplitudes $\mathcal{L}_1, \mathcal{L}_2, \mathcal{L}_3, \mathcal{L}_4$ and $\mathcal{L}_{5+\alpha}$ must be specified whereas the outgoing wave-amplitude $\mathcal{L}_5$ is computed from the characteristic equation. In a constant-density inflow BC, the density ρ to be prescribed is known at the inlet as well as the species mass-fractions Y_α and the velocity components u_i . These are used in the computation of the characteristic wave-amplitudes $\mathcal{L}_i$ along with the Taylor's hypothesis which allows calculation of the velocity components and the velocity gradients.

With the longitudinal component u_1 set to a specified mean velocity $\langle u_1 \rangle$ in flame simulations, the laminar flame speed s_L , the unsteady velocity field in the other two directions is obtained by scanning a frozen field of homogeneous isotropic turbulence. Relating the unsteady local velocity field to spatial traversal in a frozen velocity field is valid strictly when

$$u' \ll \langle u_1 \rangle \quad (2.40)$$

in which case Taylor's hypothesis provides the unsteady velocity

$$\frac{\partial u_i}{\partial t} = \langle u_1 \rangle \frac{\partial u_i}{\partial x} \quad (2.41)$$

in terms of the spatial velocity gradient required for closing the inflow boundary

2. The Direct Numerical Simulation method

condition. The temperature at the inlet is calculated using the LODI form of the energy equation.

Subsonic non-reflecting outflow

At the outlet, all waves are outgoing except $\mathcal{L}_1$. The value of this amplitude can be obtained using a steady-state approximation of the corresponding characteristic equation. The value $\mathcal{L}_1 = \mathcal{S}_1$ is then obtained upon setting all other wave-amplitudes to 0. However, it is observed that with such a prescription, the pressure in the domain tends to drift (Poinsot and Lele, 1992). Hence, in order to relax the boundary condition towards the steady-state value, a pressure-correction term is added as

$$\mathcal{L}_1^{(x)} = S_1 + \frac{\sigma}{2L} a (1 - \mathcal{M}^2) (p - p_\infty) \quad (2.42)$$

which accounts for the initial differences in pressure that may not satisfy the steady state equation of the characteristic. Rudy and Strikwerda (1980) provided an approximate constant value for $\sigma = 0.287$. The ambient pressure is set to $p_\infty = 1 \text{ bar}$, and the Mach number is specified as $\mathcal{M} = 5 \times 10^{-3}$ (Cant, 2013).

2.3 Numerical method

Upon prescribing the boundary conditions, the closed system of boundary-value-problem equations can be solved numerically as a time-varying ODE

$$\frac{\partial \mathbf{U}}{\partial t} = \mathbf{R}(\mathbf{U}, t) \quad (2.43)$$

such that the r.h.s. is composed of source-terms and first and second order spatial derivatives $\hat{f}' \equiv \partial/\partial x_i$ and $\hat{f}'' \equiv \partial/\partial x_i \partial x_j$ of primitive variables $\mathbf{U}$. The exact re-arranged form of the basic equations consists of a skew-symmetric decomposition of the terms so as to reduce numerical error. Further details are discussed in the **SENGA2** User Manual (Cant, 2013).

Spatial Discretisation

The derivatives f' and f'' are estimated at coordinate points obtained by discretising the domain uniformly along each direction. At any interior mesh point, the derivatives are computed to 10^{th} order accuracy using a centred finite difference scheme. The first order approximation

$$f' = \sum_{m=1}^5 a'_m \frac{f_{i+m} - f_{i-m}}{2mh_i}, \quad (2.44)$$

as well as the second approximation

$$f''_i = \sum_{s=1}^5 a''_m \frac{f_{i+m} - 2f_i + f_{i-m}}{(mh_i)^2}, \quad (2.45)$$

of the derivatives require 5 points on each side of the chosen point. Similar expressions are formed for mixed second order derivatives $\partial/\partial x_i \partial x_j$, $i \neq j$. The respective coefficients a'_m and a''_m are obtained by solving the a system of equations formed by the Taylor series expansions at each of the 11 points. Points on a periodic boundary are treated the same as general interior points. For points on a non-periodic boundary, if the chosen point is less than 5 points away from a non-periodic boundary (inlet and outlet), the order of the method is sacrificed. At points less than 3 points away from the boundary, the 4^{th} order centred scheme (used 3 points away) is skewed towards the interior so as to maintain the order of the method. The coefficients a'_m and a''_m are altered to accommodate for these changes. Values for these coefficients are provided in the **SENGA2** User Manual (Cant, 2013).

Time Marching

Upon computing the spatial differences, the r.h.s. of Equation 2.43 is known completely, and the ODE

$$\frac{d\mathbf{U}}{dt} = \mathbf{R}(\mathbf{U}, t), \quad (2.46)$$

can be solved using a 4^{th} -order explicit 5 stage explicit Runge-Kutta scheme (classified as $RK4(3)5[2R+]C$) due to Kennedy and Carpenter (2003). In this

2. The Direct Numerical Simulation method

method, the conservative solution $\mathbf{U}$ is advanced at each time step t_n by a discrete interval Δt over successive stages. At any intermediate stage i , the solution is calculated as

$$\mathbf{U}^{(i)} = \mathbf{U}^{(n)} + \Delta t^{(n)} \sum_{j=1}^{i-1} a_j^{(i)} \mathbf{R}^{(j)} \quad (2.47)$$

and in the final stage, the time-advanced solution is obtained using all the solutions at previous stages as

$$\mathbf{U}^{(n+1)} = \mathbf{U}^{(n)} + \Delta t^{(n)} \sum_{j=1}^5 b_j \mathbf{U}^{(j)} \quad (2.48)$$

where the stage coefficients $a_j^{(i)}$ and b_j are pre-computed to match the order of the method. The Butcher array is used to obtain the coefficients in a straightforward manner as described in the **SENGA2** User Manual (Cant, 2013). Hence, in principle, this can be performed using two registers – one for the solution vector $\mathbf{U}^{(i)}$ and another for the r.h.s. vector $\mathbf{R}^{(j)}$ required at each stage.

Adaptive Time-step Control

The error incurred over the numerical time marching can be estimated using the truncation error with respect to a lower-order scheme. As the solution is advanced using a 4th-order scheme as shown above, a 3rd order scheme is used in parallel. This approach is referred to as ‘embedded method.’ The difference between the two solutions in an embedded method provides an estimate of the error. This error may be used to compute adaptively the timestep for the next iteration of the algorithm. A PID controller due to Kennedy and Carpenter (2003) takes the form

$$\Delta t^{(n+1)} = \text{TOL} \cdot \left(\frac{\hat{\epsilon}}{\hat{r}_{n+1}} \right)^\alpha \left(\frac{\hat{\epsilon}}{\hat{r}_n} \right)^\beta \left(\frac{\hat{\epsilon}}{\hat{r}_{n-1}} \right)^\gamma \Delta t^{(n)} \quad (2.49)$$

where $\alpha = 0.49/p$, $\beta = 0.34/p$ and $\gamma = 0.1/p$ given $p = 3$ is the order of the embedded method. The error-bound $\hat{\epsilon} = 10^{-3}$ and the tolerance variable

$TOL = 0.9$ allows for a safety-factor in the timestep estimation. The use of such controllers in the time-marching schemes for PDEs has a rich background in dynamical control theory. This PID controller is used as is for Chapter 3 through Chapter 5. An improved form of the controller (Söderlind, 2002) is developed in the final chapter.

Computational Algorithm

Numerical solutions of the governing equations may be computed using the schemes described above. In order to exploit parallel computing resources, a parallel decomposition of the domain is performed. The numerical solution is thus computed simultaneously over various sub-domains mapped to individual cores on a supercomputing cluster. In order to compute gradients using finite difference approximations described above, points close to the edges of the sub-domain require information from neighbouring sub-domains. For this purpose, a `HALO` array is constructed where the necessary information from the neighbouring sub-domain is stored during the computation procedure. For optimised fast I/O operations and optimised overall performance of the CFD solver, the `HDF5` library is used. This allows collective `MPI` I/O operations using an `API`. The `DARWIN` (Intel Sandy Bridge E5-2670) cluster and the massively parallel `ARCHER` (Cray XC30) supercomputer were used to conduct all simulations in the present work. Post-processing of data is conducted using various tools including `Python`, `Jupyter` and an in-house `FORTRAN95` code called `SATN`.

2.4 Benchmark solutions

Standard test cases have been performed using `SENGA2` to validate the framework. These include, in order of increasing flow complexity, a) 1D laminar propagating flame solutions, b) 2D vortex advection study, and c) homogeneous isotropic decaying turbulence. These serve to verify respectively: a) combustion chemistry calculations, b) the inflow and outflow boundary conditions, c) computation of 3D Navier-Stokes equations with turbulent spectra. Hence, all necessary components of a 3D turbulent flame propagation problem

2. The Direct Numerical Simulation method

are benchmarked in this manner.

1D Laminar Flame

A benchmark for flame chemistry models is the 1D laminar flame propagation solution. The 1D domain with inflow and outflow boundary conditions is set up. A steady inlet velocity is set approximately equal to the unstretched laminar flame speed s_L expected *a priori* under the specified ambient conditions $p^\circ = 1$ bar and $T^\circ = 300K$. The initial thermochemical field is specified as

$$Y_R(x; t = 0) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{x - x_0}{\delta} \right) \right] \quad (2.50)$$

for the reacting species R . The density and temperature are set in a similar manner using error function profiles. Using a single-step description of chemistry, a converged solution for 1D laminar flame propagation is obtained for these conditions after approximately 1600000 time steps. Figure 2.1 shows the key profiles obtained in terms of flame coordinates x (Figure 2.1a) as well as in the progress variable space c (Figure 2.1b). A thin reaction zone is evident (red line in Figure 2.1a). A peak reaction rate of $\dot{\omega}_{max} \approx 2000 \text{ s}^{-1}$ is computed for the stoichiometric mixture. In terms of the progress variable, this peak occurs

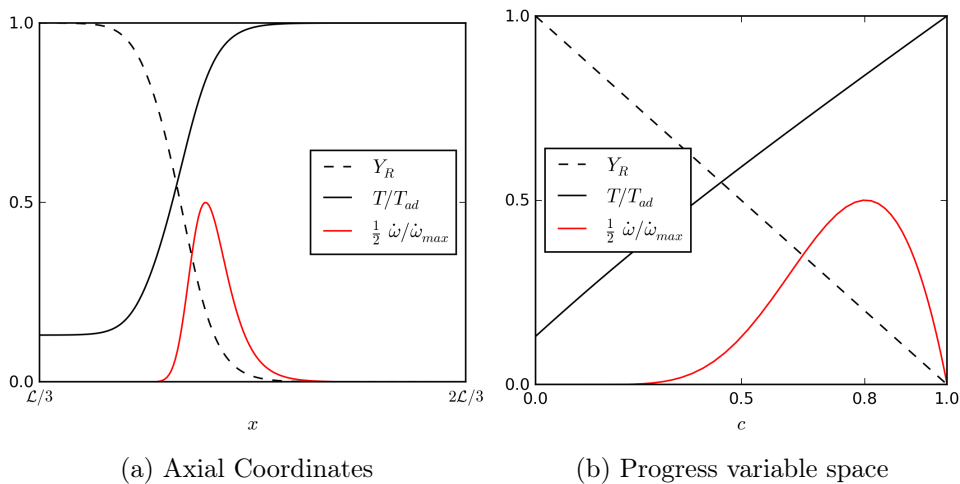


Figure 2.1 Laminar propagating 1D flame solution modelled using single-step kinetics and unity Lewis number. A spatially-thin reaction zone (left) is simulated. The peak reaction rate occurs at $c = 0.8$ (right).

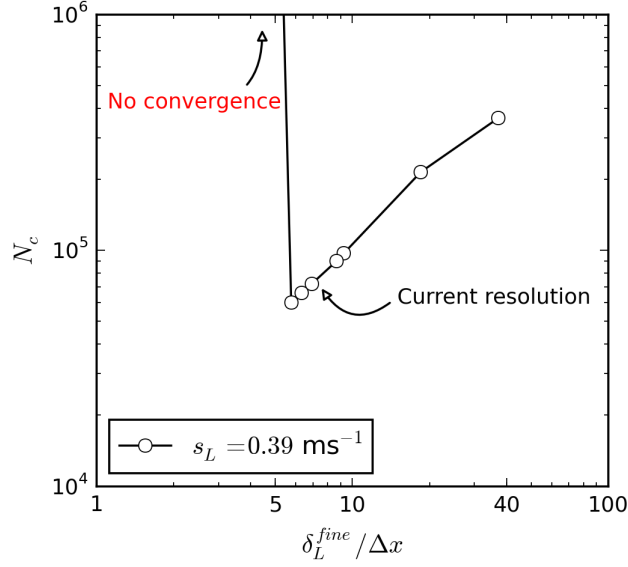


Figure 2.2 Grid resolution study to determine the bounds for flame chemistry resolution. Convergence fails for grids with resolution $\Delta x \gtrsim \delta_L/5$ where $\delta_L = 0.36 \times 10^{-3} m$ is obtained *a priori* on the finest grid.

at $c = 0.8$; this is an important aspect that will be used later on in the subsequent analysis. A laminar flame speed $s_L \approx 0.39 m s^{-1}$ and flame thickness $\delta_L \approx 0.36 mm$ are computed. All other relevant thermo-chemical parameter values will be discussed in Chapter 3. The discussion here is intended solely to verify the framework.

In order to verify further the dependence of the solution on the mesh properties, a mesh convergence study was conducted. This helps also find the resolution constraint imposed by the chemical flame structure of a 1D laminar flame. The laminar flame thickness δ_L was computed first using a fine mesh with nearly 40 points across this flame width δ_L . This corresponds to the right most point $\delta_L^{fine} / \Delta x \approx 40$ in Figure 2.2. Subsequently, the mesh was coarsened by increasing Δx so that $\delta_L^{fine} / \Delta x$ decreases (from right to left in Figure 2.2). In the coarsest mesh, (left most point in Figure 2.2), the flame was resolved using nearly 5 points. Inclusive of the fine and coarse extremes, all intermediate mesh configurations provided the same converged laminar flame speed and similar laminar flame structure as the fine-mesh result. The added benefit of using coarser meshes is that the number of steps N_c (ordinate in Figure 2.2) required to attain convergence is reduced. Meshes with coarser

2. The Direct Numerical Simulation method

resolution failed to provide a converged solution (marked using red text).

2D Vortex Advection

A benchmark case for boundary conditions is performed in a 2D domain with the left and right boundaries specified with inflow-outflow NSCBCs along the longitudinal direction and periodic BCs along the span-wise directions. The initial condition for a 2D vortex is given by the velocity field

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u_0 \\ 0 \end{pmatrix} + \frac{1}{\rho} \begin{pmatrix} \frac{\partial \psi}{\partial y} \\ -\frac{\partial \psi}{\partial x} \end{pmatrix}, \quad (2.51)$$

and is determined using the potential flow coordinate

$$\psi = C \exp \left(-\frac{x^2 + y^2}{2R_c^2} \right), \quad (2.52)$$

where C determines the vortex strength and R_c the core radius. The pressure p for this flow field is initialised as

$$p - p_\infty = \rho \frac{C^2}{R_c^2} \exp \left(-\frac{x^2 + y^2}{2R_c^2} \right) \quad (2.53)$$

where $p_\infty = 1$ bar is the ambient pressure. The mean axial inflow $u_0 = 5 \text{ m s}^{-1}$ is subsonic unlike in the study by Poinso and Lele (1992).

Figure 2.3 shows various snapshots of vorticity during the time-evolution of the snapshot. As the vortex approaches the outflow boundary, it is distorted and squeezed out of the domain through its lower half (x velocities are higher in this region of the vortex). Acoustic waves (small vertical lines at $t = 1 \text{ ms}$) are traced travelling away from the inflow boundary in one of the snapshots. A region of weak vorticity is generated near the inflow from the interaction of this wave with the boundary. These vorticity regions may contaminate the solution and are the subject of ongoing investigation. In particular, an improved formulation is sought for the outflow boundary condition prescribed in the

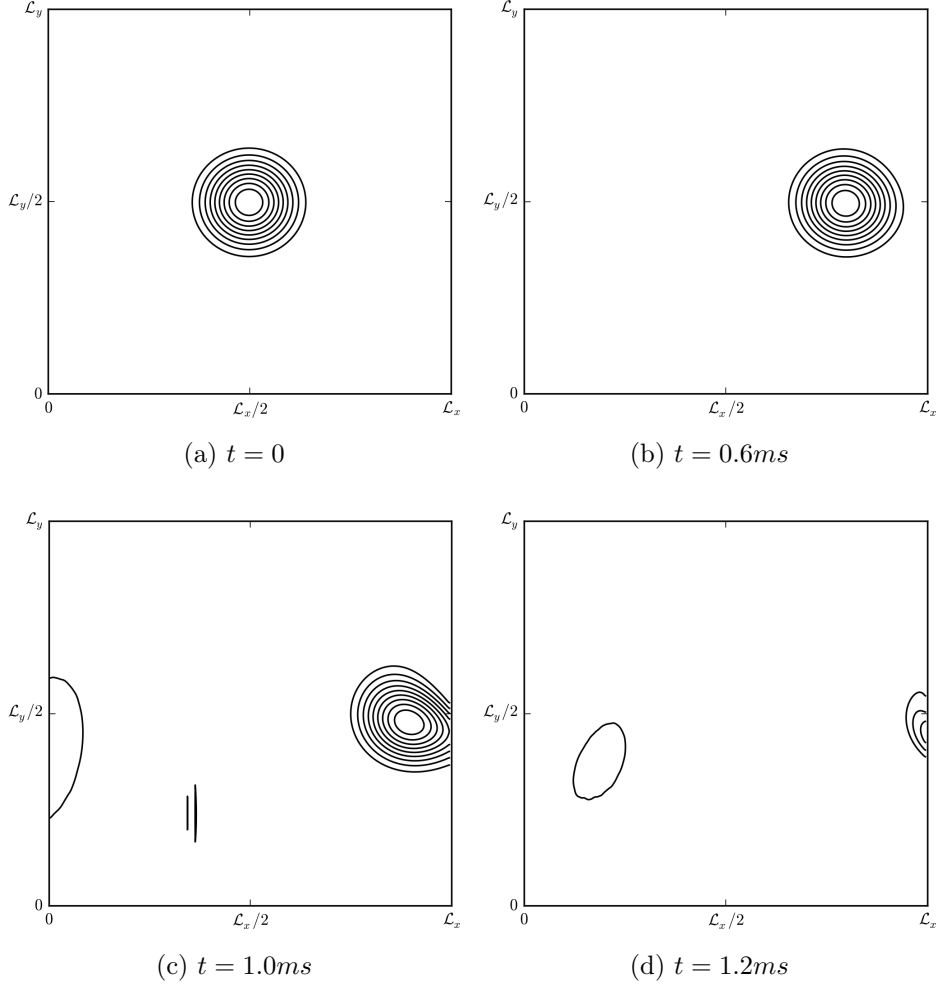


Figure 2.3 Simulation snapshots of a counter-clockwise rotating vortex advected through a 2D inflow-outflow domain with inlet velocity $u_0 = 5 \text{ m s}^{-1}$.

current work. At present, however, this serves to verify the general framework of NSCBCs for computing solutions in an inflow-outflow configuration.

3D Turbulent Non-reacting Flows

Finally, a benchmark is performed to verify the 3D computation of turbulent energy spectra. In turbulent flows, the initial turbulent velocity field $\mathbf{v}(\mathbf{x}, t = 0)$ for a cubic domain of size L is computed by specifying an energy spectrum due to Batchelor and Townsend (1948) as follows

$$E(\boldsymbol{\kappa}) = \frac{c_0 L}{\kappa_0} \left(\frac{\boldsymbol{\kappa}}{\kappa_0} \right)^4 \exp \left[-2 \left(\frac{\boldsymbol{\kappa}}{\kappa_0} \right)^2 \right], \quad (2.54)$$

2. The Direct Numerical Simulation method

in the wavenumber $\boldsymbol{\kappa}$ space such that κ_0 denotes the wavenumber with the maximum turbulent kinetic energy. The constant c_0 corresponds to the initial mean turbulent kinetic energy $k_0 \equiv 1/2\langle \mathbf{v} \cdot \mathbf{v} \rangle$ at $t = 0$ using the relation

$$c_0 = \frac{32}{3} \sqrt{\frac{2}{\pi}} k_0. \quad (2.55)$$

For a specified initial energy spectrum $E(\boldsymbol{\kappa})$, one instantiation $\mathbf{v}(\boldsymbol{\kappa})$ of the possible velocity fields is obtained in wavenumber space using the method proposed by Orzsag discussed in Cant (2013). A Fourier transform allows the initial velocity field $\mathbf{v}(\boldsymbol{\kappa}, t = 0)$ to be transformed into the velocity field $\mathbf{v}(\mathbf{x}, t = 0)$ in Cartesian space. Hence, a homogeneous isotropic turbulence (HIT) field is obtained as the initial condition. With the periodic BCs specified in all three directions, the turbulent decay of this HIT field can be simulated. The various regions of the energy spectrum are illustrated in Figure 2.4a for a time-evolved solution of an HIT field. The central region (red) denotes the energetic modes κ_E whereas the inertial subrange (orange/yellow) denotes the modes where dissipation is independent of the wavenumber. The spectrum extends up to κ_{max} where the dissipation range terminates.

The instantaneous turbulent kinetic energy $k(t)$ is expected to follow the

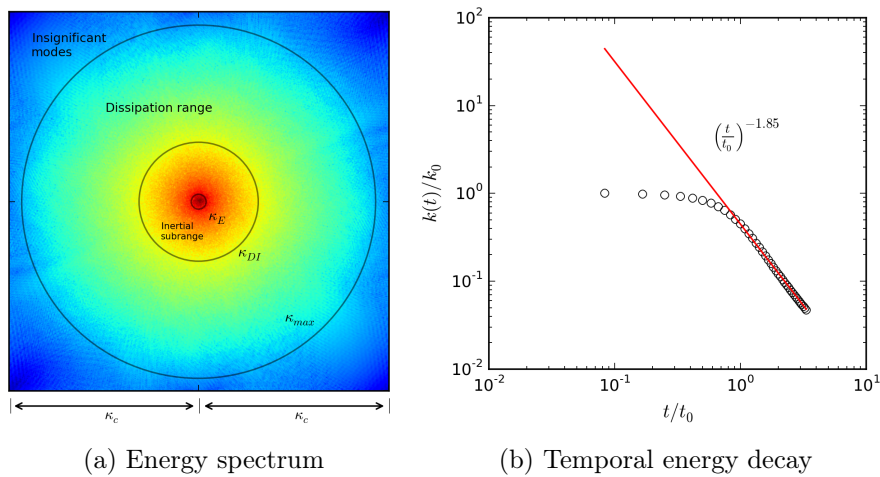


Figure 2.4 Turbulent kinetic energy computed in a periodic $128 \times 128 \times 128$ HIT simulation. Panels show a) snapshot of energy spectrum in Fourier space and b) temporal decay of kinetic energy.

temporal relationship

$$k = k_0 \left(\frac{t}{t_0} \right)^{-n}, \quad (2.56)$$

with the exponent n constant for a developed flow signifying a constant dissipation rate ϵ (Pope, 2001). Figure 2.4b shows the temporal evolution of mean kinetic energy $k(t)$ obtained using DNS with grid size $128 \times 128 \times 128$. Initial kinetic energy k_0 represents a flow with $u' = 10s_L$. The value of the decay exponent $n \approx 1.85$ achieved after a time $t \approx t_0$ is found to be close to that expected in the final period of decay (Batchelor and Townsend, 1948; Pope, 2001). The exponent stays constant for the remaining time at least until the kinetic energy attains a small fraction $k \approx 0.05k_0$ of the initial value. This serves to verify the 3D computations of the Navier-Stokes solutions in the present framework.

Summary: computational framework

The computational framework used in the subsequent investigations is laid out. The Navier-Stokes equations are framed in a 3D compressible form along with thermo-chemical transport (Cant, 2013). A 10^{th} -order centred finite difference operator evaluates spatial derivatives and reduces to 4^{th} -order at the inlet and outlet faces. In the stream-wise direction, inflow-outflow boundaries is specified using the Navier-Stokes characteristic boundary conditions (Sutherland and Kennedy, 2003). At the inlet, a reflecting constant-density condition with specified velocity components is imposed, whereas at the outlet, a non-reflecting outflow condition is imposed. The transverse directions are specified with periodic boundary conditions. A 4^{th} -order explicit Runge-Kutta method is used for time-marching along with adaptive time-stepping implemented using an error controller (Kennedy and Carpenter, 2003).

Chapter 3

Parametric Simulations of the Bending Effect

The goal of the present chapter is to use the computational framework described in the previous chapter to simulate turbulent premixed flame propagation. Selection of relevant simulation parameters has been informed by the conditions of bending recalled below. Recorded images of the turbulent flames, the pre-heat and reaction zone structures, as well as the associated turbulent burning velocities are discussed.

3.1 Design conditions for bending

Generalising the expression discussed in Chapter 2, Driscoll (2008) has provided a general dependence of s_T on physico-chemical parameters as

$$s_T = f(u', \ell_0, \bar{U}_{in}; s_L, \delta_L, Le; L) \quad (3.1)$$

where u' , ℓ_0 , $\bar{U}_{in}$ are physical properties, namely the turbulence intensity, integral length scale and mean inlet velocity of the premixture, whereas s_L , δ_L and Le are thermo-chemical properties of the mixture, namely the unstrained laminar flame speed, laminar flame thickness, and the Lewis number. Further, the dependence on flame configuration established experimentally by Shepherd et al. (2002) is considered within a characteristic length scale L .

3. Parametric Simulations of the Bending Effect

The bending effect refers (Bradley, 1992; Lipatnikov and Chomiak, 2002; Driscoll, 2008) to the non-linear variation of the curve $s_T(u')$. Hence, in order to capture the bending effect, it is essential that $\ell_0, \bar{U}_{in}, s_L, \delta_L, Le$ and the flame configuration parameter L remain unchanged between any two measurements. This constraint has been emphasised by Driscoll (2008) in light of recent experiments as well as simulations wherein other parameters vary simultaneously with u' . Such simulations may result in capturing a different parametric variation of s_T and, therefore, may not capture the bending effect or lead to different conclusions on the same. Therefore, the focus here is to design a set of simulations wherein u' is the only parameter varied systematically. Furthermore, values of u' are varied in a regime where the emergent curve $s_T(u')$ bends, i.e. s_T records a bending effect. The selection of each parameter maintained across the simulations is discussed as follows.

Thermo-chemical parameters

The thermochemical parameters: Lewis number Le , laminar flame speed s_L and laminar flame thickness δ_L are related to the choice of fuel-air mixture. Combustion of stoichiometric methane-air mixtures is considered here for which the Lewis number $Le \sim 1$. Effects of pyrolysis as well as radiative heat transfer are negligible for methane-air combustion. Hence, a relatively simple thermochemical model can describe flame propagation accurately for these mixtures. This has motivated the investigation of methane-air flames in many experimental and simulation databases as listed by Lipatnikov and Chomiak (2002).

Subsequently, methane-air combustion chemistry is described using a single-step kinetic model with unity Lewis number (see Chapter 2). The assumptions of single-step chemistry together with a unity Lewis number drastically simplify the modelling framework. Indeed, this provides a basic set of conditions in which to investigate the salient mechanisms of a particular combustion phenomenon. So this was thought to be a reasonable starting point for the investigation of the bending effect. It has been pointed out since that stretch effects, especially the contributions of local flame curvature, may be significantly different for non-unity Lewis number flames. Hence, in Chapter 6,

3.1. Design conditions for bending

Table 3.1 Thermo-chemical input parameters.

Ambient pressure, P_a	1.01×10^5 Pa
Inlet temperature, T_u	300 K
Pre-exponential constant, A	2.75×10^7 m ³ kg ⁻¹ s ⁻¹
Activation energy, E_a	10^8 Jkg ⁻¹
Gas constant, R	287.1 Jkg ⁻¹ K ⁻¹
Lewis number, Le	1.0
Prandtl Number, Pr	0.7
Schmidt Number, Sc	0.7
Heat release parameter, τ	6.7
Equivalence ratio, ϕ	1.0
Laminar flame speed, s_L	0.39 ms ⁻¹
Laminar flame thickness, δ_L	3.6×10^{-4} m
Reaction zone FWHM, δ	1.65×10^{-4} m

these assumptions are lifted. Nevertheless, the relative simplicity of the simulations discussed here and until Chapter 6 has provided several insights in a relatively inexpensive manner.

An unstrained 1D laminar flame solution profile calculated using the framework discussed above is used as the initial thermo-chemical field: density ρ , temperature T , and species mass-fractions Y_α . The laminar flame speed s_L is calculated by integrating the unburned mixture reaction rate $\dot{\omega}_R$ across an unstrained 1D laminar premixed flame

$$s_L = -\frac{1}{\rho_u Y_{R,u}} \int_{-\infty}^{\infty} \dot{\omega}_R(x) dx \quad (3.2)$$

where ρ_u is the density of the unburned mixture and $Y_{R,u}$ is the reactant mass fraction in this mixture. The unstrained laminar flame thickness $\delta_L = \delta_L^0$ is calculated using the maximum temperature gradient method

$$\delta_L = \frac{T_b - T_u}{(|dT/dx|)_{max}} \quad (3.3)$$

where $T_u = 300$ K is the unburned gas temperature and $T_b = 2300$ K is the adiabatic burned gas temperature. The values of s_L and δ_L are provided in Table 3.1 along with other relevant thermo-chemical parameters.

3. Parametric Simulations of the Bending Effect

3.1.1 Flame configuration and regime

Flame configuration plays an important role in determining the burning velocity s_T of the flame. Several realistic flame configurations have been considered by previous researchers as discussed in Section 1.2. A freely propagating flame is considered here instead for the following reasons

1. Jet flames and bluff-body stabilised flames require a huge domain to account for the turbulent spread. Freely propagating flames require only that the axial extent of the domain be several times the turbulent flame brush thickness. Undue computational expense is, therefore, mitigated in the latter.
2. Turbulent flow properties vary considerably over the flame surface in realistic flame configurations. Freely propagating flames offer a means to specify a single turbulence intensity u' and quantify its effects on s_T .
3. Effects of mean curvature are absent in statistically-planar propagating flames. Therefore, the problem of turbulent burning velocity in this configuration is the true analogue of the 1D propagating laminar flame.

Figure 3.1a illustrates the flame configuration using a typical 3D snapshot obtained from one of the simulations. The flame surface (denoted by a single

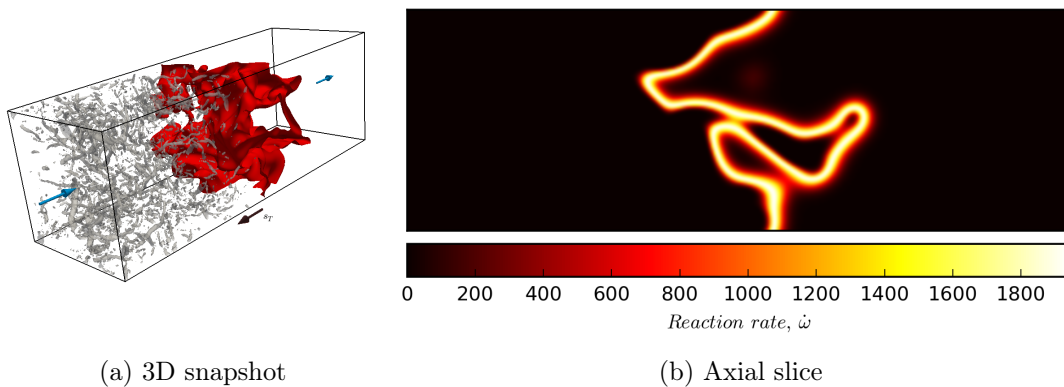


Figure 3.1 Inflow-outflow flame configuration used in the simulations. Left: 3D rendering of a propagating flame isosurface interacting with upstream turbulent eddies in the domain. Right: 2D axial slice showing the location of the flame and relative size of the domain.

progress variable isosurface: red contour) propagates into upstream turbulence (denoted by high-enstrophy contours: grey eddies) with a speed s_T (red arrow). In Figure 3.1b, a 2D axial slice is shown. The axial length of the domain is 3 times its width in spanwise directions. This helps accommodate flame propagation in the axial direction and, at the same time, avoids flame-boundary interactions. As discussed in Chapter 2, the transverse directions are specified with periodic boundary conditions, whereas the upstream and downstream faces (marked using blue arrows in Figure 3.1a) are specified with inflow and outflow NSCBCs respectively.

Turbulence initialisation

Turbulence is initialised using a procedure outlined by Rogallo (1981). First, a velocity field of desired turbulence intensity u' is generated using an energy spectrum for homogeneous isotropic turbulence proposed by Batchelor and Townsend (1948). As discussed in Chapter 2, the spectrum is specified in Fourier space using two parameters: 1) u' , which specifies the turbulent kinetic energy and 2) k_0 , which specifies the wavenumber of peak turbulent kinetic energy. Next, the corresponding Cartesian field is computed using a Fourier transform and applied to a cubic periodic domain of width L . The Cartesian periodic velocity field is allowed to evolve for a brief period. No forcing has been employed in the present simulations so that the turbulence decays ever so slightly during this period. This time-evolved homogeneous isotropic turbulence (HIT) solution is used as the initial velocity field in the flame domain.

Since the stream-wise extent of the flame domain is 3 times its width L , three identical HIT solutions are copied adjacent to each other for initialisation. Further, an identical HIT solution is convected through the inlet. Due to the time-evolution of the initial HIT solution, fewer transients are induced in the corresponding flame simulation.

The parameters k_0 and L together determine the integral length scale ℓ_0 and the Taylor length scale λ for the initialised spectrum (Batchelor and Townsend,

3. Parametric Simulations of the Bending Effect

Table 3.2 Turbulence properties and dimensionless parameters.

Case $\longrightarrow$	I	II	III	IV	V
Inlet/Initial u'	u'_i/s_L	1.50	7.50	10.00	20.00
leading edge u'	u'_{le}/s_L	0.94	4.50	6.00	12.00
Turbulent KE	k	m^2/s^2	11.7	20.6	82.5
Peak KE wavenumber	κ_0		2.0		185.6
Integral length scale	ℓ_0	mm	0.99		$\longrightarrow$
Kolmogorov scale	η	μm	33.35	28.89	20.42
Domain length	$L_x = 3$	cm	1.5		16.67
Domain width	L_y, L_z	cm	0.5		$\longrightarrow$
Grid size	$N_x \times N_y \times N_z$		$288 \times 96 \times 96$		$\longrightarrow$
Axial mesh resolution	Δx	μm	52.26		
Span-wise resolution	$\Delta y, \Delta_z$	μm	52.63		
LETOT	τ_0	ms	1.59	0.34	0.25
Chemical time	τ_c	ms	0.93	0.93	0.93
Total run time	$T = 4\tau_0$	ms	6.36	1.28	0.48
Damköhler number	Da		1.71	0.36	0.13
Karlovitz number	Ka		1.20	12.36	53.96
			19.08		99.82

[†] Arrows indicate that empty fields have the same value as the centre column field of the corresponding row.

* Acronyms: LETOT (Large-Eddy Turn-Over Time) and KE (Kinetic Energy).

3.1. Design conditions for bending

1948; Cant, 2013) as follows

$$\ell_0 = \frac{L}{\sqrt{2\pi k_0}}; \quad \lambda = \frac{L}{2\pi k_0}. \quad (3.4)$$

Therefore, these parameters have been fixed throughout the dataset with the intention of controlling ℓ_0 and λ of the prescribed turbulent flow field across the entire dataset (refer to Table 3.2 for values). In fact, L is chosen so that the integral length scale is several times the laminar flame thickness: $\ell_0 \approx 3\delta_L$.

As the flame simulation evolves in time, the inflow establishes a statistically-stationary spatial profile of turbulence from the inlet to the leading edge of the flame after a few eddy turn-over times. The intensity u' of turbulence varies to noticeable degree over this region. Hence, a leading edge turbulence intensity u'_{le} calculated at a planar section corresponding to $\bar{c} = 0.01$ has been supplied alongside the inlet turbulence intensity u'_i in Table 3.2. The length scales ℓ_0 and λ vary to a relatively minor extent in comparison. The leading edge values of these scales have, therefore, not been reported. Conforming with standard practice, all following values of u' correspond to the inlet or initial intensity.

Since the integral length scale ℓ_0 is fixed across all simulations, the Kolmogorov scale η becomes very small in high u' turbulence. Due to this, complete resolution of high u' turbulence up to the Nyquist frequency imposes a severe computational challenge. Hence, a fixed mesh spacing of the order $\Delta x \sim \mathcal{O}(\eta)$ of Kolmogorov scales is specified throughout the dataset. In the high u' cases, Δx is up to a few times the Kolmogorov length scale η calculated based on the Batchelor-Townsend spectrum as

$$\eta = \left[\frac{\nu^2}{15u'^2\pi^2\bar{k}_0^2} \right]^{1/4} \quad (3.5)$$

where $\bar{k}_0$ is the wavenumber of peak turbulent kinetic energy normalised by the domain width L . Coarse-grained simulations such as these have been conducted previously (Poludnenko and Oran, 2011). The relatively larger grid sizes contribute small-scale dissipation by numerical means, so that this framework is numerically valid. Nevertheless, fine-grained simulations are being

3. Parametric Simulations of the Bending Effect

conducted (see Chapter 6) to ascertain the ramifications of the present study.

Combustion regime

The selection of all parameters on the r.h.s. of Equation 3.1 has been discussed above. The integral length scale ℓ_0 together with the chosen turbulence intensity u' specifies the regime of the simulation. The combustion regime of simulations is estimated here using a Karlovitz number

$$\text{Ka} \equiv \left(\frac{u'}{s_L^0} \right)^{\frac{3}{2}} \left(\frac{\delta_L^0}{\ell_0} \right)^{\frac{1}{2}}, \quad (3.6)$$

based on the Taylor scale strain rate (Bradley, 1992). The Borghi diagram in Figure 3.2 shows the regime of each of the simulations marked as a single point (labelled I - V). The choice of u' values for the simulations has been such that by increasing u' successively between each simulated case, the dataset bridges the flamelet regime and the Broken Reaction Zones (BRZ) regime. These values of the Karlovitz number were calculated using inlet/initial turbulence properties. These values have been reported along with the Damköhler number

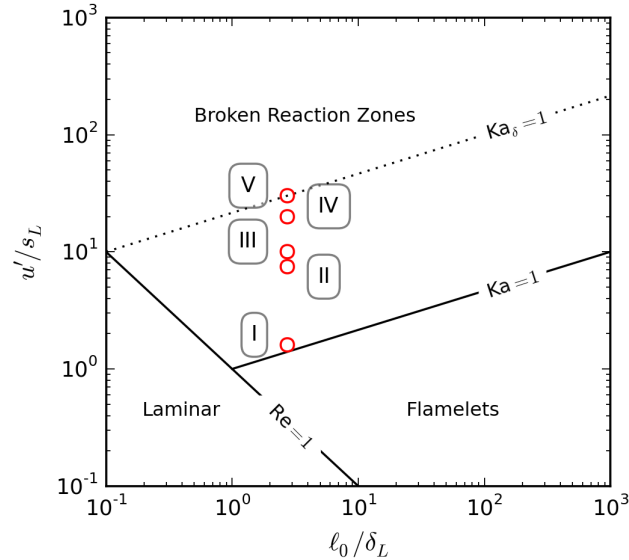


Figure 3.2 Regime diagram showing the region of parameter space covered by the present simulations. The entire region between the flamelet regime and broken reaction zones regime is spanned by increasing u' successively across five simulations labelled I - V.

3.2. Recorded effects of turbulence intensity

Da for the entire dataset in Table 3.2.

The dataset as prepared above consists of 5 different simulations each with a specified inlet u' . The DARWIN (Intel Sandy Bridge E5-2670) and ARCHER (Cray XC30) supercomputers were used to compute the solutions. Each simulation used approximately $T_c \sim 2.5 \times 10^4$ core-hours. The simulations were each run for $t = 4\tau_0$ where $\tau_0 = \ell_0/u'$ is the integral time scale. During this period, an initial phase of monotonic growth in s_T is observed up to $t \lesssim 2\tau_0$, followed by a phase of oscillations in s_T about an average value specific to each case. All statistics are collected during this phase at the instant $t = 4\tau_0$ as it provided representative results for the period of statistical-stationarity. Averaging, for instance, is conducted at the snapshot corresponding to this instant over the spanwise directions.

3.2 Recorded effects of turbulence intensity

3.2.1 Images of the turbulent flame brush

Figure 3.3 shows cropped slices of the domain corresponding to each of the simulations along the columns with the turbulence intensity noted on top. The time evolution of each of the flames is shown up to 4 eddy turn-over times τ_0 across the different rows. Each panel shows a 2D slice of the instantaneous progress variable contours at the corresponding time noted on the left. It is evident that the turbulent flame brush thickness increases across the simulations as u' is increased from $1.5s_L$ to $30s_L$ (left to right along any row in Figure 3.3). This thickness also increases over time in each simulation up to a certain maximum thickness as presented in (Nivarti and Cant, 2015a). Whereas wrinkling governs the flame brush thickness in the low to moderate intensity cases, considerable pocket-formation takes place in the high-intensity cases $u' > 10s_L$ determining the overall flame brush thickness.

A closer look at the time-evolution of flame wrinkling behaviour shows that wrinkling takes place at a much smaller time scale and much smaller length scales in the high-intensity cases. Low-intensity cases with $u' < 10s_L$ are dominated by slowly evolving, large-scale wrinkling behaviour; i.e. each

3. Parametric Simulations of the Bending Effect

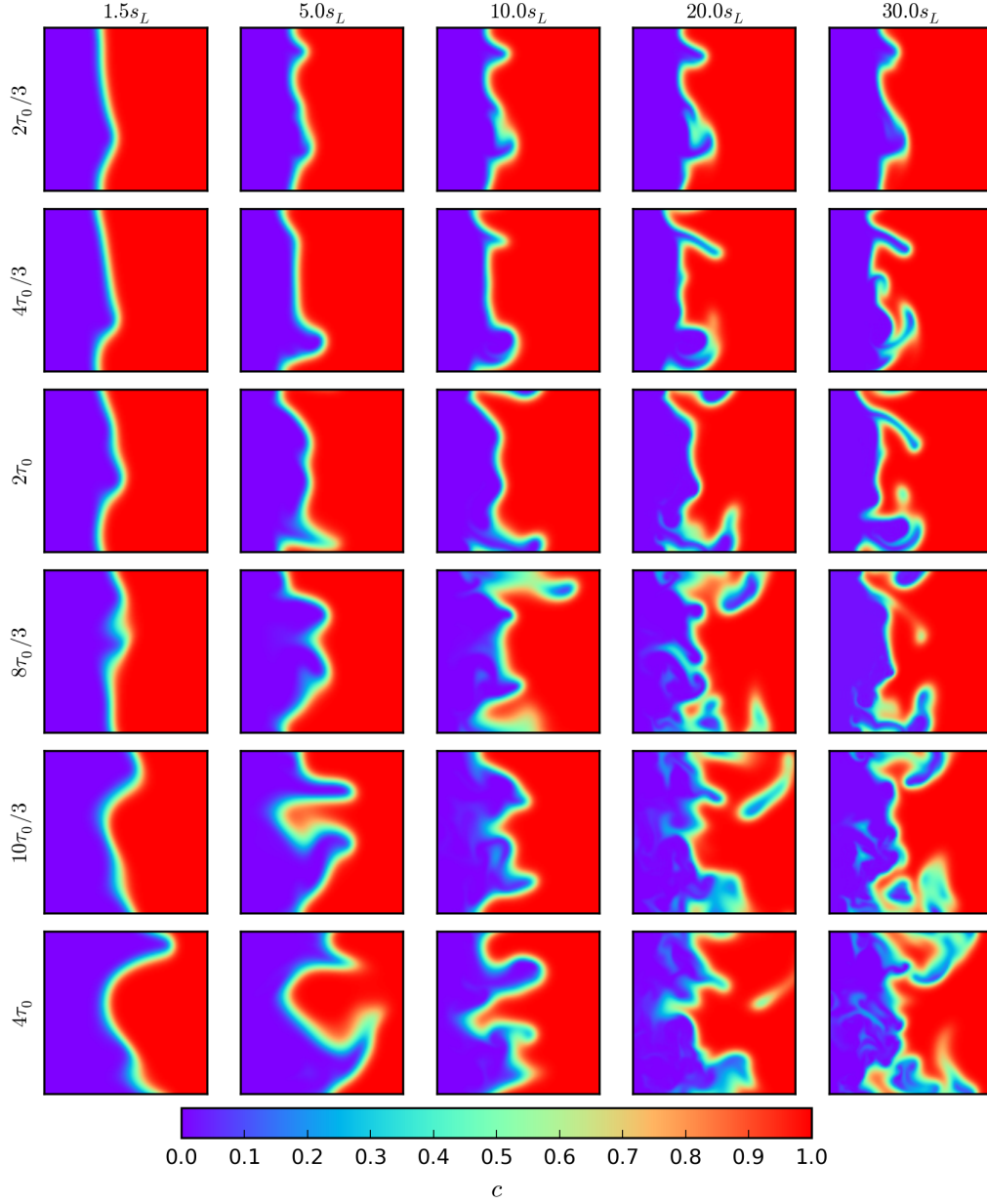


Figure 3.3 Contours of progress variable (colour) for each of the five simulations (columns, with u' value noted on top). Time evolution of the respective flame occurs down each column, with elapsed time noted on the left in each row.

wrinkle evolves over a significantly greater number of rows in the columns to the left. This highlights an interesting divide between low- and high-intensity cases. Given the constraints of the physical geometry, large-scale wrinkles of low-intensity turbulence cases keep the flame wrinkled for longer durations of time. In contrast, the wrinkling is dominant at smaller scales in the high-

3.2. Recorded effects of turbulence intensity

intensity cases so that the flames are flatter on average than the low-intensity cases.

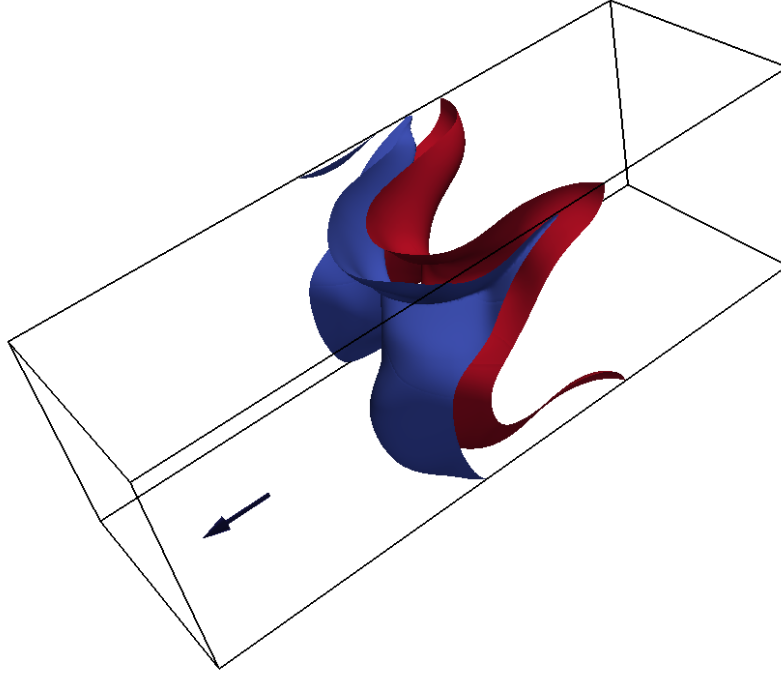
In order to inspect further the physical differences between the low- and high-intensity cases, three dimensional instantaneous snapshots at $t = 4\tau_0$ of the lowest and highest u' flame brushes are presented in Figure 3.4. The differences are striking. In the low u' case (Figure 3.4a, above), the leading edge $c = 0.01$ isosurface (coloured blue) and the trailing edge $c = 0.99$ isosurface (coloured red) are close to and roughly parallel to each other: the flame brush is thin. Moreover, the wrinkles scale with the domain size $\ell_w \sim \mathcal{O}(L)$. Similar large-scale wrinkling was also observed previously in laminar flame simulations of low-Karlovitz flame-vortex interaction (Poinsot et al., 1991b).

In contrast, the high u' flame brush (Figure 3.4b, below) has an extremely irregular and fragmented leading edge. Only a few large-scale wrinkles are noticeable (analysed quantitatively later). The instantaneous flame surface consists instead of many small-scale wrinkles $\ell_w \ll \mathcal{O}(L)$. The trailing edge is also highly wrinkled, but the size of these wrinkles is larger than those on the leading edge. The two edges of the flame brush are much farther apart than in the low u' case. These images resemble DNS results obtained for premixed single-step flames with $u' \approx 35s_L$ in the BRZ regime by Poludnenko and Oran (2011). This sharp contrast between the two instantaneous flame brushes illustrates visually the relationship between u' and the dominant scale of flame wrinkling ℓ_w .

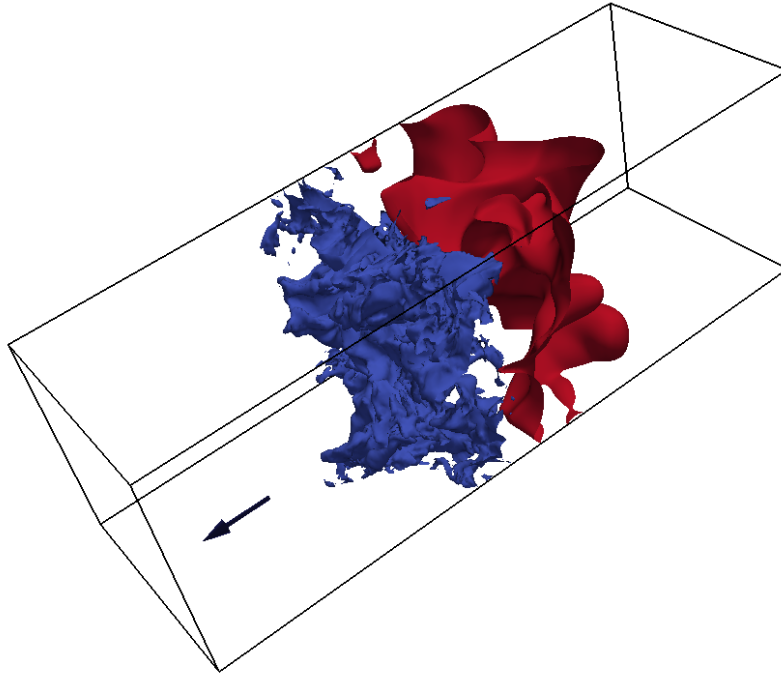
Flame brush edges

In Figure 3.4, the effects on the leading edge appear to be different from those on the trailing edge. A quantitative analysis of these surfaces is presented in Figure 3.5. Distributions of mean curvature h_m and curvature shape factor S_h are shown for low-intensity (black lines) and high-intensity (red lines) instantaneous flame brush edges. The leading edge (solid lines) has been taken as the $c = 0.01$ contour and the trailing edge (dashed lines) has been taken as the $c = 0.99$ contour. Previous DNS studies have adopted related definitions with slightly different choices of progress variable contour values (Lipatnikov and

3. Parametric Simulations of the Bending Effect



(a) Lowest intensity case I: $u' = 1.5s_L$



(b) Highest intensity case V: $u' = 30s_L$

Figure 3.4 Instantaneous snapshots of the turbulent flame leading edge $c = 0.01$ (coloured blue) and trailing edge $c = 0.99$ (coloured red) in cases with the lowest and highest u' , respectively. The arrow indicates the direction of flame propagation.

3.2. Recorded effects of turbulence intensity

Chomiak, 2002; Driscoll, 2008). It has been verified in the present cases that the precise choice does not have a significant effect on the statistics obtained.

Mean curvature statistics

Figure 3.5a shows a comparison of distribution of mean curvature given by $h_m = (h_l + h_u)/2$, the mean of local principal curvatures h_l and h_u , for the flame surfaces shown in Figure 3.4. The low- u' flame brush edges (black lines) exhibit little variation in h_m about the mean in comparison to the broad range of mean curvatures observed in the PDF for the high u' case (red lines). This shows that the flame surface is wrinkled at smaller scales at higher intensities; i.e. the scales of flame surface wrinkling are inversely related to the intensity of turbulence. In both cases, however, the mean value of mean curvature is close to zero for both leading (solid lines) and trailing edges (dashed lines). In the higher u' case, the peak probability of h_m occurs closer to zero than in low u' for both edges. This represents quantitatively the reduced large-scale curvature in the higher u' case noticed qualitatively in Figure 3.3 and Figure 3.4.

Furthermore, in the low- u' case (black lines in Figure 3.5a), the leading edge (solid black line) has a high likelihood of positive mean curvature – the

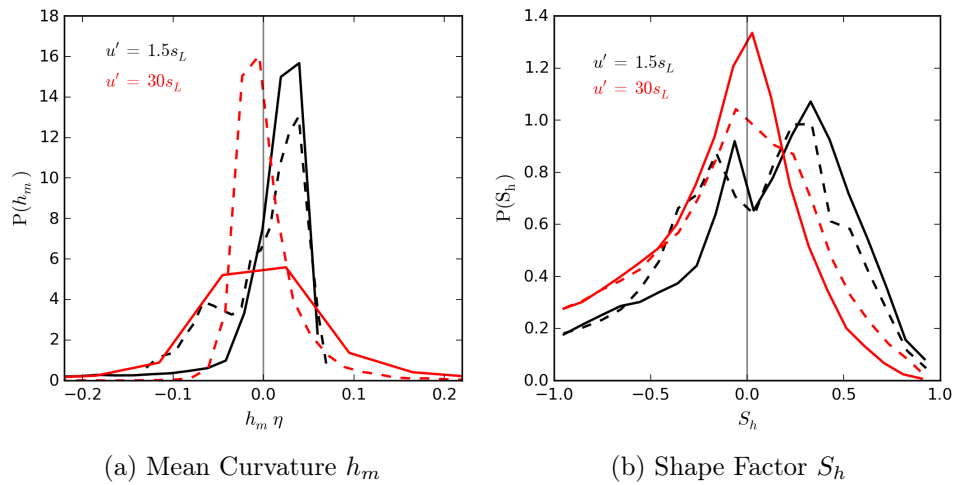


Figure 3.5 Distributions of the instantaneous mean curvature h_m and curvature shape factor S_h for the leading edge (solid lines) as well as trailing edge (dashed lines) surfaces in cases I and V (black and red lines, respectively).

3. Parametric Simulations of the Bending Effect

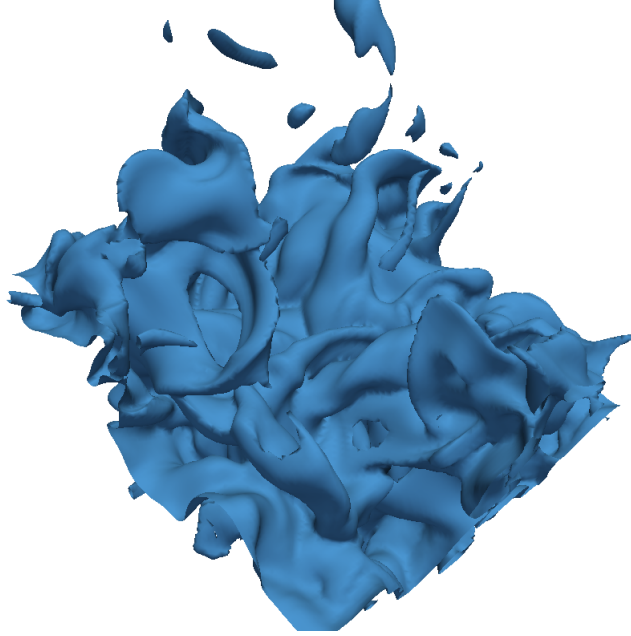
trailing edge (dashed black line) follows this distribution except for a slightly higher probability of negative curvature. In the high u' case (red lines), both leading as well as trailing edges have significant probability of negative mean curvature. The distribution of h_m on the trailing edge in the high u' case (dashed red line in Figure 3.5a) resembles the distribution on the leading edge of the low u' case (solid black line in Figure 3.5a) but with the mean value negative $\langle h_m \rangle < 0$.

Curvature shape factor statistics

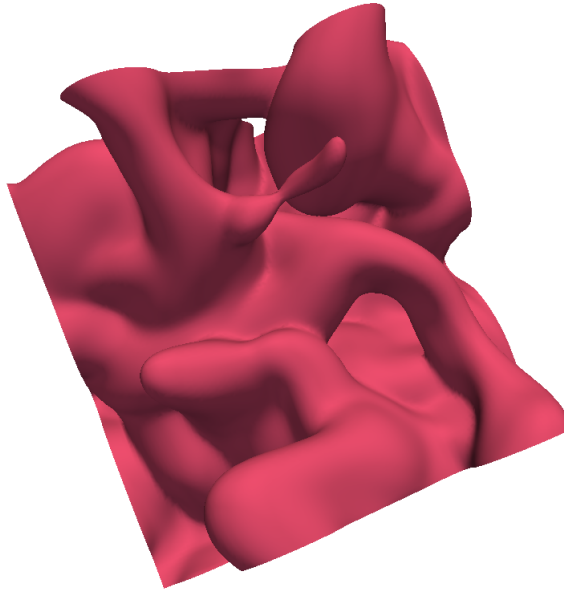
Figure 3.5b presents statistics of the curvature shape factor $S_h = h_l/h_u$ defined as the ratio of the minimum (h_l) and maximum (h_u) local principal curvatures by magnitude. Broadly, three shapes are captured: a) $S_h = 1$ represents locally spherical topology, b) $S_h = 0$ represents cylindrical topology, and c) $S_h = -1$ represents saddle shapes. These topologies are evident upon closer visual examination of the flame brush surfaces in Figure 3.4.

The wrinkles in the low u' flame brush (pictured in Figure 3.4a) form smooth and rounded ridges. Notably, the wrinkles do not protrude into the reactants or products but instead are gently warped in between. No “finger”-like structures have been seen here such as those observed more recently elsewhere (Lipatnikov et al., 2015). Since the trailing edge is parallel to the leading edge in this case, both surfaces have a similar distribution $P(S_h)$ (black lines in Figure 3.5b). Except for a small probability of saddle shapes ($S_h = -1$), the surfaces tend to have cylindrical topology ($|h_l| \ll |h_u|$) as is apparent in the large-scale thin rounded ‘folds’ in Figure 3.4a described earlier. This distribution of S_h has been noted previously in the simulation of material surfaces evolving in turbulence (Pope et al., 1989). It has also been observed more recently in the DNS of a slot-jet premixed flame in shear turbulence (Griffiths et al., 2015). A non-negligible probability of spherical shapes $S_h = 0$ is noted here in addition.

Spherical and ellipsoidal shapes with $h_l, h_u > 0$ are less common in high u' flames (red lines in Figure 3.5b) as opposed to the low u' flames (black lines). Instead, the high u' flame brush shows a greater probability of saddle-like



(a) Leading edge, $c = 0.01$



(b) Trailing edge, $c = 0.99$

Figure 3.6 Magnified view of the instantaneous leading edge (blue) and trailing edge (red) surfaces at $t = 4\tau_0$ as computed for case V with $u' = 30s_L$.

(given by $S_h \approx -1$) as well as of cylindrical ($S_h \approx 0$) shapes. Unlike the mean curvature PDFs, the distributions of $P(S_h)$ on the trailing edge of the high u' case (dashed red line in Figure 3.5b) is not similar to that on the leading edge of the low u' case (solid black line in Figure 3.5b).

3. Parametric Simulations of the Bending Effect

The topological features of the high u' case are inspected further in Figure 3.6 using a magnified view of the surfaces. The leading edge (coloured blue in Figure 3.6a) is highly convoluted and consists mainly of twisted ‘folds’ and the edges of these folds have a locally cylindrical topology. The sides of these folds are twisted at scales larger than the maximum principal curvature at the edge. Evidently, these folds contribute to the increased probability of $S_h = 0$ (cylindrical shapes) and $S_h < 0$ in the high u' distribution in Figure 3.5b. The relatively smooth trailing edge consists of long extended ‘fingers’ instead. The fingers have spherical tips which contribute to $S_h \approx 1$; the sides of these fingers are cylindrical, and the base forms a saddle shape. Some of the fingers merge into each other and form large-scale toroidal structures. Ongoing work is focused on investigating further the preference for these topological shapes.

Reaction zone contours

Evidently, the 20-fold increase in u' from case I to case V has a marked influence on the turbulent flame brush. The topological observations noted above may suggest that the internal turbulent flame structure might also differ markedly. In Figure 3.7, reaction rate contours are shown (panels above) using black and white shades in axial sections of the domain. Progress variable contours (black lines) shown alongside indicate that reaction $\dot{\omega} \neq 0$ is confined to thin regions between $c = 0.5$ and $c = 0.99$. At higher u' (Figure 3.7b), this zone of reaction appears broadened yet it remains confined to within the same contour lines. The reaction rate scatter $\dot{\omega}(c)$ shown below in Figure 3.7 indicates only slight deviations from the laminar flamelet profile (red line). The reaction rate peak occurs at $c \approx 0.8$, exactly as for a flamelet. Even for the highest u' flame (Figure 3.7d), a magnified view of the scatter reveals very minor differences from the flamelet profile. In other words, the reaction zones are not affected even though the surface topology changes drastically.

In Figure 3.8, 3D contours of the progress variable isosurface $c = 0.8$ are shown to emphasise this point further. In the backdrop, slices of the reaction rate $\dot{\omega}(\mathbf{x})$ have been shown to reveal the reaction profile alongside the convoluted surface. In the low u' flame (above), the $c = 0.8$ isosurface is attached

3.2. Recorded effects of turbulence intensity

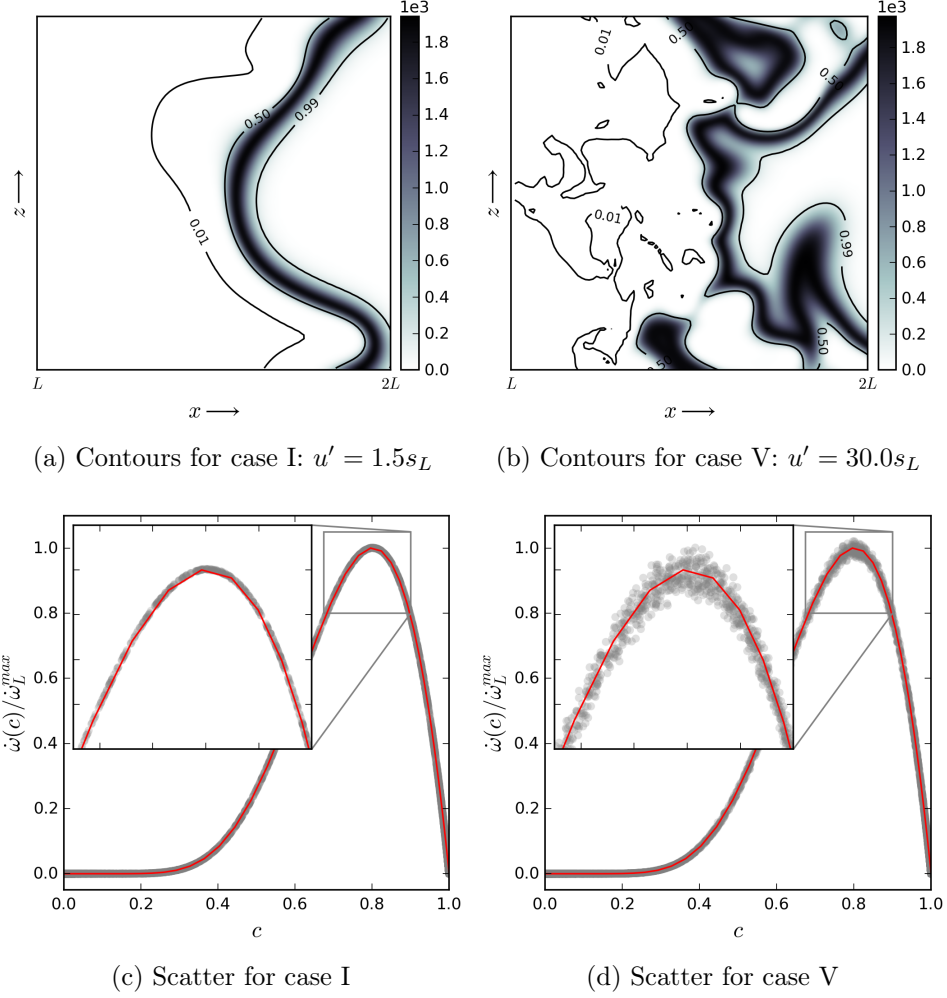
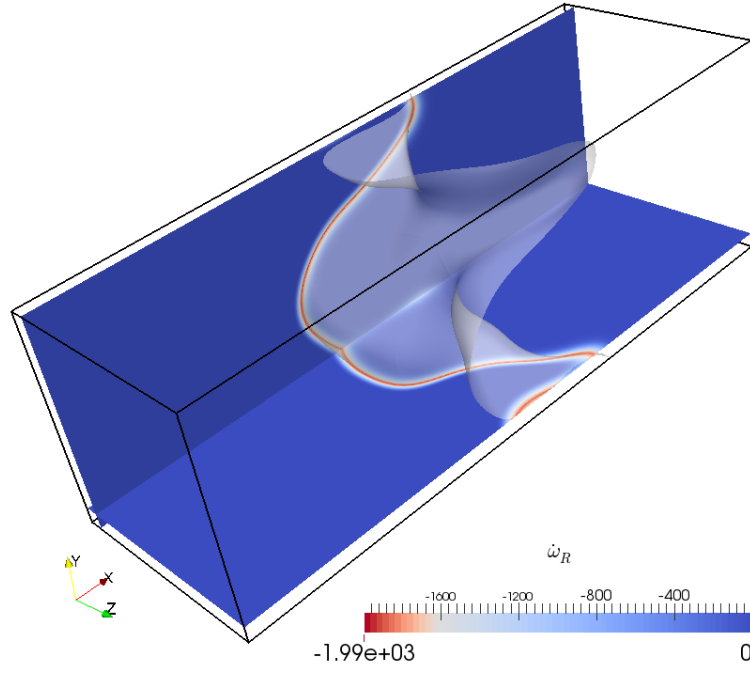


Figure 3.7 Reaction rate contours $\dot{\omega}(x, z; y = 5L/6)$ in cropped axial slices of the domain (above) and reaction rate scatter $\dot{\omega}(c)$ across the entire domain (below) at $t = 4\tau_0$ for cases I and V.

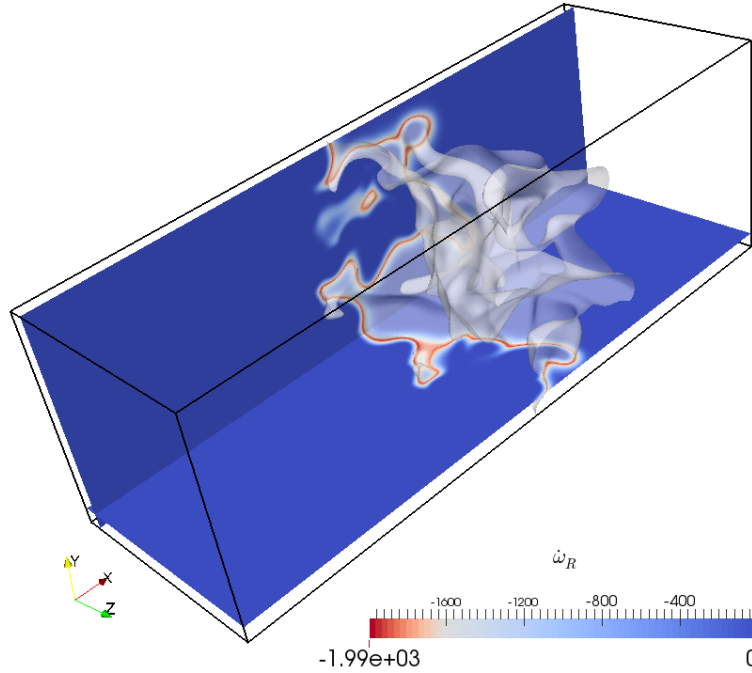
to the reaction zone as expected. This continues to be the case even in the highest u' case (below) where the $c = 0.8$ isosurface undergoes considerable wrinkling. The reaction rate contours (visible as a thin red band in the slices) continue to remain smooth and connected with the exception of minor local variations due to occasional flame self-intersections.

Both visual and statistical assessments presented here indicate clearly that even though the turbulent flame brush is affected severely under increasing u' , the reaction zone (i.e. the region corresponding to $0.7 < c < 0.9$) retains a laminar flamelet structure even up to $u' = 30s_L$. These observations, therefore,

3. Parametric Simulations of the Bending Effect



(a) Case I: $u' = 1.5s_L$.



(b) Case V: $u' = 30.0s_L$.

Figure 3.8 Progress variable isosurface $c^* = 0.8$, corresponding to the peak reaction rate, in the lowest and highest intensity cases. Axial sections of the domain show the variation of reaction rate $\dot{\omega}$ across the domain.

conform with the scaling arguments for the TRZ regime (Peters, 1999) as discussed in Section 1.2.2. This provides an indication that flame propagation and the associated turbulent burning velocity s_T is not affected by quenching since that would necessarily cause the reaction zone to change.

3.2.2 Computation of turbulent burning velocity

The turbulent burning velocity s_T is calculated as the integral

$$s_T \equiv \frac{\dot{m}_F}{\rho_u Y_{u,F} A_0} = -\frac{1}{\rho_u Y_{u,F} A_0} \int_V \dot{\omega}_F dV, \quad (3.7)$$

thereby defining s_T as the global fuel consumption speed expressed using the mass transformation rate $\dot{m}_F$ or, equivalently, the integrated reaction rate $\dot{\omega}_F$ of fuel in an unburned premixture of density ρ_u and fuel mass fraction $Y_{u,F}$; finally, A_0 is the flow cross-section area. Here, F denotes the fuel which corresponds to the unburned reactant mixture.

In each of the simulations, s_T is computed using the expression above. It is observed that s_T grows with time up to a period of $t \sim 2\tau_0$ after which the value of s_T oscillates about a value specific to the specific case. In Figure 3.9, the computed values for turbulent burning velocity at $t = 4\tau_0$ are shown for each of the cases. The inset shows the temporal variation for a typical case; oscillations after a certain period of time are within a small error margin of the value at $t = 4\tau_0$ (grey line and circle) used to plot the variation of s_T across the dataset. Since all parameters other than u' are fixed across the set of simulations, the graph in Figure 3.9 shows the curve $s_T(u')$. Clearly, the bending effect has been captured – the deviation from linear enhancement of s_T is prominent for cases IV and V with $u' > 10s_L$.

The normalized turbulent burning velocity s_T/s_L values shown in Figure 3.9 are similar in order of magnitude $\mathcal{O}(s_T/s_L)$ to the values obtained in previous DNS studies (Aspden et al., 2008; Poludnenko and Oran, 2011; Savard and Blanquart, 2015). The order of magnitude $\mathcal{O}(s_T/s_L)$ obtained using DNS is typically smaller than that obtained experimentally (Bradley, 1992; Shy et al., 2000b; Gülder and Smallwood, 2007). For example, stoichiometric methane-air

3. Parametric Simulations of the Bending Effect

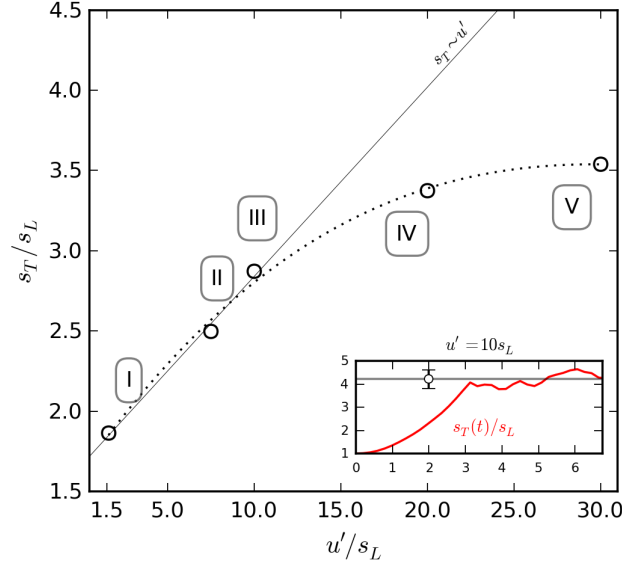


Figure 3.9 Computed variation of the normalized turbulent burning velocity s_T/s_L with normalized turbulence intensity u'/s_L . The inset shows a typical variation of $s_T(t)$ and the corresponding value of s_T chosen from this variation.

flames have been considered experimentally in downward propagating flames (Shy et al., 2000b) up to $u'/s_L \approx 15$. The corresponding measurements indicate $s_T/s_L \approx 10 - 12$; i.e. a few times the predictions obtained using DNS. These differences may arise due to the differences in Lewis numbers of chemically reacting species between experimental and simulated flames. Perhaps more importantly, these differences may be due to the dependence of s_T on the geometry. In other words, the relatively low values of s_T/s_L observed here in comparison to experiments could be related to the small geometrical extent of the DNS. The relatively larger integral length scales $\ell_0 \approx 10 - 20$ cm in the experiments of Shy et al. (2000b) are as yet unable to be considered by DNS. Nevertheless, the present DNS dataset provides the ability to investigate the mechanism of the observed bending effect.

3.3 Summary: on the bending effect recorded

A parametric DNS dataset has been designed with due considerations of the notion of the bending effect. The most basic conditions that can reproduce the bending effect are prescribed upon an initially-laminar stoichiometric methane-

3.3. Summary: on the bending effect recorded

air flame. All controllable thermo-chemical and turbulence parameters are maintained across the set of simulations; these include the flame configuration and domain size as well as numerical parameters such as the mesh spacing. The turbulent intensity u' is the only parameter varied across the simulations. The curve $s_T(u')$ thus obtained records a bending effect which is, therefore, a consequence of increasing u' only.

The present thermo-chemical framework relies on the twin assumptions of unity Lewis number and single-step chemistry. This has helped simplify the description and analysis and narrow the potential causes of bending to kinematic rather than chemical effects such as local quenching. Since the framework indeed records a bending effect (Figure 3.9), it follows that the mechanism responsible for the bending effect recorded must be kinematic and not chemical in nature. It is plausible that the underlying mechanism in the present dataset may also operate in flames with more complicated thermo-chemical properties although the significance of such a mechanism remains to be evaluated by using precisely such a framework (see Chapter 6). In the following two chapters, the validity of Damköhler's hypotheses is investigated in the present DNS dataset with the objective of highlighting the mechanism of the bending effect recorded.

Chapter 4

Damköhler's First Hypothesis

In this chapter, the validity of Damköhler's first hypothesis (DH1) is investigated within the bending effect recorded in the previous chapter. Recall the modified form of DH1

$$\frac{s_T}{s_L} = I_0 \frac{A_T}{A_L} \quad (4.1)$$

where I_0 the so-called stretch factor is a function of Le . The equivalent laminar flame surface area A_L is the square cross-section area of the domain. Hence, given a fuel-air mixture, the primary task that remains to validate DH1 is to compute the turbulent flame surface area A_T . This computation is pursued within the framework of the Flame Surface Density (FSD) approach. The FSD approach was discussed in Chapter 1; it provides a measure of the flame surface area A_T . Moreover, it provides the factors influencing this measure; namely, the stretch rate components. Hence this allows for a conceptualisation of the bending effect in terms of the stretch rate components: strain rate and curvature propagation. In the passages below, relevant concepts are discussed followed by its application to the bending effect recorded.

4.1 Flame Surface Density approach

Any progress variable isosurface $c = c^*$ within the turbulent flame brush may be considered as a constant-property material surface (Pope, 1988) and may hence be used for the computation of A_T . In the framework of the FSD ap-

4. Damköhler's First Hypothesis

proach, each point on such an instantaneous surface is specified by an infinitesimal area δA within a fixed infinitesimal volume δV . The local surface-to-volume ratio may then be defined as

$$\Sigma'(\mathbf{x}, t; c = c^*) \equiv \frac{\delta A(\mathbf{x}, t; c = c^*)}{\delta V}, \quad (4.2)$$

at each point $\mathbf{x}|_{c=c^*}$ on the surface. The local surface area δA may be calculated using components of the local gradient $\nabla c(\mathbf{x}, t)$ of the isosurface. It has been found (Boger et al., 1998), however, that in the limit of LES filter width $\lim_{\Delta \rightarrow 0} \Sigma' = |\nabla c|$. This approximation holds in DNS because $\Delta \rightarrow 0$ necessarily. Hence, $\Sigma' = |\nabla c|$ in the present study.

The quantity Σ' is a local measure of the degree to which a progress variable isosurface $c = c^*$ is wrinkled because points on the surface that have a larger surface area within a local infinitesimal volume necessarily have higher local mean curvatures. At the same time, it is noteworthy that the progress variable gradient ∇c is high only where reaction rate is non-zero. Hence, the flame surface-to-volume ratio when defined using the progress variable gradient $\Sigma' \equiv |\nabla c|$ combines two aspects – the physical: surface wrinkling and the chemical: reaction rate.

Generalised FSD profiles

The expectation of Σ' is denoted by Σ which represents the mean flame surface to volume ratio. It is calculated here as

$$\Sigma(\mathbf{x}, t) \equiv \langle \Sigma'(\mathbf{x}, t) \rangle = \langle |\nabla c(\mathbf{x}, t)| \rangle, \quad (4.3)$$

and it is, therefore, a statistical quantity – also known as Flame Surface Density (FSD) – that is often measured in experiments (Driscoll, 2008), and is central to combustion modelling (Trouvé and Poinso, 1994; Veynante and Vervisch, 2002). Indeed, the transport of this quantity was discussed earlier in Section 1.2 as a modelling framework. The averaging in Equation 4.3 may be performed temporally over different ensembles or spatially over statistically homogeneous regions in the domain. In the present study, the averaging is performed at a

4.1. Flame Surface Density approach

specific instant ($t = 4\tau_0$) over span-wise planes of the domain which provide a statistically homogeneous sample. In such statistically-stationary flames, the FSD is expected to be a function $\Sigma(x)$ of axial distance only.

The profile $\Sigma(x)$ is compared with the laminar profile (red line) in Figure 4.1a for three cases of the present dataset (I: $u' = 1.5s_L$, III: $u' = 10s_L$ and V: $u' = 30s_L$). The broadening of the $\Sigma(x)$ profile with increasing u' indicates that the flame surface extends over a larger portion of the domain, i.e. the mean turbulent flame brush thickens with increasing u' . This is in agreement with the images shown earlier in Figure 3.4 as also with experimental measurements of FSD discussed by Driscoll (2008).

Conventionally, the variation of FSD over mean progress variable $\bar{c}$ values is compared with the laminar flamelet FSD to assess the effects of turbulence on the flame brush. Figure 4.1b shows Σ as a function of $\bar{c}$ for three representative cases (I, III and V) exhibits a peak in Σ close to $\bar{c} \approx 0.6$ similar to the laminar flamelet profile (blue line). In comparison, the Σ peak shifts towards a lower value of $\bar{c}$ at $u' = 10s_L$ (dashed line). At higher intensities still (dotted line), the peak shifts further towards the leading edge. While the figure includes only three of the cases for clarity, the remaining cases in the

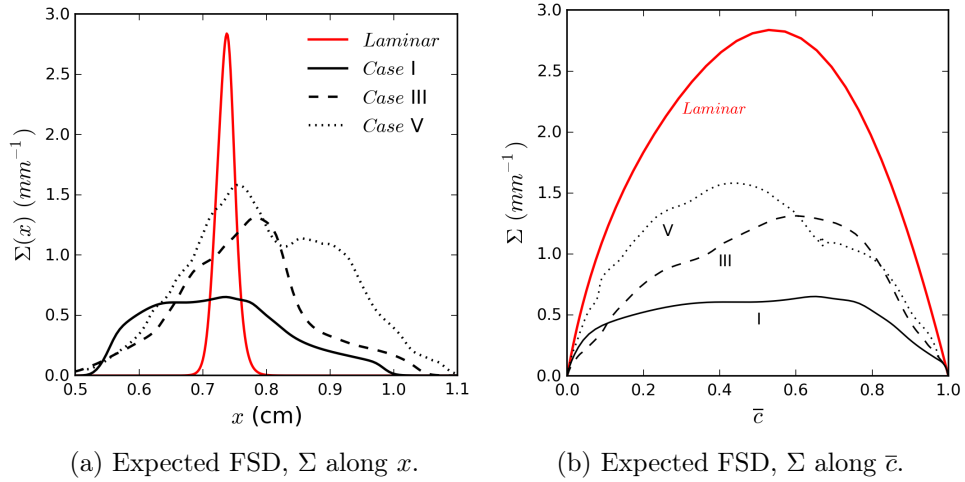


Figure 4.1 Expectation of FSD Σ as a function of the axial coordinate x (left) and mean progress variable $\bar{c}$ (right) for three cases (I, III, and V) spanning the dataset. The laminar flamelet solution (red line) is shown for comparison.

4. Damköhler's First Hypothesis

dataset also follow this trend. Such a shift in the peak of Σ with increasing u' has been reported in a recent experimental study (Kheirkhah and Gülder, 2015) where it is linked with counter-gradient and gradient transport regimes. Further inspection of Figure 4.1b shows that the FSD values for turbulent flames are lower than the laminar flamelet values. This again conforms with the measurements of the aforementioned experimental study (Kheirkhah and Gülder, 2015). However, the trend observed here is that the FSD values for turbulent flames increase with increasing u' which stands in contrast to the previous measurements (Kheirkhah and Gülder, 2015).

Scatter in progress variable space

A key challenge in the analysis of turbulent premixed flames is to compare the local internal flame structure with a 1D laminar flamelet profile. Due to wrinkling of the flame surface, the surface normal vector is not always aligned with the streamwise direction. It is common practice to sample over span-wise sections instead of progress variable isosurfaces. The section-sampling method is often applied for evaluating mean profiles of Σ as a function of $\bar{c}^*$ obtained by averaging $\Sigma'(x, y = y^*, z = z^*)$ throughout a slice which corresponds to an av-

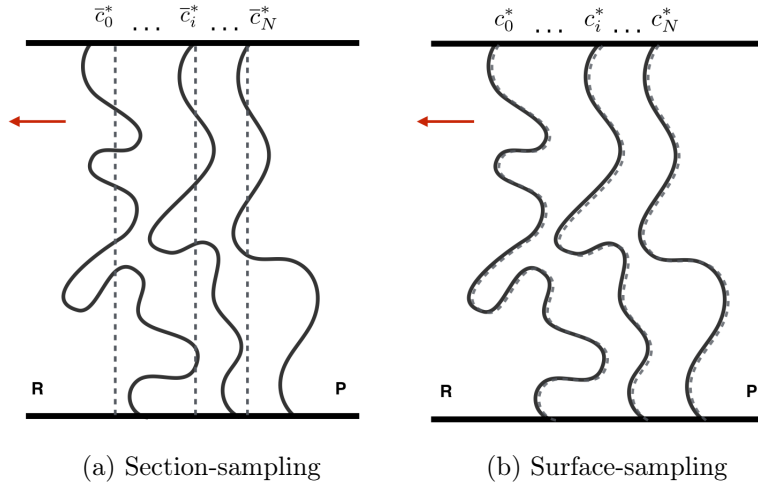


Figure 4.2 Illustration of sampling methods (dashed lines). Left: sampling over spanwise sections of the domain across the mean turbulent flame brush ($\bar{c}_0^* < \bar{c} < \bar{c}_N^*$). Right: sampling over instantaneous progress variable c isosurfaces (solid lines) within the instantaneous turbulent flame brush ($c_0^* < c < c_N^*$).

4.1. Flame Surface Density approach

erage progress variable $\bar{c}^*$ (illustrated in Figure 4.2a). Since wrinkling changes the direction of the local structure from that of the slices, the slice-sampling method can provide a misleading comparison between the local turbulent flame structure and the laminar flamelet structure. A similar concern was expressed previously (Shepherd et al., 2002) in order to avoid incorrect assessments of “flame broadening” relying on slice-sampling. Hence, $\Sigma'(x; y^*, z^*)$ is not an appropriate benchmark of comparison with the laminar flamelet profile $\Sigma'_L(x)$ even in the statistically 1D case considered here.

Instead, the scatter of points over the progress variable space $\Sigma'(c)$ makes for a more direct comparison with the laminar flamelet profile. Geometrically, this method is analogous to sampling over progress variable isosurfaces $c = c^*$ as shown in Figure 4.2b and is, therefore, termed surface-sampling. The comparison with the laminar flamelet profile is direct and any deviations from the flamelet profile can be noticed straightforwardly. Hence, even though the exact spatial point corresponding to a given value of FSD may not be clear in the scatter, this is the apt and preferred method of comparison of turbulent local internal structure with laminar flamelets.

The scatter $\Sigma'(c)$ obtained using the surface-sampling method is presented in the left column in Figure 4.3 for the three cases I, III and V. For the low u' case I, the overall Σ' profile is not disturbed noticeably in comparison to the laminar flamelet profile $\Sigma'_L = |\nabla c|_L$ (red line). As u' is increased, the deviation of Σ' from the flamelet profile at any given value of c (isosurface) increases. For $u' \geq 10s_L$, large deviations from the flamelet profile are evident close to the leading edge $c \leq 0.4$. The reaction zone $c \geq 0.7$, however, is much less affected under increasing u' . Even for the highest u' flames, only minor deviations are visible. These correspond to the minor deviation in reaction rate profile observed in Figure 3.7. This implies that the flame brush tends to be wrinkled by length scales that do not disturb significantly the internal progress variable gradient ∇c in the reaction zone.

Instantaneous slices of $\Sigma'(x, y = 5/6L_y, z = 5/6L_z)$ at $t = 4\tau_0$ are shown alongside on the right column in Fig. 4.3 for the same three cases. The extent of the turbulent flame brush is shown by overlaying progress variable con-

4. Damköhler's First Hypothesis

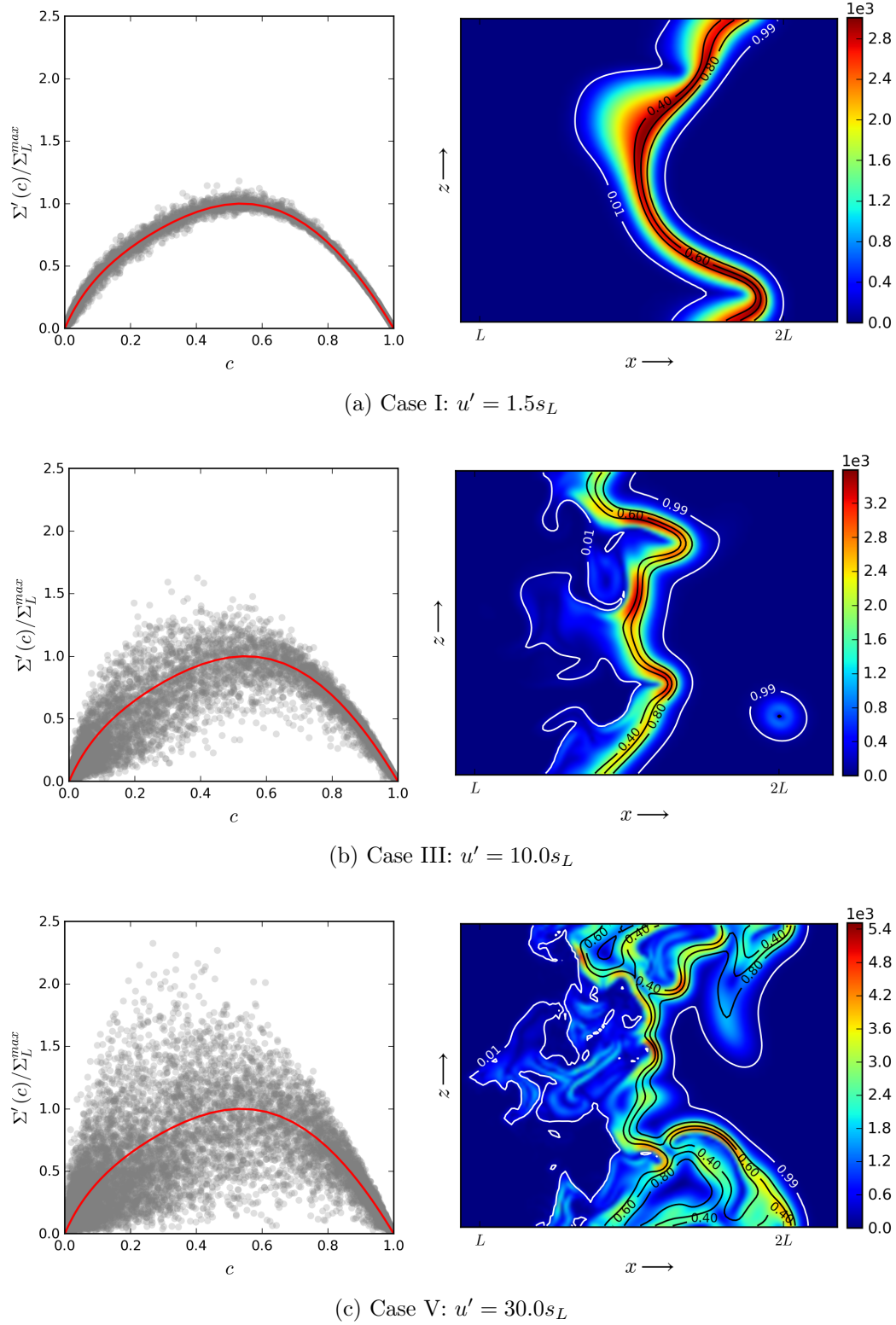


Figure 4.3 Instantaneous normalized $\Sigma'(c)$ scatter (left column) at $t = 4\tau_0$ compared with the laminar flamelet profile (red line). Corresponding contours of $\Sigma'(\mathbf{x})$ (right column) are shown in an axial section overlaid with progress variable contours (black and white lines).

4.1. Flame Surface Density approach

tours in white. The contours in black represent the interior flame structure $0.4 < c < 0.8$. The colour bars show clearly that the peak magnitude Σ'_{max} (red colour) in a given slice increases with u' . Since this magnitude is higher than the that in laminar flames, these regions indicate steepening of the gradients and, thereby, thinning of flame thickness by turbulence. In addition, the spatial region where the peak is observed appears to be increasingly fragmented, occurring selectively in regions of negative curvature (note: the flame is propagating to the left). This localisation of $\Sigma'_{max} = |\nabla c|_{max}$ has been attributed to a preferential “tight packing” of progress variable contours due to turbulence (Poludnenko and Oran, 2011). Elsewhere (Steinberg et al., 2012), the same behaviour is referred to as the preferential alignment of the compressive eigenvector of strain rate with the c gradient. Further investigation of flame surface topology will help establish reasons for this observation.

4.1.1 Computation of flame surface area

As discussed in the previous chapter as well as in the passages above, the reaction zone appears to retain integrity across the entire dataset. Hence, the turbulent flame surface area A_T may be estimated to within a scaled constant using an isosurface within the reaction zone (Filatyev et al., 2005; Driscoll, 2008). In the FSD approach, the area A_T can be expressed as the volume integral

$$A_T = \int_{-\infty}^{\infty} \Sigma' \delta(c - c^*) dV, \quad (4.4)$$

of the surface-to-volume ratio Σ' conditioned on the progress variable value $c = c^*$ corresponding to the reaction zone isosurface considered. Presently, this is chosen as the peak reaction rate isosurface, i.e. $c^* = 0.8$, but it was found that any value $0.6 < c^* < 1.0$ corresponding to the reaction zone is appropriate. The Dirac delta function is evaluated by conditioning the integral to the spatial region corresponding to $c = c^* \pm 0.01$. Hence, the DH1 expression

$$\frac{s_T}{s_L} = I_0 \frac{A_T}{A_L} = I_0 \frac{1}{A_L} \int_{-\infty}^{\infty} \Sigma' \delta(c - c^*) dV \quad (4.5)$$

4. Damköhler's First Hypothesis

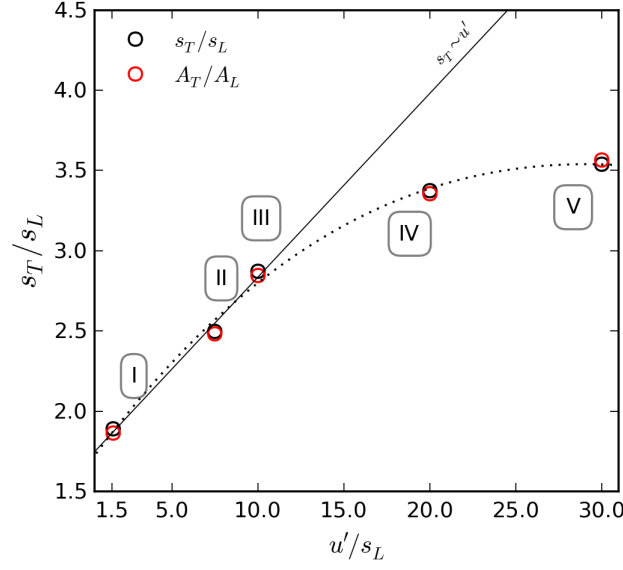


Figure 4.4 Computed flame surface area ratio A_T/A_L compared with normalised turbulent burning velocity s_T/s_L in the recorded bending effect.

may be validated using the conditioned Σ' volume integral. This approach may only be followed in DNS studies where the local progress variable corresponding to the local FSD Σ' is available for computation. Hence, this equation is used here and is consistent with with other DNS studies (Aspden et al., 2011; Lapointe et al., 2015; Poludnenko, 2015). In experimental studies (Bagdanavicius et al., 2015), however, this approach using Equation 4.5 is often not feasible. Therefore, in such studies, a mean flame surface area to volume ratio of the entire flame surface is computed (also, confusingly, denoted Σ in such studies) and integrated over the entire volume to calculate A_T . These differences in the computation procedure are considered in Chapter 6 where comparisons are being made with experiments in the explosion vessel references above.

In Fig. 4.4, it is seen that the ratio of the reaction zone surface area $A_T(c^* = 0.8)$ to that of the laminar surface area A_L indeed matches closely the burning velocity ratio s_T/s_L . Hence, Damköhler's first hypothesis (Equation 1.4, Equation 4.1) is valid for the entire range of u' simulated with the stretch factor $I_0 \approx 1$ throughout. Any deviations in s_T/s_L from A_T/A_L are within a few percent of the s_T/s_L value as was also noted by previous DNS works (Sankaran et al., 2007; Poludnenko and Oran, 2011). Even in the highest u' case, which lies at the TRZ/BRZ regime boundary, A_T predicts accurately

the burning velocity s_T . Such a close correspondence of s_T/s_L and A_T/A_L stands in contrast to some recent experiments in “V” and Bunsen configurations (Filatyev et al., 2005; Gülder and Smallwood, 2007; Bradley et al., 2013). Ongoing work (Ahmed et al., 2017) is aimed at understanding the role of turbulence length scale ℓ_0 and flame configuration in effecting these differences.

Preliminary validation with detailed chemistry

The validity of DH1 throughout the bending effect carries significant implications. The present framework considers a simplistic 1-step chemical kinetic model elaborated in Chapter 2. In order to verify the scope and validity of further analysis conducted on this dataset, comparisons were made (Nivarti and Cant, 2015b) using a detailed 25-step chemical kinetic model due to Smooke and Giovangigli (1991) as discussed briefly in Chapter 2 and elaborated in Chapter 6. Parametric simulations of flame propagation using this detailed model have not been feasible due to high computational expense. Therefore, the case III with $u' = 10s_L$ was chosen as a point of verification. Using the identical flame configuration, ICs and BCs a case was set up with the only difference that the initial laminar flame was described using the detailed chemical kinetic model.

Results of the chemical mechanism comparisons are shown in Figure 4.5. A snapshot at $t = 4\tau_0$ of the propagating flame as recorded using 1-step chemistry in the present dataset is shown in Figure 4.5a. In line with the discussions above, the pre-heat zone appears thickened (between the black progress variable contour lines 0.01 and 0.5), whereas the reaction zone (between contour lines 0.5 and 0.99) remains thin and the respective contour lines remain parallel to each other. The corresponding snapshot for detailed chemistry is shown in Figure 4.5b. The similarity with the 1-step chemistry simulation is striking. Most importantly, the reaction zone remains thin throughout, even though a similar degree of pocket formation is evident in both cases.

Investigating further, the time-evolving turbulent burning velocity $s_T(t)$ is plotted against the turbulent flame surface area $A_T(t)$ for both cases in Figure 4.5c. As expected from the discussions so far, the 1-step chemistry flame

4. Damköhler's First Hypothesis

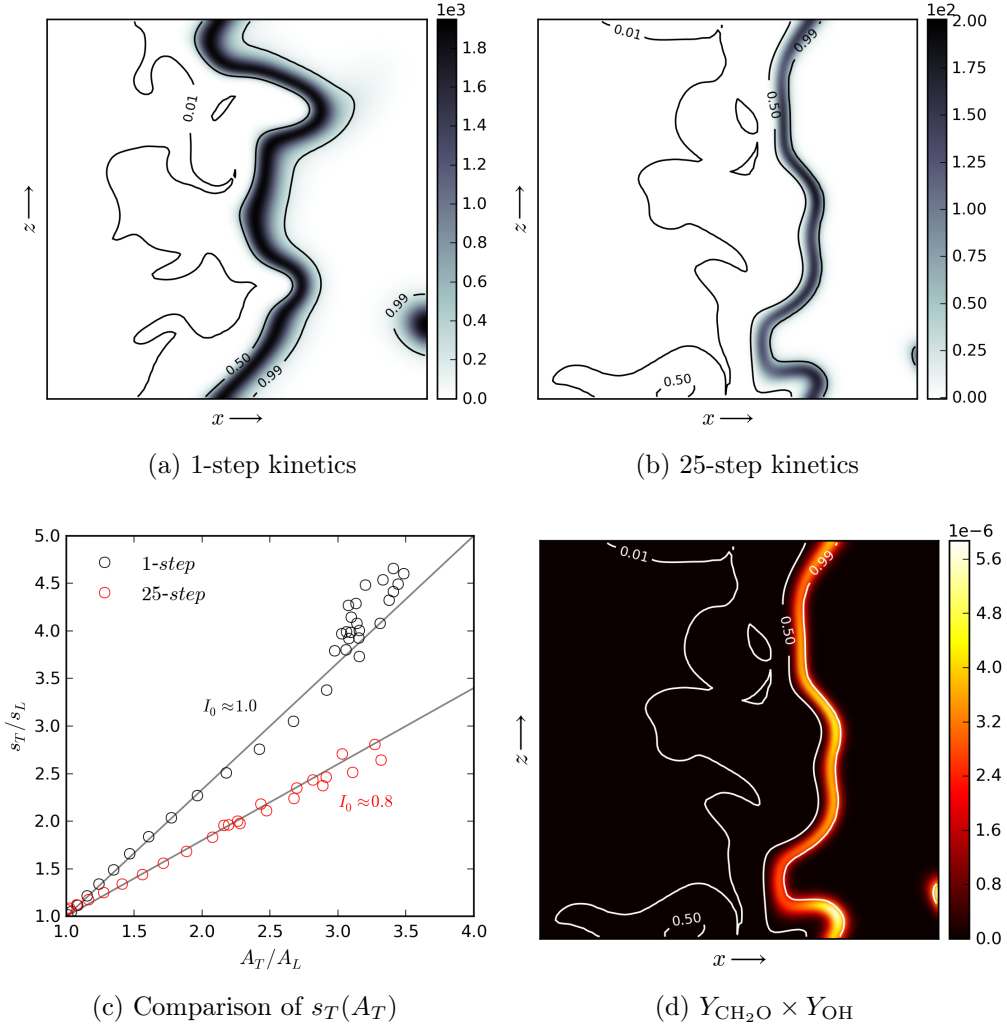


Figure 4.5 Comparisons of turbulent flame structure and propagation characteristics simulated using 1-step and 25-step reduced chemical kinetic models for case III with $u' = 10s_L$.

(black circles) displays conformance with Damköhler's first hypothesis (DH1) at all times. This corresponds to a stretch factor value $I_0 \approx 1$. The conformance with DH1 remains true, however, for the 25-step chemistry flame as well, with the only difference that the stretch factor $I_0 \approx 0.8$ is slightly lower in comparison. Qualitatively, the conformance with DH1 is also noted in the contours of heat release indicated using the product of mass fractions $Y_{\text{CH}_2\text{O}} \times Y_{\text{OH}}$. No signs of localised flame extinctions have been evident. These comparisons seem to suggest that differences in s_T recorded by adopting detailed chemistry models may be subject to thermo-diffusive effects which influence I_0 rather

than localised flame extinctions which influence the validity of DH1. Still, the study pursued in Chapter 6 aims to address comprehensively the flame propagation behaviour using detailed chemical kinetics. At present, however, this comparative study serves to give additional weight to the results obtained in the present dataset using single-step chemistry.

Based on the discussions above, it is apparent that the reaction zone retains globally its internal structure. DH1 is satisfied for all turbulence intensities within the dataset. Hence, the wrinkled turbulent reaction zone can be treated as an ensemble of locally-laminar reaction zones without serious loss of accuracy. This implies that the bending effect recorded within the dataset must also be explained in terms of a flamelet description of the turbulent flame. Further investigation of the FSD equation and its source-terms is carried out in order to find possible underlying mechanisms of the bending effect.

4.2 Stretch rate components

An equation for the turbulent transport of the local surface-to-volume ratio $\Sigma'(\mathbf{x})$ of a surface propagating in turbulence has been derived previously (Pope, 1988; Candel and Poinso, 1990) as

$$\frac{\partial \Sigma'}{\partial t} + \nabla \cdot (\dot{\mathbf{X}} \Sigma') = \dot{s} \Sigma' \quad (4.6)$$

where $\dot{\mathbf{X}}(\mathbf{x}) = \mathbf{u} + s_d \hat{n}$ is the total velocity of the point which propagates with displacement speed s_d along its normal $\hat{n}$ given by $\hat{n}(\mathbf{x})|_{c=c^*} = -(\nabla c / |\nabla c|)|_{c=c^*}$. Equation 4.6 shows that stretch rate $\dot{s}$ regulates the local production and destruction of surface-to-volume ratio $\Sigma'(\mathbf{x}, t > t^\circ)$ in proportion to the available local surface-to-volume ratio at a given instant t° . The role of the stretch rate is, therefore, investigated across the dataset. First, it is recalled that stretch rate $\dot{s}$ can be decomposed (Pope, 1988) into

$$\dot{s} = a_t + s_d h_m, \quad (4.7)$$

where a_t and $s_d h_m$ correspond to local tangential strain rate and local flame

4. Damköhler's First Hypothesis

propagation rate respectively. These are given by

$$a_t = \nabla \cdot \mathbf{u} - \hat{n} \hat{n} : \nabla \mathbf{u}, \text{ and} \quad (4.8)$$

$$h_m = \frac{1}{2} \nabla \cdot \hat{n}, \quad (4.9)$$

and the local surface normal $\hat{n}$ is defined (as above) to be positive in the direction of the unburned mixture. These individual components of the stretch rate source term are analysed in the following passages.

4.2.1 Statistics of strain and propagation terms

Tangential strain

The distribution of tangential strain rate a_t on the $c^* = 0.8$ isosurface is shown in Figure 4.6a. The strain rate has been normalized using the Taylor scale strain rate u'/λ . It is evident that turbulent straining of the flame surface occurs close to the Taylor length scale λ as suggested previously (Bradley, 1992; Bray and Cant, 1991). With increasing u' the Taylor scale strain rate u'/λ increases, so that the similarity of distributions implies that the prescribed tangential strain rate a_t increases in accordance. All the cases exhibit an ex-

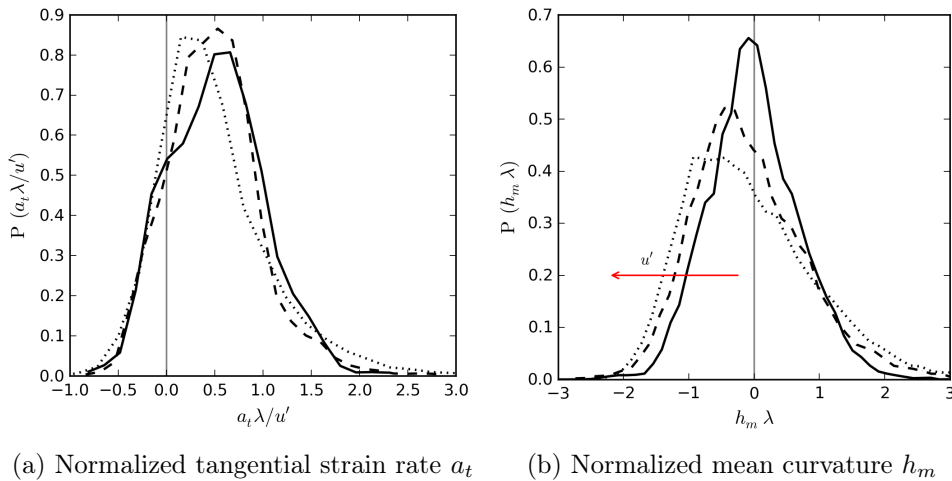


Figure 4.6 Distribution of strain a_t and curvature h_m over the peak reaction rate isosurface $c^* = 0.8$ for three cases (lowest u' : solid line, highest u' : dotted line) spanning the entire dataset.

tensional mean surface strain $\langle a_t \rangle_{c=c^*} > 0$ consistent with theory on turbulent transport of material surfaces (Pope, 1988) and with previous results on flame surfaces (Echekki and Chen, 1998; Chakraborty and Cant, 2007). Further, the distribution shapes are similar to those observed previously in lower intensities of turbulence (Bray and Cant, 1991) throughout the dataset.

Mean curvature

The variation of local mean curvature h_m of the $c^* = 0.8$ isosurface is shown in Figure 4.6b for the same three cases. For consistency with strain rate scaling, the Taylor length scale λ is chosen here as the scaling parameter. For all cases, the surface average of mean curvature $\langle h_m \lambda \rangle_{c=c^*} \approx 0$. With increasing u' , the likelihood of negative mean curvatures increases (indicated by red arrow). At the same time, the spread of the curvature distribution also increases. The shapes of these distributions also conform with previous observations (Bray and Cant, 1991). The variation of strain (as shown in Figure 4.6a) is contrary to the variation of curvature (as shown in Figure 4.6b) with increasing u' .

Configurations of strain and curvature

In order to further clarify the relationship between strain a_t and curvature h_m in the discussion above, it is important to note the configuration of strain and curvature components observed in turbulent premixed flames. The effect of strain rate a_t on surface stretch is direct: extensive strain generates surface area and compressive strain destroys it. The mechanism by which propagation rate $s_d h_m$ contributes to surface stretch, however, is more subtle. The propagation rate term only contributes if a wrinkle is formed – surface elements with no mean curvature do not generate surface area due to propagation.

The relationship between curvature and strain is investigated further in Figure 4.7. The correlation between h_m and a_t scaled using the Kolmogorov scale η and Taylor scale λ respectively are shown for low- and high-intensity flames. The negative correlation at low intensities (Figure 4.7a) is striking. Previous studies conform with this observation, indicating similarly that a_t and h_m are negatively correlated up to moderate values of turbulence (Peters

4. Damköhler's First Hypothesis

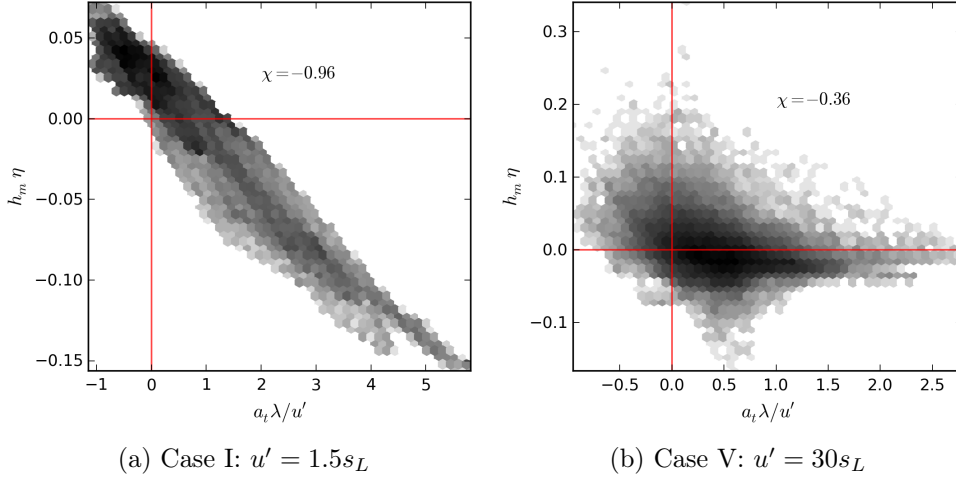


Figure 4.7 Joint probability distribution of strain rate a_t (scaled with Taylor scale strain rate u'/λ) and mean curvature h_m (scaled with Kolmogorov scale η) in the lowest and highest intensity cases.

et al., 1998; Chakraborty and Cant, 2004; Steinberg and Driscoll, 2009). The high-intensity case (Fig. 4.7b) continues to show a significant negative correlation although the correlation coefficient is lower. Hence, the effects of a_t and h_m act to oppose each other locally: for $h_m > 0$, strain rate is compressive ($a_t < 0$) and for $h_m < 0$, strain rate is extensive ($a_t > 0$). The underlying reasons for the preference of such configurations are being investigated presently.

It is emphasised that the mean curvature h_m is not a mean in the sense of Reynolds averaging. While the mean $h_m = 1/2(h_l + h_u)$ may be zero, the principal curvatures h_l and h_u that constitute the mean may not be zero. In such cases, the flame surface may have a net propagation effect which may contribute to a net stretch rate. Going back to Figure 3.6a, it is seen that a finite amount of the surface undergoes these forms of curvature. At present, we ignore this possible complication in flame surface propagation but it may be worthy of further investigation.

Displacement speed

In the overall stretch rate $\dot{s}$, the displacement speed s_d acts to regulate the propagation stretch effects of curvature h_m . According to Peters (2000), the expression for the displacement speed s_d of a point $\mathbf{x}$ on an isosurface $c = c^*$

is given by

$$s_d(\mathbf{x}; c = c^*) = \left[\frac{\nabla \cdot (\rho D \nabla c) + \dot{\omega}}{\rho |\nabla c|} \right]_{c=c^*}, \quad (4.10)$$

where D is the local molecular diffusivity. The first term $\nabla \cdot (\rho D \nabla c)$ in the numerator is molecular diffusion and the second term $\dot{\omega}$ is the reaction rate. Figure 4.8 shows profiles of displacement speed s_d at the isosurface $c^* = 0.8$ for the same three cases I, III and V spanning the lowest to highest turbulence intensity. In the lowest intensity case (solid line), a relatively narrow distribution of s_d/s_L about the expected value corresponding to the density ratio at this surface is evident. Under higher levels (dashed line) of turbulence intensity $u' = 10s_L$, the variance of $s_d|_{c^*=0.8}$ increases due to increased turbulent fluctuations experienced by the reaction layer. In the highest intensity case (dotted line), the variance spans a significantly larger range denoting the increased scatter due to turbulent fluctuations. In accordance, negative s_d becomes increasingly common in higher intensities of turbulence. This is in line with previous 2D DNS studies (Echekki and Chen, 1996; Peters et al., 1998).

The surface mean $\langle s_d \rangle_{c=c^*}$ is close to the value expected for a laminar flamelet at the isosurface $c^* = 0.8$ for case I (solid line in Figure 4.8). A

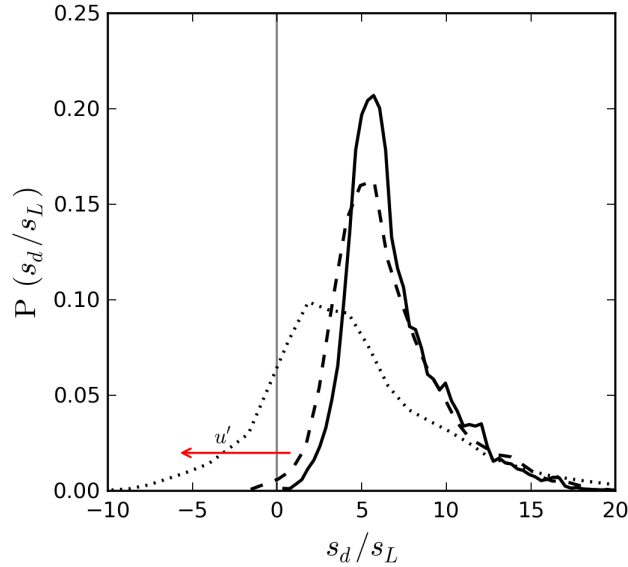


Figure 4.8 Distribution of displacement speed s_d over the peak reaction rate isosurface $c^* = 0.8$ in three cases spanning the dataset (solid line: lowest intensity and dotted line: high-intensity).

4. Damköhler's First Hypothesis

minor reduction of the peak value is noted for case III (dashed line). In the highest intensity case V, however, a further reduction is observed indicating a greater role played by turbulent fluctuations. The increasing scatter in $s_d(c)$ in high u' may be attributed to the diffusive term in Equation 4.10 because the reaction rate term $\dot{\omega}$ retains to a great extent the laminar flamelet profile (as discussed in Section 1.2.2). Ongoing investigation is aimed at addressing these observations.

Configuration of curvature and displacement speed

The net stretch rate contribution due to the propagation term $s_d h_m$ relies on both aspects: the creation of mean curvature h_m and the propagation of these curved elements s_d . The consequent curvature propagation behaviour may be revealed in the correlations between quantities h_m and s_d appearing in the propagation term $s_d h_m$ shown in Figure 4.9. It is clear that at low intensities (Figure 4.9a), s_d and h_m are negatively correlated; i.e. s_d is higher when mean curvatures are negative $h_m < 0$, and vice versa. In high intensities (Figure 4.9b), the correlation continues to remain negative, but a considerable amount of negative displacement speed $s_d < 0$ is also observed. Nevertheless, of

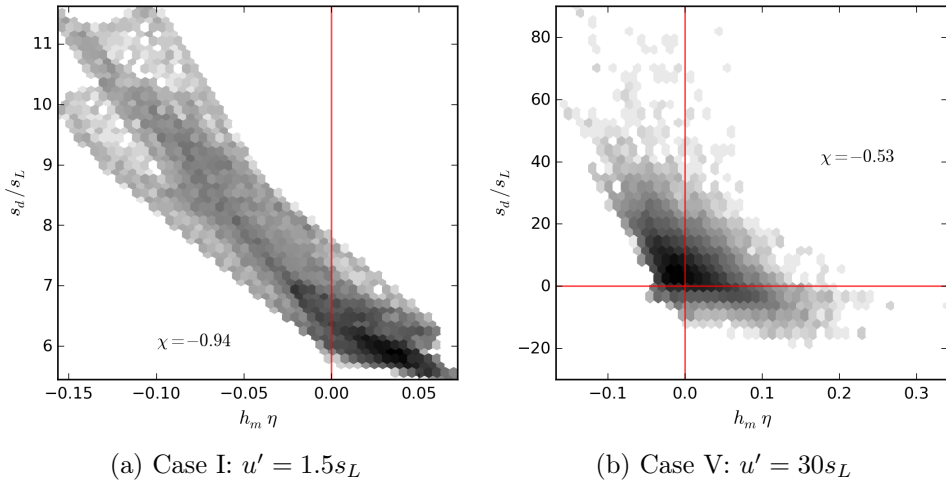


Figure 4.9 Joint probability distribution of s_d (scaled with laminar flame speed s_L) and h_m (scaled with Kolmogorov scale η) in the lowest and highest intensity cases.

the four possible configurations between $\pm s_d$ and $\pm h_m$, the two configurations with opposite signs ($s_d < 0$, $h_m > 0$ and vice versa) are most common. Some sections of the surface with $s_d > 0$ and $h_m > 0$ are observed, but nearly no sections with $s_d < 0$ and $h_m < 0$ are observed.

Assuming s_d has a laminar flamelet behaviour in the mean, the local mean curvature h_m determines the sign of the propagation rate term $s_d h_m$: a positively curved surface element $h_m > 0$ contributes productively Σ (given $s_d > 0$) and a negatively curved surface element $h_m < 0$ contributes destructively to Σ .

4.2.2 Balance of strain and propagation

It has been argued by Bradley et al. (1992) that the increase in tangential strain rate a_t with u' causes localised flame extinctions at sufficiently high u' . This has been attributed historically as the primary cause of the bending effect in $s_T(u')$. In particular, increased a_t reduces s_d locally causing the flame surface area A_T to decrease by virtue of holes. The role of curvature h_m has been considered minimal thus far. Informed by the evolution of non-reacting scalar surfaces, turbulence has been expected to even out flame surface curvatures. This picture conforms with the observation that $\langle h_m \rangle \approx 0$ for all u' values considered in the present dataset.

However, the true effect of curvature on the flame surface area A_T (as computed in Equation 4.5) is manifested through propagation rate $s_d h_m$ and not merely curvature h_m . Hence, the actual individual contributions of the stretch rate components a_t and $s_d h_m$ are identified (Nivarti and Cant, 2017) here by calculating volume-averaged quantities

$$\bar{a} = \frac{1}{V} \int_V a_t dV, \text{ and } \bar{h} = \frac{1}{V} \int_V s_d h_m dV, \quad (4.11)$$

where V is the domain volume. These volume integrals are graphed together in Figure 4.10 over the entire range of u' simulated presently.

On the one hand, it is observed that the volume-averaged tangential strain rate $\bar{a}$ is positive for all the turbulence intensities considered, and its mag-

4. Damköhler's First Hypothesis

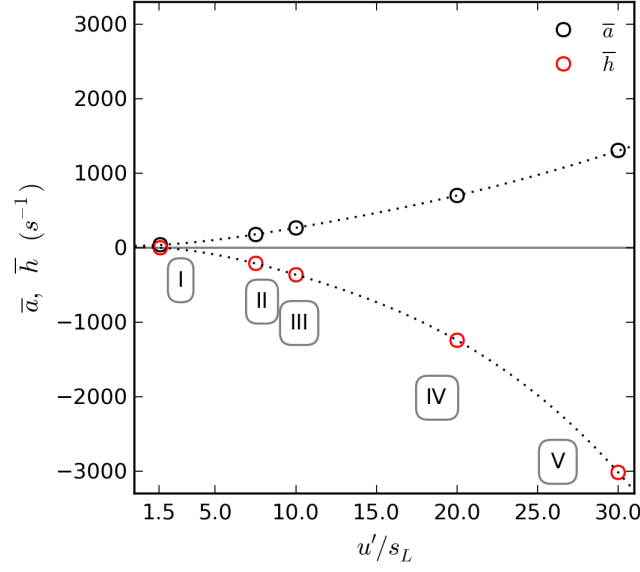


Figure 4.10 Variation of volume-integrated source-terms $\bar{a}$ and $\bar{h}$ of the transport equation for Σ' with increasing normalized turbulence intensity u'/s_L .

nitude $|\bar{a}|$ increases monotonically with u' . Hence, net turbulent strain rate contributes productively to Σ' over the entire range of simulations. This conforms indeed with the previous studies as well as the figures discussed above. On the other hand, the volume-averaged propagation rate $\bar{h}$ contributes destructively to Σ' and its magnitude increases by several orders over the same range of u' . Therefore, the two source-terms appear to regulate together the total flame surface area A_T . A balance between the two terms determines the value of this area at a given u' . Since DH1 is satisfied as per Figure 4.4, the surface area A_T governs the turbulent burning velocity s_T . Hence, it may be inferred that the bending effect recorded in $s_T(u')$ is related to this balance of strain rate a_t and propagation rate $s_d h_m$.

A phenomenological explanation of bending

The results presented above outline a self-regulating mechanism which maintains on average the value of Σ in a prescribed turbulent flow field. For a given u' , production of Σ due to extensive turbulent strain is opposed by destruction of Σ due to flame propagation in negative curvature regions. The overall effect of strain and curvature is to regulate Σ . As u' increases, the magnitude of

extensive strain a_t increases resulting in increased production of Σ . This is balanced by increased destruction of Σ because larger portions of the brush have $s_d h_m < 0$. The steady-state Σ attained for any given u' is directly related to the flame surface area A_T and, consequently, determines s_T . Hence, the variation of $s_T(u')$ relies on a competition between strain and curvature – the source-terms of Σ transport – that determines the steady-state Σ attained. The conditions of bending may therefore be sought by posing the question: what are the relationships that determine the Σ attained for a given u' ?

The key mechanism of bending seen in Figure 3.9 is highlighted in unison by Figure 4.4 and Figure 4.10. These figures indicate that turbulent burning velocity s_T is governed by the flame surface area A_T (Figure 4.4) but the monotonic increase in extensive strain rate a_t with u' does not result in a monotonic increase in A_T due to the destructive role of negative mean curvature (Figure 4.10). This non-monotonic variation of A_T results in the bending of $s_T(u')$ (seen earlier in Figure 3.9).

For a given geometry L and integral length scale ℓ_0 , the most significant change with increasing u' is the production of an increasing number of small-scale eddies. It may be concluded, therefore, that these small-scale eddies are less efficient at generating flame surface area. This reduced efficiency may be due to the fact that these eddies have shorter lifetimes in comparison to the overall time scale of flame wrinkling as proposed by Meneveau and Poinso (1991). The reduced efficiency may also result from a shift in balance between the relevant time scales of strain rate as well as of propagation rate. For example, the images in Section 3.2.1 show that the shapes and sizes of wrinkles change with increasing u' . The ‘folds’ and ‘fingers’ seen in high u' turbulence act to increase the significance of propagation rate effects over strain rate effects. Further, small-scale wrinkling causes higher propagation speeds (Figure 4.8) due to enhanced molecular diffusion between flames in close proximity. This combination of increased small-scale wrinkling and increased propagation speed may, therefore, also reduce the time scale of self-intersections.

4.3 Summary: the role of DH1 in bending

Turbulent surface strain rate a_t and flame surface propagation rate $s_d h_m$ have opposing effects on the surface area A_T . While strain tends to produce A_T , flame propagation tends to destroy A_T . With increasing u' , propagation rate effects dominate and tend to reduce the overall flame surface density Σ attained. An explanation for this imbalance and the resulting decreased Σ in high u' turbulence is sought. Two distinct signatures of the governing mechanism are

1. increased negative mean propagation (Figure 4.10) in high u' turbulence,
2. and increased displacement speed s_d in regions of negative curvature (Figure 4.8 and Figure 4.9) which exaggerates the previous effect.

Hence, a possible mechanism of the bending effect is framed in terms of kinematic effects as opposed to chemical effects such as localised extinctions. Since all parameters but u' are held fixed, an increased number of small-scale eddies are expected with increasing u' . Further investigation will be focused on investigating the role of small-scale eddies on flame surface topology and propagation.

Chapter 5

Damköhler's Second Hypothesis

Damköhler proposed both hypotheses (DH1 and DH2) as primary mechanisms for s_T enhancement in the respective regimes of operation. As the primary mechanism operates in a given regime, the secondary mechanism was expected to ‘recede in the background’ contributing alongside albeit to a lesser degree. This raises an important question: when does one primary mechanism transition to being a secondary mechanism? Alternatively, is there a limit to the applicability of a single primary mechanism? Over the years, the range and upper u' limit of validity for DH1 has received significant attention, and this has been the focus of the previous chapters. The validity limit for DH2 remains unknown.

As discussed in Chapter 1, Damköhler (1940) reasoned that the enhancement of s_T in ‘fine-body’ turbulence arises as a consequence of the enhancement of the local internal transport process. Therefore, DH2 concerns the effects of turbulence on the diffusive component of the expression $s_L \sim A\sqrt{D\dot{\omega}}$. The local reaction rate $\dot{\omega}$ as well as the global flame surface area A_T were assumed to be unaffected. Reasoning along these lines, the ratio of flame speed in ‘fine-body’ turbulence to the unstrained laminar flame speeds may be expressed as

$$\frac{s_T}{s_L} = \sqrt{\frac{D_T}{D_L}}, \quad (5.1)$$

where D_T and D_L represent the transport coefficients in turbulent and laminar flames respectively. Recent investigations in intense (Poludnenko and Oran,

5. Damköhler's Second Hypothesis

2011; Savard and Blanquart, 2015) and extreme (Wabel et al., 2016) intensities of turbulence have highlighted the possible significance of diffusive transport processes in determining s_T in such conditions. Appropriate modifications of DH2 are, therefore, being proposed so as to fit the s_T data acquired from experiments and DNS. Motivated by these investigations, the present work focuses on outlining the regimes where DH2 is applicable. In this chapter, the scalar flux transport recorded using the present DNS is analysed and its implication for the minimal conditions of validity for DH2 is discussed.

5.1 Scalar flux transport in turbulence

In cold non-reacting flows, the ratio $D_T/D_L > 1$ because turbulent mixing and transport of the scalar flux enhances effectively the diffusive transport coefficient. This enhanced turbulent scalar flux transport leads to increased propagation rates of scalar isosurfaces. Most importantly, the enhancement abides by the mathematical validity of Equation 5.1 which requires that $D_T/D_L > 0$.

Bray-Moss-Libby formulation

In laminar premixed flames, the analogous scalar which designates propagation of flame isosurfaces is the reaction progress variable c introduced earlier in Chapter 1. For turbulent premixed flames, the Favre mean progress variable $\tilde{c}$ provides an appropriate framework (Veynante and Vervisch, 2002) to quantify the mean transport of the propagating isosurfaces. Favre mean quantities $\tilde{q} = \overline{\rho q}/\bar{\rho}$ represent density-weighted averages whereas q'' denotes the respective fluctuations so that $q = \tilde{q} + q''$. As introduced in Section 1.2, the Favre average framework provides an equation for the transport of the scalar $\tilde{c}$ as

$$\nabla \cdot \bar{\rho} \tilde{u} \tilde{c} = -\nabla \cdot \bar{\rho} \widetilde{u'' c''} + \bar{\omega}, \quad (5.2)$$

according to the Bray-Moss-Libby (BML) formulation due to Bray (1980). In this framework, the viscous term is neglected under the assumption $\text{Re} \gg \text{Da} \gg 1$, and the unsteady term is neglected considering a statistically-steady state. Although these assumptions may not hold strictly in the present dataset,

5.1. Scalar flux transport in turbulence

this framework serves to highlight the key physical mechanisms governing the propagation of the mean flame surface. In the present study, c denotes the progress variable based on reactant mass-fraction $c = (Y_{R,u} - Y_R)/(Y_{R,u} - Y_{R,b})$ where the subscripts u and b stand for unburned and burned components respectively. Alternatively, the temperature T may also be used in which case the diffusivity will correspond to thermal diffusivity.

In the BML framework, flame propagation is linked with the convection term on the l.h.s. in Equation 5.2 as well as the two terms on the r.h.s. which denote

1. $-\nabla \cdot \bar{\rho} \widetilde{\mathbf{u}'' c''}$ is the scalar flux term which describes turbulent mixing across the Favre mean $\tilde{c}$ isosurface, and
2. $\bar{\omega}$ is the reaction source-term which describes the mean chemical transformation of the reactive scalar $\tilde{c}$ from $0 \rightarrow 1$.

Hence, Equation 5.2 extends the mechanics for laminar flame propagation to the context of mean flame propagation in turbulence. Indeed, this framework forms the basis for several modelling approaches for turbulent flame propagation (Veynante et al., 1997; Lipatnikov and Chomiak, 2002).

The discussions so far suggest that the second term $\bar{\omega}$ is not influenced significantly in the present dataset (see Figure 3.7). The first term, however, may be expected to change in turbulence if the effects on transport of the scalar flux $\widetilde{\mathbf{u}'' c''}$ are considered. Supporting evidence is provided by the previous discussions which indicate that the pre-heat zone thickens considerably (see Figure 4.1). Diffusive transport processes occur in this very region and, hence, the role of turbulence must be examined in this context.

5.1.1 Gradient transport hypothesis

The enhancement of molecular diffusivity D_T due to turbulence may be seen in the same vein as the diffusion of passive scalars due to molecular transport. The application of Fick's law to turbulent transport of passive scalars suggests that scalar fluxes must be transported favourably down the scalar gradient

5. Damköhler's Second Hypothesis

(Pope, 2001); i.e. from higher to lower concentrations. Such a model of turbulent transport conforms with the qualitative picture where turbulence aids mixing.

A ‘gradient transport’ expression for the turbulent reactive scalar flux $\widetilde{u''c''}$ has been hypothesised as

$$\widetilde{u''c''} = -D_T \frac{\partial \tilde{c}}{\partial x}, \quad (5.3)$$

based on an analogy with Fick’s law. This expression models the transport of the scalar flux $\widetilde{u''c''}$ down the mean scalar gradient $\partial \tilde{c}/\partial x$ for which the diffusion coefficient $D_T > D_L > 0$; i.e. turbulence enhances mixing of different concentrations of the reactive scalar according to gradient (G) transport.

Effect on flame propagation

In premixed flames, the propagation of the mean flame brush is enhanced by the mixing of products and reactants. Hence, gradient transport of reactive scalar is favourable to flame propagation. This is visualized in Figure 5.1. Since $\widetilde{u''c''} < 0$ in gradient transport, it follows that turbulent fluctuations u'' that arise from turbulent vortical motion (red arrows in Figure 5.1) support progress variable fluctuations c'' convoluting further an initially disturbed

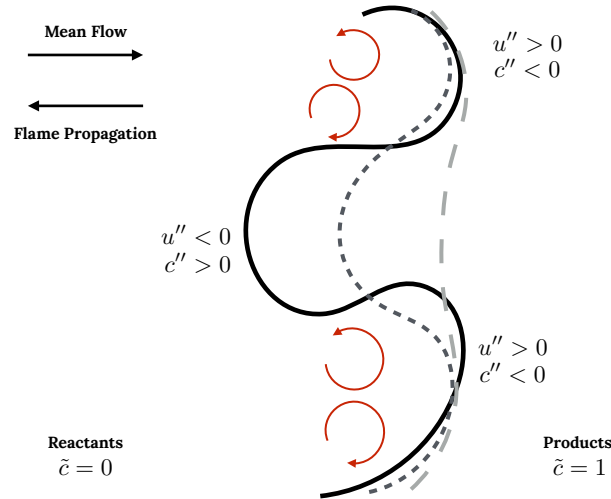


Figure 5.1 Schematic showing gradient (G) transport of the progress variable flux. A disturbed flame surface (light dashed line) is wrinkled further (progressively darker solid curves) by vortical activity. The flame does not counteract this tendency, and is simply convoluted by turbulent fluctuations.

flame surface. Hence, the turbulent diffusivity $D_T > 0$ based on gradient hypothesis in Equation 5.3. As a consequence, the ratio D_T/D_L is applicable under the square-root operation in the DH2 expression (Equation 5.1).

5.2 Counter-gradient transport

Numerical (Libby and Bray, 1981; Rutland and Cant, 1994) and experimental studies (Shepherd et al., 1982) suggest that gradient transport is not the only mechanism of scalar flux transport in premixed flames. In other words, the turbulent scalar flux $\widetilde{u''c''}$ (l.h.s. in Equation 5.3) does not always have the opposite sign (direction) to the scalar gradient $\partial\tilde{c}/\partial x$ (r.h.s. in Equation 5.3). In such a case, Equation 5.3 provides $D_T < 0$ posing a threat to the validity of the DH2 expression (Equation 5.1). Such a mode of scalar flux transport is referred to as counter-gradient (CG) transport (Libby and Bray, 1981).

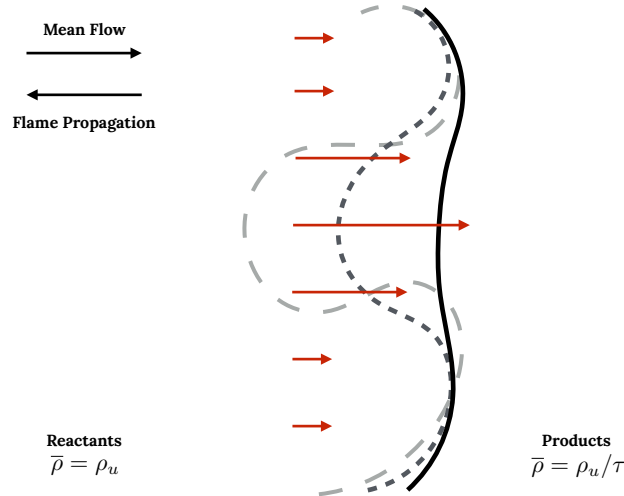


Figure 5.2 Schematic of the counter-gradient (CG) transport mechanism. At sufficiently high heat release factors $\tau = \rho_u/\rho_b$, the flame has a tendency to act against gradient transport. An initially wrinkled flame surface (dashed convoluted curve) may un-wrinkle as the lighter product peninsula is differentially accelerated in the direction of products (along red arrows, away from the direction of propagation).

5. Damköhler's Second Hypothesis

Mechanism of counter-gradient transport

CG transport has been attributed (Veynante et al., 1997) to a counter-acting mechanism in premixed flames which acts to inhibit flame surface wrinkling. This mechanism arises due to gas expansion across the flame, and it competes with the wrinkling action of turbulent vortical motion (as seen in G transport). DNS analysis of mean scalar flux transport has highlighted the role of pressure gradients (Rutland and Cant, 1994; Veynante et al., 1997) in the CG/G transition. The concept that emerges from these studies has been illustrated in Figure 5.2. Thermal expansion gives rise to a self-induced pressure gradient which scales with the heat release factor $\tau \sim \rho_u/\rho_b > 1$. Wrinkled flame surfaces may be characterised by a peninsula of lighter products (as shown in Figure 5.2); these regions are accelerated differentially in comparison to neighbouring reactant gulfs under the same pressure gradient. Hence, an initially convoluted flame surface (dark contour) may un-wrinkle if the effect of heat release is large enough to compensate for the wrinkling effect of turbulence.

Hence, CG transport results from a shift in balance between flame-induced gas expansion (represented by τ) and flow-imposed turbulent fluctuations (represented by u'). An appropriate model that captures the accompanying change in sign of $\widetilde{u''c''}$ is written (Veynante et al., 1997) as follows

$$\widetilde{u''c''} = \tilde{c}(1 - \tilde{c})(\tau s_L - 2\alpha u'), \quad (5.4)$$

wherein the ratio $N_B = \tau s_L/2\alpha u'$ (called the Bray number) dictates the CG/G transition in scalar flux transport (since $\tilde{c}(1 - \tilde{c}) > 0 \forall \tilde{c} \in [0, 1]$).

In more recent works, the influence of flame-generated vorticity has been investigated (Louch and Bray, 2001). Wenzel and Peters (2000) have verified the role of gas expansion using G-equation model simulations of flame propagation with added heat release (discussed in Section 1.2). The simulations recorded a bending effect in $s_T(u')$ akin to the present dataset. The simulations of Wenzel and Peters (2000) also recorded a CG/G transition in the scalar flux transport, but the implication of this transition on Damköhler's formulations for s_T enhancement was not addressed. In fact, a connection of the CG/G

transition with the DH2 expression for s_T has not been considered to date.

Scalar flux and gradient computations

In Figure 5.3, each panel shows the variation of Favre averaged turbulent scalar flux $\widetilde{u''c''}$ with the Favre averaged scalar gradient $\partial\tilde{c}/\partial x$ for the specified case with corresponding u' . Each point $(\partial\tilde{c}/\partial x, \widetilde{u''c''})$ is coloured according to the corresponding value of $\tilde{c}$, indicating its position in the mean flame brush $0.01 < \tilde{c} < 0.99$. The leading edge $\tilde{c} \approx 0$ (cold unburned reactants) is coloured blue, whereas the trailing edge $\tilde{c} \approx 1$ (hot burned products) is coloured red. In all of the cases, $\partial\tilde{c}/\partial x > 0$ throughout the mean turbulent flame brush, i.e. points lie to the right of the dotted vertical line at $\partial\tilde{c}/\partial x = 0$. An exception is the small region close to $\tilde{c} \approx 0.6$ (marked pink points in Figure 5.3c) in case IV. This exception may be attributed to excessive entrainment of unburned reactants within the preheat zone of the mean flame brush (visualised below in Figure 5.4). In contrast to the scalar gradient, the scalar flux $\widetilde{u''c''}$ transitions from being entirely positive to entirely negative across the different cases. These four representative cases (I, III, IV and V) are discussed below to highlight the salient features of this transition.

In case I (Figure 5.3a), $\widetilde{u''c''} > 0$ throughout the Favre mean flame brush. In addition, $\widetilde{u''c''}$ appears to have a direct correspondence with mean scalar gradient $\partial\tilde{c}/\partial x$, both terms attaining a maximum in the preheat zone between $\tilde{c} \approx 0.4$ and $\tilde{c} \approx 0.6$. Similarly, case II (not shown) as well as case III (Figure 5.3b) exhibit $\widetilde{u''c''} > 0$ across most of the brush; i.e. all points lie above the dotted horizontal line. The correspondence of $\widetilde{u''c''}$ with $\partial\tilde{c}/\partial x$ follows in similar fashion, but with the exception that $\widetilde{u''c''} < 0$ close to the leading edge, exhibiting a local minimum close to $\tilde{c} \approx 0.01$ (marked dark blue dots in Figure 5.3b). Clearly, the upstream turbulence intensity u' in case IV begins to overturn the counter-gradient (CG) transport $\widetilde{u''c''} > 0$ that existed throughout the flame brush in the low u' case I. This shift in the behaviour of $\widetilde{u''c''}$ in the preheat zone is, therefore, a signature of the imminent transition to gradient (G) transport at higher intensities.

Upon increasing u' , the magnitudes of $\widetilde{u''c''}$ and $\partial\tilde{c}/\partial x$ do not change sig-

5. Damköhler's Second Hypothesis

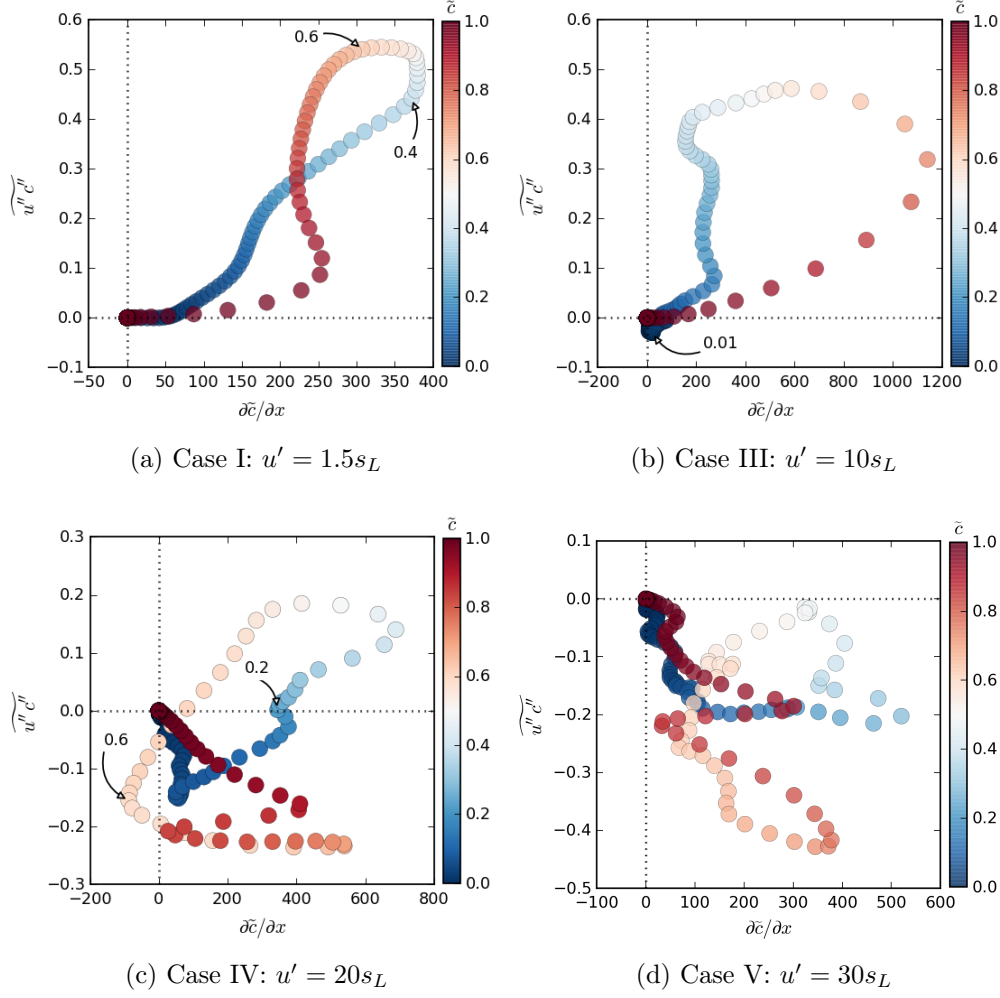


Figure 5.3 Variation of mean scalar flux $\widetilde{u''c''}$ with the mean scalar gradient $\partial\tilde{c}/\partial x$. Colours denote corresponding values of the mean progress variable $\tilde{c}$ (blue: leading edge $\tilde{c} = 0.01$, red: trailing edge $\tilde{c} = 0.99$).

nificantly (as seen in the axes of panels in Figure 5.3). Instead, the sign of $\widetilde{u''c''}$ and the correspondence between $\widetilde{u''c''}$ and $\partial\tilde{c}/\partial x$ is affected considerably. In case IV (Figure 5.3c), $\widetilde{u''c''} < 0$ through most of the flame brush (barring a small region between $\tilde{c} \approx 0.2$ and $\tilde{c} \approx 0.6$) whereas in case V (Figure 5.3d), $\widetilde{u''c''} < 0$ across the entire flame brush. The high degree of scatter that accompanies this transition marks a departure from a smooth wrinkled flame to a highly convoluted flame. This follows from the discussion above: in gradient transport wrinkling is enhanced by turbulence resulting in convoluted flames, whereas in CG transport wrinkling is diminished resulting in relatively smooth flames.

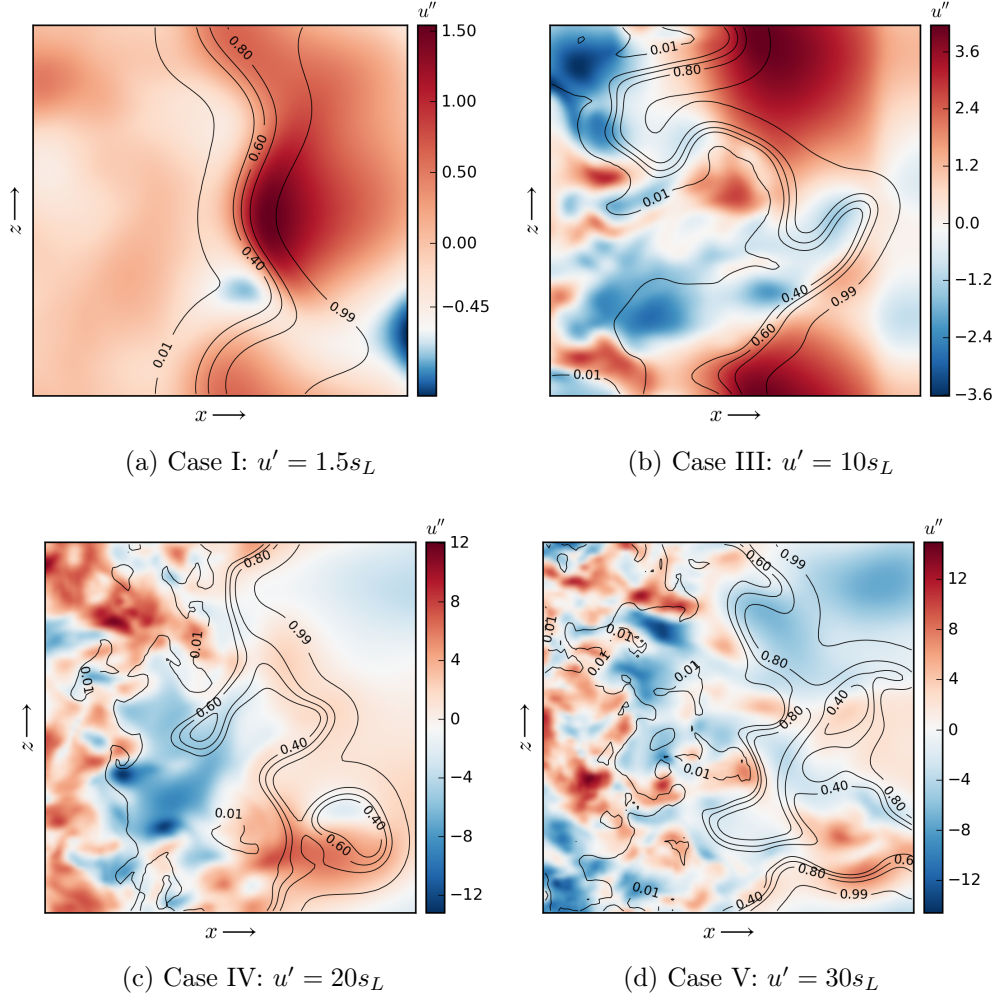


Figure 5.4 Instantaneous progress variable contours (black lines) and Favre velocity fluctuations u'' (background colours) in an axial cross-section $y = \frac{L}{2}; L < x < 2L, z$ of the domain.

Figure 5.4 shows flame surface contours corresponding to the cases I, III, IV and V within streamwise slices of the domain. The flame is propagating to the left in all panels. The departure from a smooth wrinkled flame in case I to the highly convoluted flame in cases IV and V is seen readily. This corresponds to the contrast in scatter of points in the respective cases noticeable in Figure 5.3. Such a change in the pattern of wrinkling has also been noted in the CG/G transition captured in other simulations conducted previously (Veynante et al., 1997; Chakraborty and Cant, 2009).

Each panel of Figure 5.4 also shows the velocity fluctuations u'' using colours (blue: negative, and red: positive) in the backdrop of the contour

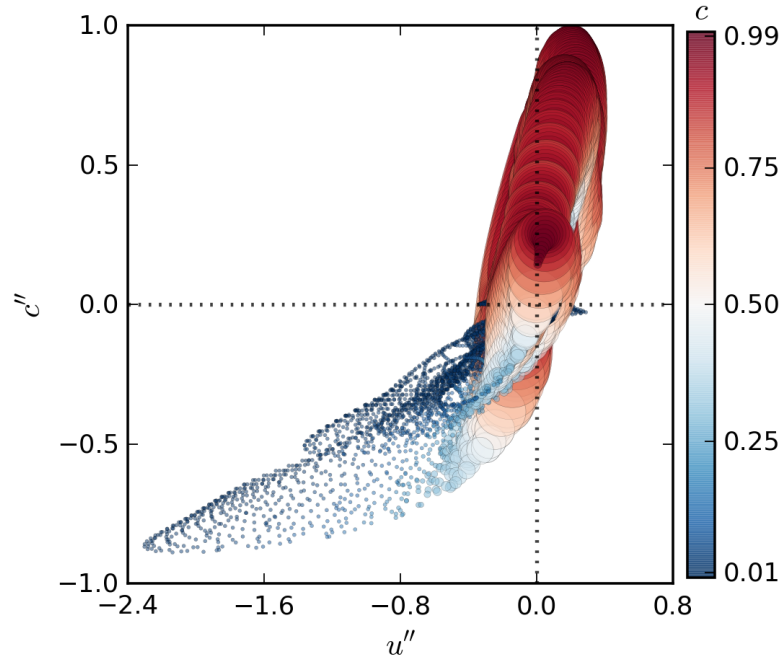
5. Damköhler's Second Hypothesis

lines. The decreasing size of turbulence small-scales with increasing u' may be observed in the gradually changing distribution of coherently coloured flow field regions. On closer inspection, it is seen additionally that while positive velocity fluctuations (red colour) appear predominantly behind the flame in case I (Figure 5.4a), such fluctuations appear ahead of the flame to a significantly higher extent in case V (Figure 5.4d). This transition provides visual evidence of a shift in balance within the dataset between velocity gradients of two varieties: 1) those *generated* behind the flame due to gas expansion, and 2) those *present* ahead of the flame in the turbulent flow field.

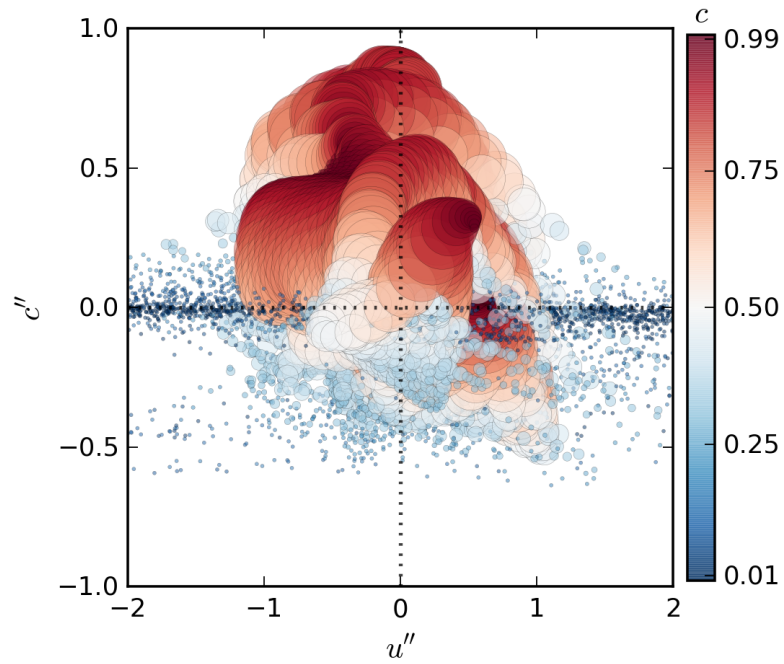
5.2.1 Regime of counter-gradient transport

The role of the balance between the flame imposed gas expansion and the flow imposed turbulence in the CG/G transition was investigated by Wenzel and Peters (2000). By using a G-equation model of the flame surface with added heat release, they were able to compute the two corresponding components of turbulent velocity fluctuations $u'' = u_f'' + u_g''$. The shift in favour of the gas expansion induced fluctuations u_g'' as opposed to the flow field fluctuations u_f'' explained the CG/G transition recorded between two separate simulation cases. In the simulations of Wenzel and Peters (2000), the gas expansion factor τ was varied. Here the turbulence intensity u' is varied instead with τ held constant across the dataset. Hence, $u_g'' = g(\tau s_L)$ and its corresponding flux component $\widetilde{u_g'' c''}$ is expected to be constant, while $u_f'' = f(u')$ and $\widetilde{u_f'' c''}$ are expected to change as u' increases from case I to case V. The shift in balance between these quantities accompanies the CG/G transition recorded in the present dataset.

In case I (Figure 5.5a, low u'), u'' and c'' are positively correlated through most of the flame brush. Either $u'' < 0$ and $c'' < 0$ (seen in the long trail of blue dots from the leading edge) or $u'' > 0$ and $c'' > 0$ (seen predominantly in the big red dots of the reaction zone region). A small number of points (in the preheat and reaction zones) display a negative correlation, but their contribution to the mean scalar flux $\widetilde{u'' c''}$ is insignificant as the corresponding correlations do not carry over to the averaged values (shown in Figure 5.3a).



(a) Case I: $u' = 1.5s_L$



(b) Case V: $u' = 30s_L$

Figure 5.5 Recorded correlations between u'' and c'' for case I (above) and case V (below). Colours indicate the progress variable value (blue: reactants, red: products) and size is proportional to the reaction rate magnitude. The transition from positive to negative correlation corresponds to the G/CG transition.

5. Damköhler's Second Hypothesis

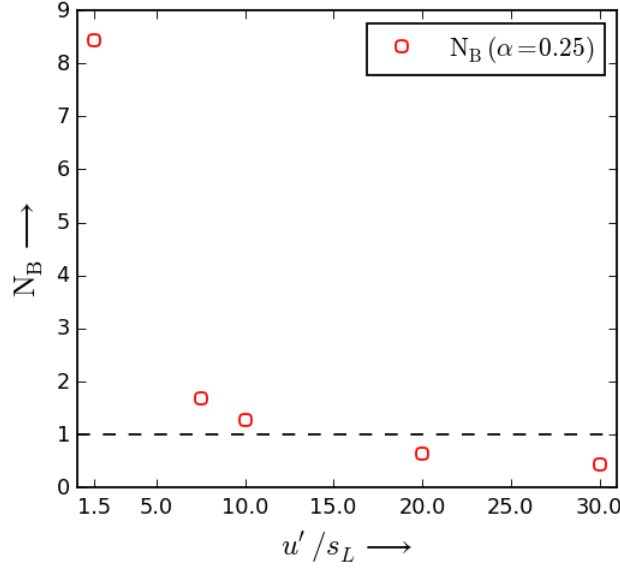


Figure 5.6 The Bray number N_B for each case simulated in the present dataset delineating the gradient/counter-gradient transport regimes at unity.

A more complicated correlation is evident in case V (Figure 5.5b, high u') which exhibits G transport. Regions with positive correlations continue to be present, indicating the constant contribution of gas expansion in both cases. On the other hand, a large portion of the preheat and reaction zone shifts to a negative correlation, representing the overturning of this contribution by the turbulent flow field. In fact, the negative correlations are more significant in the mean (as seen in Figure 5.3d). From the preceding discussion, it is clear that this qualitative change in the different behaviour of the scalar flux $\widetilde{u''c'}$ occurs at a certain threshold u' between $10s_L$ and $20s_L$ within the dataset.

Veynante et al. (1997) provided a simple criterion to delineate the CG/G regimes with contrasting $\widetilde{u''c'}$ behaviour. According to Equation 5.4, $\widetilde{u''c'}$ has opposite signs across a Bray number of unity, $N_B \equiv \tau s_L / 2\alpha u' = 1$. In the present context, u' is the only parameter relevant to the criterion that is being varied between any two cases. Moreover, the integral length scale ℓ_0 is also held constant ($\ell_0/\delta_L = 2.75$) across all the cases. The corresponding graph $N_B(u'/s_L)$ is shown in Figure 5.6. With $\alpha = 0.25 \pm 0.1$, the predicted transition matches (to within $\pm 5s_L$ between $10s_L < u' < 20s_L$) the transition observed between cases III (Figure 5.3b) and IV (Figure 5.3c).

Veynante et al. (1997) hypothesised α to be a function of ℓ_0/δ_L . Ignoring further the possible dependence on u'/s_L , they found that $N_B = 1$ delineates the CG/G transition in their dataset for $\alpha(\ell_0/\delta_L = 11) = 0.5$. The present analysis, with $\alpha(\ell_0/\delta_L \approx 3) = 0.25$, indicates that α is a gradually increasing function of ℓ_0/δ_L . A recent experimental investigation (Kheirkhah and Gülder, 2015) of counter-gradient transport in V-shaped flames suggests a logarithmic variation of α with ℓ_0/δ_L supporting the assumption of a monotonic variation considered here. Kheirkhah and Gülder (2015) further report $\alpha(\ell_0/\delta_L = 4) \approx 0.3$ which is very close to the values obtained here. This value of α , therefore, provides a valuable datapoint pertinent to subsequent investigations on the general behaviour of the efficiency function α . It is noted that the CG/G transition is reported here for a planar flame, and such transitions may occur locally and under slightly different conditions for more complicated geometries. For example, Kheirkhah and Gülder (2015) observe a CG/G transition at $u'/s_L \approx 3$ which is lower than the conditions $u'/s_L \approx 10$ observed here. The shift in balance between τ and u' in the CG/G transition at $N_B(\alpha = 0.25) = 1$ occurs as u' is increased with ℓ_0 held constant in this dataset. Hence, the recorded CG/G transition is linked to a transition in the role of turbulence small-scales.

5.2.2 Computation of the diffusion coefficient

Knowing the scalar flux $\widetilde{u''c''}$ and the Favre mean progress variable gradient $\partial\tilde{c}/\partial x$, the corresponding turbulent diffusivity D_T may be computed. This can be compared with the laminar diffusivity D_L to provide the overall enhancement of diffusivity due to turbulence.

The molecular diffusivity D_L of a species in laminar flow is calculated as

$$D_L = \frac{\lambda}{\rho C_p \text{Le}}, \quad (5.5)$$

given its Lewis number (here, $\text{Le} = 1.0$). It is recalled that DH2 refers to the turbulent amplification of molecular diffusion ‘between the preheat zone and the reaction zone’. In order to produce the diffusion coefficients for evaluating

5. Damköhler's Second Hypothesis

DH2, values must then be chosen within this ($0.6 \leq c \leq 0.9$) region. In the present work, D_L is calculated as $D_L = (\lambda/\rho C_p)|_{c=0.8}$ at the $c = 0.8$ axial location where the reaction rate attains a maximum in a laminar flame. Similarly, the turbulent diffusivity D_T is evaluated at $\tilde{c} \approx 0.8$ in the turbulent premixed flame brush.

In Damköhler's original work (Damköhler, 1940), D_T was estimated for turbulent flames using Prandtl's mixing length hypothesis (Prandtl, 1925). According to this hypothesis, the diffusivity may be approximated as the product of a length scale and a turbulent velocity scale. These scales are chosen respectively as the integral length scale ℓ_0 and the turbulence intensity u' to provide the expression

$$D_T \sim u' \ell_0 \quad (5.6)$$

which is expected to be positive for all turbulent flows because $u', \ell_0 > 0$ necessarily. For laminar flames, the relevant scales may be chosen as the flame thickness δ_L and flame speed s_L respectively to provide $D_L \sim \delta_L s_L \sim \nu$. These expressions may then be used to compute s_T as

$$\frac{s_T}{s_L} \sim \sqrt{\frac{D_T}{D_L}} \sim \sqrt{\frac{u' \ell_0}{s_L \delta_L}} \sim \sqrt{\frac{u' \ell_0}{\nu}} \quad (5.7)$$

where $\nu \sim s_L \delta_L$ is based on a constant Prandtl number assumption. In fact, Damköhler used this very line of reasoning to arrive at $s_T \sim \sqrt{Re_0}$, the final term in the above equation, for 'fine-body turbulence.' More recently, improved formulations of D_T have been used instead of Prandtl's method using parameters of the k - ϵ model of turbulence (Lipatnikov and Chomiak, 2002; Savard and Blanquart, 2015).

While these approaches to calculate D_T may be adopted here, the focus here is to understand what it means to use the gradient hypothesis instead. Since the gradient hypothesis is closely linked with flame propagation behaviour, it has the ability to shed light on the underlying physical mechanisms and their limitations. The counter-gradient transport mechanism was one such instance which exposed a limitation of the gradient hypothesis and consequently suggested the existence of a different mode of flame propagation. Therefore, D_T

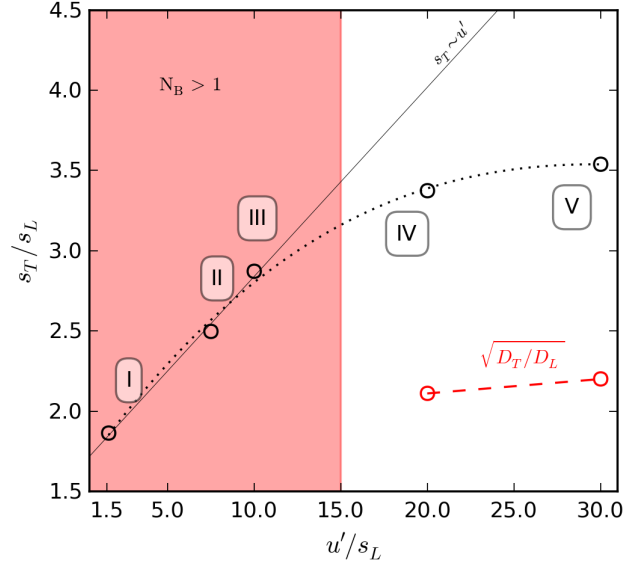


Figure 5.7 Computed normalized turbulent burning velocity s_T/s_L compared with predictions $\sqrt{D_T/D_L}$ of DH2 in the gradient diffusion regime $N_B < 1$. DH2 is invalidated in the CG transport regime denoted by $N_B > 1$ (shaded red).

is computed here using the gradient hypothesis expression of Equation 5.3 as

$$D_T = -\frac{\widetilde{u''c''}}{\partial \tilde{c}/\partial x} \Big|_{\tilde{c}=0.8}. \quad (5.8)$$

at the Favre mean reaction zone $\tilde{c} = 0.8$. In the presence of a CG/G transition, D_T is expected to change in sign. Given the formulation of DH2 as presented in Equation 5.1, the applicability of a negative D_T is prohibited.

DH2 states that the role of ‘fine-body turbulence of size $\ell \ll \delta_L$ ’ is to enhance s_T ‘by amplifying the microscopic (diffusive) transport processes’ within the flame brush. As discussed above, $\widetilde{u''c''} < 0$ only in a small portion of the dataset corresponding to the cases IV and V (as shown in Figure 5.6). Numerical evaluation of Equation 5.1 for these cases is shown in Figure 5.7. For the remaining cases, $N_B > 1$ and the diffusion coefficient $D_T < 0$. Hence, Equation 5.1 cannot be evaluated. In other words, Damköhler’s second hypothesis (DH2) applies strictly to the gradient transport regime where $N_B < 1$. This is illustrated in Figure 5.7 by marking the region of inapplicability $N_B > 1$ in red.

5. Damköhler's Second Hypothesis

Consequently, it appears that the general claim that ‘turbulence always acts to enhance the flame speed’ might only apply in certain special limiting conditions. In fact, for $N_B > 1$, the turbulence scales may have an inhibitive effect on s_T because $\widetilde{u''c''} > 0$ is transported against the gradient $-\partial\tilde{c}/\partial x$ favourable to flame propagation. The difference between values of $\sqrt{D_T/D_L}$ and s_T/s_L in Figure 5.7 opens a further question: to what extent do DH1 and DH2 influence s_T individually in this region of overlapping validity? As yet, the evidence is inconclusive and further investigation is necessary to understand fully the significance of DH1 and DH2 in the thin reaction zones regime. An investigation of higher u' in a regime corresponding precisely to DH2, i.e. with $\ell \ll \delta_L$, will help understand when it is that the diffusive processes begin to govern decisively the enhancement in s_T . The present analysis elucidates rather the minimal criteria for the applicability of Damköhler's second hypothesis.

5.3 Summary: validity regime of DH2

In low u' turbulence, DH1 applies and turbulent motion both roughens and stabilizes the surface. These simultaneous effects result in a positive correlation between u'' and c'' , i.e. CG transport prevails. Referring to Equation 5.3, this implies that the l.h.s. $\widetilde{u''c''} > 0$ whereas the r.h.s. $\partial\tilde{c}/\partial x > 0$. Hence, since $D_T < 0$, it is clear that DH2 cannot operate.

In high u' turbulence, DH1 continues to apply as the large-scales serve to deform the surface. In this regime, however, G transport ($\widetilde{u''c''} < 0$) prevails. Hence, DH2 is applicable and operates alongside DH1. The transition between CG/G transport, therefore, delineates the regimes of applicability of DH2.

Hence, contrary to Damköhler's original conclusion, it appears that ‘fine-body turbulence with $\ell \ll \delta_L$ ’ may not always act to enhance the propagation speed s_T by ‘amplifying microscopic transport processes.’ In fact, this is plausible solely beyond the threshold u' (i.e. for $N_B < 1$) in a regime where G transport prevails.

Two aspects solicit further investigation: 1) the nature (positive or negative) of effect of ‘fine-body’ turbulence $\ell \ll \delta_L$ on s_T below the threshold u' (i.e.

5.3. Summary: validity regime of DH2

for $N_B > 1$) and its associated expression, and 2) the underlying causes that govern the shift between different effects of turbulence on flame propagation.

Chapter 6

Towards Validation with the Leeds Experiment

In the previous chapters, a mechanism of the bending effect has been proposed based on the validity of DH1. Further, a recorded transition in the scalar flux transport has revealed a limitation of DH2. These investigations suggest that flame propagation can be limited by physical mechanisms inherent to the kinematics of propagation. Experimental investigations of the Leeds explosion vessel have suggested (Bradley et al., 1992), however, that thermo-chemical processes such as flame quenching constitute the primary mechanism of bending. Hence, in order to validate these two contrasting explanations of bending, a comparative study has been initiated with Leeds group.

In the following, the Leeds experiment and its recent 3D reconstruction capability are described along with preliminary comparisons with the parametric simulations conducted so far. Subsequently, the host of modifications made to the DNS method for carrying out the present work are elaborated. These modifications have resulted in the design of a computationally-efficient DNS. The simulation results will soon be compared with experimental results.

6.1 Leeds: expanding spherical explosions

As described in Section 1.1.4, the Leeds explosion vessel provided 2D flame surface measurements of an outward expanding spherical explosion previously

6. Towards Validation with the Leeds Experiment

(Bradley et al., 2011). Ongoing PhD work conducted by Ben Thorne has focused on conducting experimental measurements leading to 3D reconstructions of the flame surface (Nivarti et al., 2017). The key features of this new setup are described in the following passages.

Experimental setup

The Leeds explosion vessel provides a constant pressure environment for the initiation and outward propagation of spherical flame kernel in a turbulent premixed charge. With the overall construction of the vessel largely unchanged (Gillespie et al., 2000), the present setup allows a spark to be generated at the centre using a high-intensity laser issue through one of the quartz faces (see Figure 1.4). The fans rotate at a constant frequency during the ensuing flame propagation, so that the turbulence intensity u' and the integral length scale ℓ_0 are maintained throughout the experiment.

A laser sheet can be issued through one of the quartz windows. This sheet excites unburned seed particles in the mixture so that an instantaneous approximate flame surface contour may be located in the vessel (Gillespie et al., 2000). The laser sheet can also be made to swing across the explosion vessel by reflecting it on a rotating mirror. As the mirror rotates, the pulsating laser sheet captures several discrete slices across the vessel volume. A set of 2D flame surface contours is obtained as a result. Provided the laser sheet sweeps the vessel fast enough in comparison to the propagation speed of the flame, these contours may be assumed to correspond to an instantaneous flame surface; subsequently, the individual contours are spliced together to form a 3D reconstruction of the flame surface.

Given the constraints of the laser pulse frequency and the angular velocity of the rotating mirror, it is noted that stoichiometric flames propagate too fast for this assumption to remain valid. Hence, lean methane-air flames with $\phi = 0.6$ are considered which have a relatively lower propagation velocity even at high intensities of turbulence. This chemical composition was, therefore, agreed upon by the two groups as the basis of the comparative study. Some comparisons were made, nevertheless, using the previous stoichiometric flame

dataset obtained in Chapter 3. These preliminary comparisons have been discussed below.

6.1.1 Preliminary comparisons

Snapshots of the reconstructed flame surface are compared with the recorded data obtained in the parametric DNS. The case $u' = 10s_L$ is chosen as the point of comparison as shown in Figure 6.1a – surfaces obtained from the Leeds experiment and Cambridge DNS (at $c = 0.5$ at $t = 4\tau_0$) are illustrated

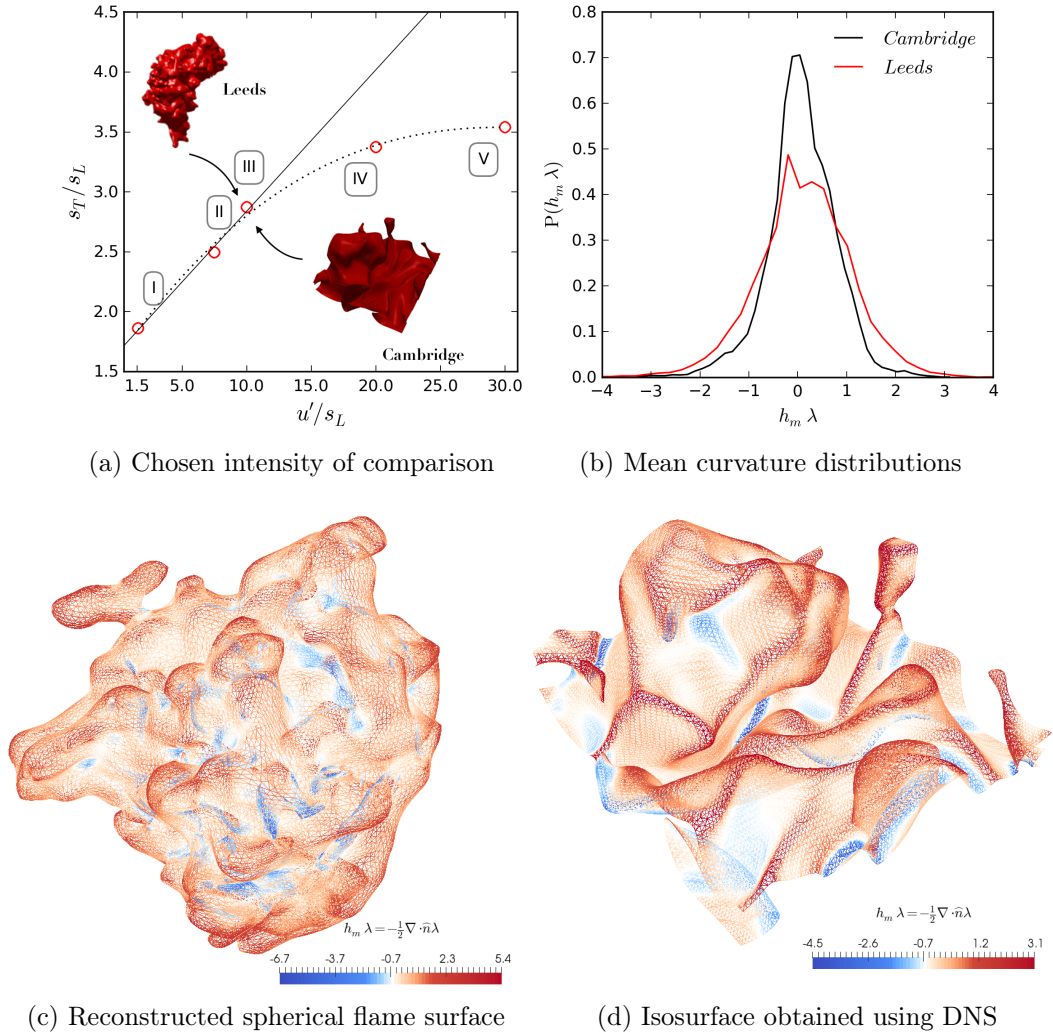


Figure 6.1 Preliminary comparisons of methane-air flame propagation in experiments (Leeds) with $\phi = 0.6$, and DNS (Cambridge) with $\phi = 1.0$. The same turbulence intensity u'/s_L is prescribed (panel a) in both cases. Curvature distributions are normalized using the Taylor length scale λ .

6. Towards Validation with the Leeds Experiment

alongside. In Figure 6.1b, these surfaces are compared quantitatively using the curvature distribution h_m obtained upon removing the average mean curvature component $\langle h_m \rangle$. Indeed h_m is found to have a very similar distribution on both flame surfaces. This indicates that the effect of various scales of turbulence on a given flame surface is similar for identical intensities. Yet it is evident that the spherical reconstruction has a wider spread of curvatures around the mean in comparison to the planar DNS isosurface. Such differences may be affected once the equivalence ratios of the two flames considered are matched.

In Figure 6.1c and Figure 6.1d the flame isosurfaces are visualized in order to aid a qualitative comparison. Local mean curvature h_m normalised with the Taylor length scale is shown using colours (red: positive, and blue: negative) on the isosurface. Significant similarities are observed in the two surfaces. Indeed, the scale of wrinkling appears to be the same for both surfaces. However, the planar isosurface tends to have locally cylindrical shapes whereas the spherical kernel exhibits more spherical shapes. Improved comparisons are sought between the experiment and DNS to elaborate on these differences. In the following, a DNS case is prepared so as to make suitable comparisons with experimental measurements in Leeds.

6.2 Cambridge: freely propagating flames

The following DNS setup is based on the method discussed in Chapter 2 with a range of modifications made to address better the experimental results.

6.2.1 Multi-step chemical kinetics

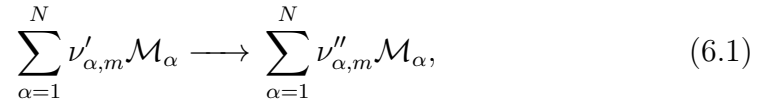
As discussed above, lean premixed turbulent flames display several phenomena that cannot be modelled adequately by the single-step chemical kinetic model used in the previous chapters. For instance, effects of non-unity species Lewis numbers are expected to be prominent in lean premixed flames. These effects may result in the modification of local mean curvatures on the leading and trailing edges. Moreover, effects of differential diffusion of various chemical species may alter flame propagation. Finally, the different reaction pathways

of these species may influence further the overall turbulent flame propagation.

In order to record the experimentally observed dynamics due to such effects in lean premixed flames, a 25-step reduced chemistry model by Smooke and Giovangigli (1991) has been used here in place of the single-step method adopted previously. The key implication of this change is that two terms of the species transport Equation 2.25 are now modelled differently. These are the reaction rate $\dot{\omega}_\alpha$ and the diffusive mass flux $\rho V_{\alpha,k} Y_\alpha$. In the previous chapters, $\dot{\omega}_\alpha$ was modelled using a single-step Arrhenius formulation (see Equation 2.5). The latter term $\rho V_{\alpha,k} Y_\alpha$ was modelled using a constant Lewis number assumption within the framework of Fick's law (see Equation 2.9). The new formulations for these terms are described below.

Reaction Rate

In an M -step reduced chemical kinetic description the overall combustion reaction (Equation 2.3) is modelled using a series of elementary reactions. A single elementary reaction may be written



where $m = 1, 2, \dots, M$ the index of the reaction. Stoichiometric coefficients of the various species α are denoted $\nu'_{\alpha,m}$ in the reactant side and $\nu''_{\alpha,m}$ in the product side. The rate of this m^{th} elementary reaction is given then by a generalised Arrhenius expression

$$\dot{\omega}_m = k_m \prod_{\alpha=1}^N \left[\frac{\rho Y_\alpha}{W_\alpha} \right]^{\nu'_{\alpha,m}}, \quad (6.2)$$

where

$$k_m = A_m T^{n_m} e^{-\frac{E_{a,m}}{R^0 T}} \quad (6.3)$$

and the constants A_m , n_m , and $E_{a,m}$ prescribed *a priori* for each elementary reaction m . It follows that the rate of formation of each chemical species α is

6. Towards Validation with the Leeds Experiment

expressed as

$$\dot{\omega}_\alpha = -W_\alpha \sum_{m=1}^M (\nu''_{\alpha,m} - \nu'_{\alpha,m}) \dot{\omega}_m, \quad (6.4)$$

which is the species-weighted sum of the rates of reaction $\dot{\omega}_m$ over all M steps. It is seen therefore, that the fuel consumption rate $\dot{\omega}_F$ for instance would depend on each elementary reaction step it participates in within this description. As a consequence, the overall rate $\dot{\omega}_F$, which dictates the value of s_T , will depend on the availability of reacting species participating in those elementary steps. Hence, the M -step reduced chemical mechanism provides a more detailed consideration of the dependence of s_T on local mixture composition. In this manner it may provide a more realistic description of the combustion process and its burning velocity.

Diffusive Mass Fluxes

In order to compute the diffusive mass flux $\rho V_{\alpha,k} Y_\alpha$ for species α , a mixture-averaged transport formulation in the absence of thermal diffusion flux (Soret effect) and diffusion thermal flux (Dufour effect) is considered here. The molecular transport coefficients for the mixture are assembled from molecular transport data for each individual species. This approach is more accurate, and also allows for greater generality in the treatment of molecular transport phenomena. Hence, for the diffusive mass flux, Fick's Law is replaced by

$$\rho V_{\alpha,k} Y_\alpha = -\rho D_\alpha \frac{\partial Y_\alpha}{\partial x_k} + \rho D_\alpha Y_\alpha \frac{1}{W_m} \frac{\partial W_m}{\partial x_k} + \rho D_\alpha Y_\alpha \left(1 - \frac{W_\alpha}{W_m}\right) \frac{1}{P} \frac{\partial P}{\partial x_k} \quad (6.5)$$

where D_α is now the mixture-averaged diffusion coefficient for species α and W_m is the effective molar mass for the mixture given by

$$\frac{1}{W_m} = \sum_{\alpha=1}^N \frac{Y_\alpha}{W_\alpha}. \quad (6.6)$$

For completeness it should be noted that the viscosity is also now a mixture-averaged quantity. Values of viscosity μ_α and thermal conductivity λ_α for each species, together with values of the binary diffusion coefficients $D_{\alpha\beta}$ for each pair of species, are obtained using a set of polynomial fits (Cant, 2013).

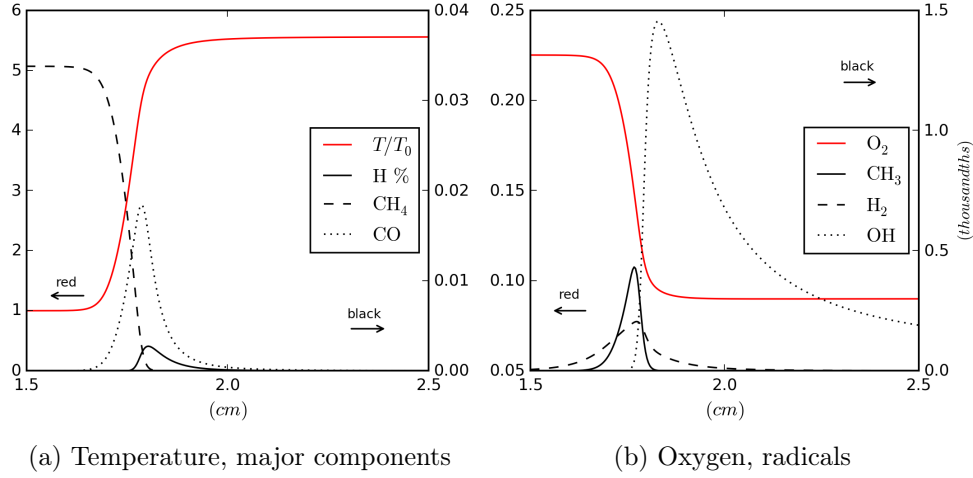


Figure 6.2 Profiles of thermo-chemical variables: temperature and chemical components (left) of the composition vector as well as radicals (right) computed using a 25-step chemical kinetic model.

In the 25-step chemical kinetic model chosen here (Smooke and Giovangigli, 1991), the composition vector consists of 16 chemical species. This is given by $[CH_4, O_2, CO_2, H_2O, H_2, O, OH, H, HO_2, H_2O_2, CO, CH_2O, HCO, CH_3, CH_3O, N_2]$. The computation of these species including formaldehyde CH_2O and hydroxyl radical OH allows for a head-to-head comparison with experimental measurements. The detailed chemical reaction rate as well as diffusion flux description in this framework allows for a more accurate simulation of the pre-heat as well as reaction zone structure. The chemical mechanism used here (Smooke and Giovangigli, 1991) has, in fact, been tailored for lean flames and excludes C_2 chemistry. Figure 6.2 shows the profiles of thermo-chemical variables computed based on this chemical mechanism.

Chemical Resolution Constraints

Initial thermo-chemical field (density ρ , temperature T , and species mass-fractions Y_α) in the turbulent flame simulation is specified with an unstrained 1D laminar flame solution profile calculated *a priori*. In the present case, the equivalence ratio $\phi = 0.6$ and inlet unburned mixture conditions $p = 1$ bar and $T = 300$ K. The laminar flame speed $s_L = 0.122$ m s⁻¹ and thickness $\delta_L = 0.928$ mm are obtained *a priori* from a 1D simulation with a fine mesh

6. Towards Validation with the Leeds Experiment

$N = 1024$ within a domain of length $L = 1\text{ cm}$. Such a fine resolution is in principle unnecessary for the turbulent flame simulation and a coarser grid may be used.

In order to find the coarsest grid that can stably simulate the chemical structure, a convergence study is conducted using 1D laminar flame simulations in this domain of length $L = 1\text{ cm}$. Beginning with an extremely fine grid $N = 1024$ that corresponds to a thermal flame thickness resolution $\delta_L^{fine}/\Delta x \approx 100$, the grid is coarsened by factors of 2 until the solution becomes unstable due to lack of adequate resolution. Close to the point of stability-loss, grids are refined gradually until the resolution requirement is narrowed to within $\delta_L^{fine}/\Delta x_c \pm 1$. Figure 6.3 shows the number of steps required N_c to obtain the converged value of laminar flame speed $s_L^{fine} = 0.122\text{ ms}^{-1}$ for each resolution level which is quantified by $\delta_L^{fine}/\Delta x$ for a fixed domain length. The resolution is found to be inadequate at $\delta_L^{fine}/\Delta x \approx 22.3$ where no convergence is achieved. Hence, this value is taken to be a resolution constraint of the present chemical kinetic model. This constraint is also used later for estimating the optimal domain size for the DNS.

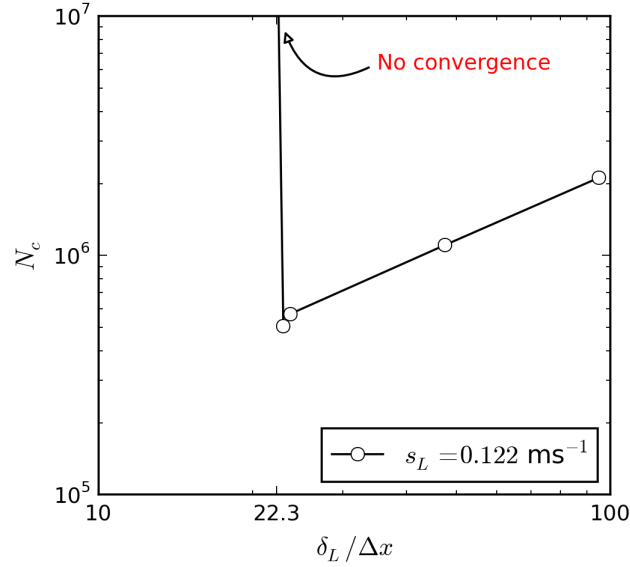


Figure 6.3 Grid resolution study to determine the spatial resolution requirement for the 25-step methane-air chemical kinetic model. Convergence fails for grids with $\Delta x \gtrsim \delta_L/22.3$, where $\delta_L = 9.3\text{ mm}$ denotes the value obtained *a priori* using a fine grid.

6.2.2 Fast adaptive timestep control

Numerical solution of 16 additional transport equations imposes a severe computational expense on the simulation. It is critical, therefore, that the desired statistically-stationary solution state be achieved in as few timesteps as possible.

A direct approach to reducing the number of timesteps would be to use large timesteps. The magnitude of timestep Δt is restricted, however, by the stability range of the numerical method. The domain of stability is characterised by a range of the Courant-Friedrichs-Lewy (CFL) number $\text{CFL} \equiv U\Delta t/\Delta x$ specific to the numerical integration scheme, where U is a characteristic velocity such as the sound speed a . In implicit integration methods, the range of CFL stability is much higher in comparison to the explicit method used presently. However, the additional stability comes with added computational expense and complexity involved in the matrix inversion that is required in implicit integration.

In explicit methods, the timestep size $\Delta t^{(n)}$ may be calculated adaptively based on a pre-specified stable CFL number for a uniform grid Δx . The adaptive timestep control strategy introduced in Section 2.3 presents yet another approach to computing timestep sizes adaptively. Rather than using a fixed CFL number, a fixed error tolerance $\hat{\epsilon}$ is specified. Thus, appropriate timestep sizes $\Delta t^{(n)}$ are computed based on PID control that maintains this error tolerance $\hat{\epsilon}$. This precludes *a priori* knowledge of stability regions of the numerical scheme.

Variation of the timestep size $\Delta t^{(n)}$ computed using PID control (Equation 2.49) is shown in Figure 6.4 using black lines. The profiles of timestep history in different simulations (shown in Figure 6.4a, Figure 6.4b and Figure 6.4c) are denoted by the PID exponents α , β and γ . These profiles illustrate a general trend; after an initial period of small step sizes the PID controller reaches a steady-state where the step size fluctuates about a fixed value. In a 1D laminar flame solution (black line in Figure 6.4a), this corresponds to $\text{CFL} \approx 1.2$, whereas in a periodic HIT simulation (black line in Figure 6.4b) this timestep corresponds to $\text{CFL} \approx 0.2$. Furthermore, a much

6. Towards Validation with the Leeds Experiment

lower CFL ≈ 0.01 is achieved in a fully-resolved turbulent flame propagation case using PID control.

This highlights that the numerical solutions so far have been performing inadequately due to an inefficient adaptive strategy of selecting timestep sizes. The timestep sizes $\Delta t \sim 10^{-10}$ s are rather small and render the overall solution to be computationally infeasible. Therefore, the control strategy is modified in order to improve timestep sizes. This is done by investigating three aspects: limiters, cutoffs and exponents.

Limiters and cutoffs

In the PID controller used so far, timestep selection has been constrained by imposing a *limiter* that restricts the maximum ratio of step size $\sigma_n = \Delta t^{(n+1)}/\Delta t^{(n)}$ provided by the controller to a small value $\hat{\sigma}_n$. In other words, the selected timestep is given by $\Delta t^{(n+1)} = \min(\hat{\sigma}_n, \sigma_n)\Delta t^{(n)}$. Limiters of this kind avoid the selection of relatively large timesteps so that large errors may be avoided at subsequent steps of the numerical solution. However, this turns out to be a rather severe restriction. The timestep profiles discussed above each indicate a period of slow growth to a steady timestep size (black lines in Figure 6.4). Such a phase of relatively-small timesteps is neither necessary numerically.

The reason for the gradual growth of $\Delta t^{(n)}$ is evident in Figure 6.4a. Timestep size ratios $\sigma_n \equiv \Delta t^{(n+1)}/\Delta t^{(n)}$ provided by the controller (black dots) are restricted to $\hat{\sigma} = 1.1$ even though the corresponding error ratios $\hat{r}_n/\hat{\epsilon}$ are small (x axis in Figure 6.4d). The error ratio shown here denotes the ratio of the maximum L_2 norm of the solution $\hat{r}_n$ to the pre-specified error tolerance $\hat{\epsilon}$. In contrast, the unlimited profile with $\hat{\sigma} = \infty$ shown alongside exhibits the same errors but with much larger step size ratios (red dots in Figure 6.4d). This suggests that the use of limiters may be abandoned entirely, saving essential computational time.

Despite the performance of the unlimited scheme (red dots in Figure 6.4d), a smooth limiter proposed by Söderlind and Wang (2006) has been implemented presently. Limiting of this sort allows large timestep ratios to be

6.2. Cambridge: freely propagating flames

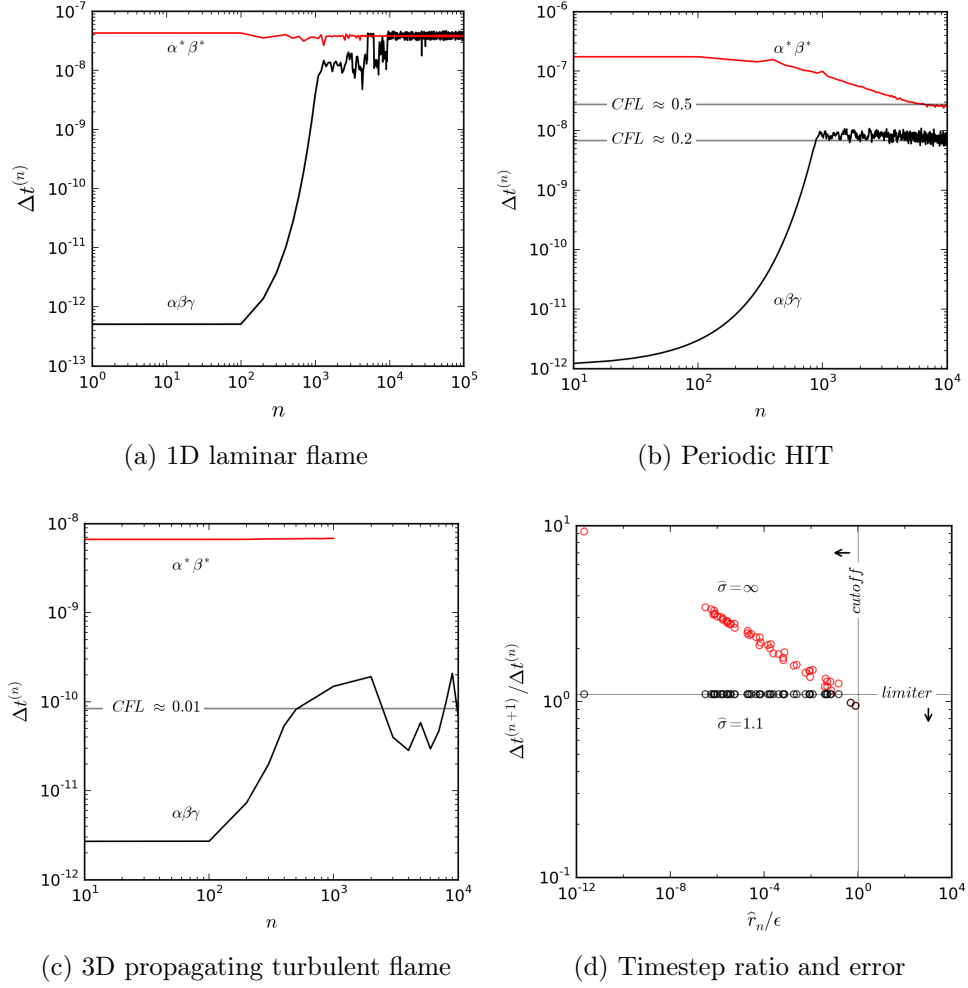


Figure 6.4 Timestep history (panels a,b, and c) as well as timestep ratios (panel d) obtained using the PID controller $\alpha\beta\gamma$ and the modified PI4.2 controller $\alpha^*\beta^*$ due to Söderlind (2002) for various test problems.

accepted in a safe manner, avoiding disastrous consequences at later steps in the numerical integration. In this approach, the timestep ratio obtained from the controller is limited as

$$\hat{\sigma}_n = 1 + \text{LIM} \cdot \tan^{-1} \left(\frac{\sigma_n - 1}{\text{LIM}} \right), \quad (6.7)$$

where LIM is a pre-specified constant value. The formulation above restricts timestep ratios σ_n to within a factor of the coefficient LIM. This means that the timestep ratio provided by the controller is bounded within $1/\text{LIM} < \sigma_n < \text{LIM}$, but in a smooth manner.

6. Towards Validation with the Leeds Experiment

Similarly, *cutoffs* are used normally to impose a restriction on the timestep selection whenever the error ratio $\hat{r}_n/\hat{\epsilon} > 1$ (as indicated by the vertical line in Figure 6.4d). Since large errors are not usually incurred in the present framework, cutoffs have not been investigated further.

Tuning exponents

Choice of controller exponents is a central issue in dynamic control of timestep selection. As part of the investigation of small step sizes provided by the previous PID controller, it was concluded that the tuning exponents were insufficiently tuned. For instance, the variation of a single exponent, say γ , would result in significant improvements of the timestep the controller converges upon. Hence, exponents suggested by Söderlind and Wang (2006) have been used in the present simulation. In fact, these correspond to the PI4.2 controller where the exponent $\gamma = 0$ (Söderlind, 2002), i.e.

$$\Delta t^{(n+1)} = \text{TOL} \cdot \left(\frac{\hat{\epsilon}}{\hat{r}_n} \right)^{\alpha^*} \left(\frac{\hat{\epsilon}}{\hat{r}_{n-1}} \right)^{\beta^*} \Delta t^{(n)} \quad (6.8)$$

where $\alpha^* = 0.6$ and $\beta^* = -0.2$ as discussed by Söderlind and Wang (2006). The error tolerance is shifted to a smaller value than before $\hat{\epsilon} = 10^{-5}$ and the safety factor is also constrained further $\text{TOL} = 0.8$. So as to make obvious the change between the previous and present controller, this is referred to as PI controller as opposed to the PID controller.

The timestep profiles obtained in this manner are presented alongside the profiles shown earlier in Figure 6.4 using red lines. In all profiles – the 1D laminar solution (Figure 6.4a), the 3D HIT solution (Figure 6.4b) and the 3D flame propagation solution (Figure 6.4c) – the timesteps rise immediately to the value converged upon due to the absence of limiting. In other words, there is no period of gradual growth beginning with the initially prescribed value as seen in the black lines. Moreover, the profiles are all much smoother than the corresponding profiles obtained using the PID controller with strict limiting (black lines). The smooth profile may also be attributed to the loss of instabilities associated with the γ term.

In Figure 6.4, it is also evident that the actual magnitude of the timestep converged upon by the PI controller is higher than the PID controller for most cases. For instance, apart from the 1D laminar flame solution case (Figure 6.4a), the timestep size improves nearly threefold for the HIT simulation (Figure 6.4b) and almost by two orders of magnitude in the turbulent flame propagation case (Figure 6.4c). Due to these merits of the PI controller, it is implemented in the present simulations. Further improvements are sought, however, including the ability to reject solutions that incur too much error. These are related to the cutoffs neglected above.

6.2.3 Linear turbulence forcing

In the Leeds setup, the intensity $u'_0 \equiv u'|_{t=0}$ of homogeneous isotropic turbulence (HIT) is maintained throughout flame propagation by keeping the fans on. In the DNS simulations conducted so far, the initial u'_0 was subject to decay. Furthermore, the rate of decay is a function of velocity gradients, so that the high-intensity cases are prone to faster turbulent decay. This is undesirable; the altered intensity u' may change the expected regime of combustion.

Investigating this effect further, the source of turbulent decay is located in the viscous term in the momentum equation

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j u_i) = -\frac{\partial}{\partial x_i}(p) + \frac{\partial}{\partial x_j}(\tau_{ji}) + f_b, \quad (6.9)$$

recalled here from Chapter 2, with the exception that a body-force f_b is also considered here. In the absence of body-forces $f_b = 0$, as in the simulations so far, the HIT simulation exhibits an exponential temporal decay of turbulent kinetic energy $\partial k / \partial t$ at the rate of turbulent dissipation

$$\varepsilon = \nu \langle \nabla \mathbf{u} : \nabla \mathbf{u} \rangle, \quad (6.10)$$

as shown in Figure 2.4. So as to mitigate the extent of turbulent decay, the flame simulations so far employed an inflow BC which convected downstream a frozen turbulence state with intensity u'_0 . Nevertheless, the convected turbulence undergoes decay from the inlet to the flame leading edge (as reported

6. Towards Validation with the Leeds Experiment

in Table 3.2). In other words, despite the inflow BC, the leading edge intensity $u'_{le} \neq u'_0$. The relatively small domain reduces the scope of this decay, but the domain size warranted by the present comparisons do not allow this simplification. Hence, a strategy of turbulent forcing is adopted here.

In an HIT simulation based on the solution of Equation 6.9, the average rate of change of turbulent kinetic energy is given by

$$\frac{\partial \rho \langle \mathbf{u} \cdot \mathbf{u} \rangle}{\partial t} = -\rho \varepsilon + \langle \rho \mathbf{u} \cdot \mathbf{f}_b \rangle, \quad (6.11)$$

in the presence of a body-force $\mathbf{f}_b$. Evidently, the body-work term $\langle \rho \mathbf{u} \cdot \mathbf{f}_b \rangle$ acts in addition to dissipation $\rho \varepsilon$. The strategy for turbulence forcing proposed by Lundgren (2003) exploits this aspect. An ‘artificial’ body-force is added in such a manner that the decay due to turbulent dissipation is balanced. Evidently, a body-force $\mathbf{f}_b = Q(\mathbf{u} - \langle \mathbf{u} \rangle)$ proportional to the local turbulent fluctuation results in the corresponding work term of form $Q \langle \mathbf{u} \cdot \mathbf{u} \rangle$ provided $\langle \mathbf{u} \rangle = 0$. Hence, the coefficient Q may then be chosen such that turbulent decay due to dissipation is balanced exactly by the work done due to forcing leading to

$$0 = -\rho \varepsilon + Q \langle \rho \mathbf{u} \cdot \mathbf{u} \rangle, \quad (6.12)$$

which provides $Q = \varepsilon / \langle \mathbf{u} \cdot \mathbf{u} \rangle = \varepsilon / 2k$ for incompressible flows where the turbulent kinetic energy $k \equiv \langle \mathbf{u} \cdot \mathbf{u} \rangle / 2$. In this manner, Lungren’s forcing strategy (Lundgren, 2003) may be used to maintain the initial turbulence intensity u'_0 throughout the simulation.

This approach to turbulent forcing has been found satisfactory in many simulations (Rosales and Meneveau, 2005; Ishihara et al., 2009). In order to extend its applicability further, Petersen and Livescu (2010) have proposed a modification to address compressible statistically-stationary turbulent flows. Such a modification has been found challenging to implement as well as unnecessary here due to the low Mach numbers involved. Carroll and Blanquart (2013), however, investigated strategies to improve the rate of convergence towards statistical stationarity. A modification of the linear forcing term was proposed as $\mathbf{f}_b = Qk_0/k\mathbf{u}$ where k_0 is the initial kinetic energy. The outcome

6.2. Cambridge: freely propagating flames

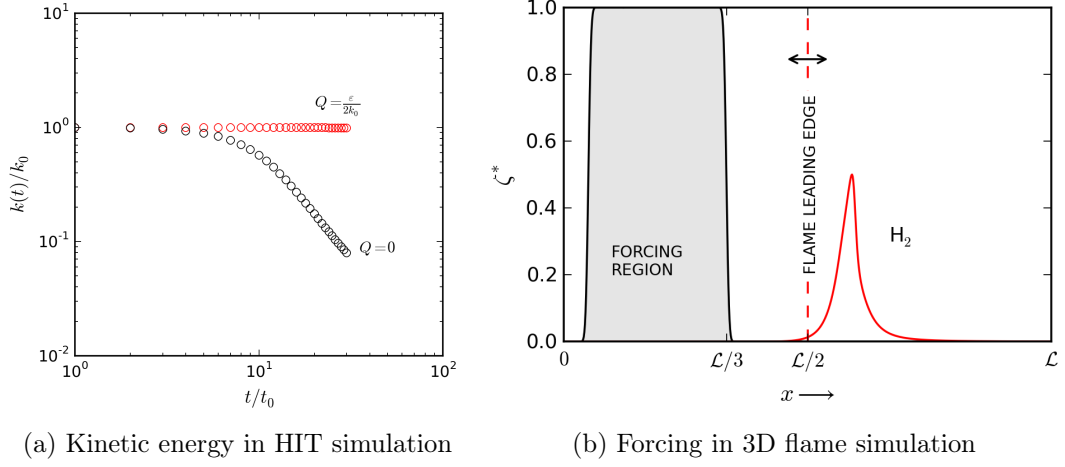


Figure 6.5 Turbulent forcing strategy. Left: time evolution of mean turbulent kinetic energy $k(t)$ for an HIT simulation with $Q = 0$ and with $Q = \varepsilon/(2k_0)$. Right: region of turbulent forcing in the flame simulation.

of this modification is that the value $Q = \varepsilon/2k_0$ thus obtained from Equation 6.11 is constant. In Figure 6.5a, results from using this forcing term are compared with the the decaying HIT simulations conducted previously. It is clear that the forced simulation (red dots) undergoes little to no fluctuation, whereas the decaying simulation (black dots) loses 90% of the energy in the same time.

Lundgren’s strategy (Lundgren, 2003) along with the modification proposed by Carroll and Blanquart (2013) is followed in the present simulations. This contrasts with some other forcing strategies developed previously. For instance, Eswaran and Pope (1988) follow a ‘naturally expected’ forcing condition in turbulent flows. Energy is injected only at low wavenumbers in spectral space. The Navier-Stokes equations are allowed to re-distribute subsequently the energy over smaller scales. Such a strategy, however accurate, is not adopted here for the sake of convenience. Nevertheless, it would be interesting to explore these alternatives in future.

Due to the merits of Lundgren’s forcing strategy (Lundgren, 2003), it has been employed recently in several DNS studies. For instance, Savard and Blanquart (2015) uses this strategy to force the turbulent flow in their simulation of high-intensity turbulent flame propagation. The forcing term is

6. Towards Validation with the Leeds Experiment

effected throughout the domain of flame propagation. Given that the forcing strategy is valid only for incompressible HIT simulations, the validity of such approaches may be questioned. Furthermore, concerns (Quadrio et al., 2016) have arisen recently regarding the effect turbulence forcing may have on the statistics collected. The present simulations, therefore, take due consideration of this, restricting the forcing to a small region of the domain upstream of the flame. The location of forcing is shown in Figure 6.5b. Both the inlet as well as the flame leading edge are avoided by using a multiplier coefficient $\zeta^* \in [0, 1]$ in $\mathbf{f}_b = \zeta^* Q k_0 / k \mathbf{u}$ such that $\zeta^* \neq 0$ only in the specified region. With the exception of a mean axial velocity, this region of forcing indeed resembles an HIT simulation case. This approach is expected to mimic the effect of fans in the Leeds experiment.

6.2.4 Computational setup and regime

Domain size optimisation

Small-scale turbulence-flame interactions are critical to the present comparison. Yet the role of large-scales must be simulated at the same time for at least two reasons. Firstly, the simulated energy spectrum represents the cascade process realistically if a large separation between integral and Kolmogorov length scales is considered (Pope, 2001). Secondly, the problem of flame propagation in the Leeds vessel corresponds to a regime between coarse-body and fine-body turbulence. Hence, it is required that ℓ_0/δ_L be as large as possible while $\eta/\delta_L < 1$. Therefore, the quality of comparison with experiment is a function of the computational domain size.

It is computationally not feasible, however, to match the experiment exactly in size. Hence, an attempt is made to maximise the possible size of the domain given the constraints of small-scale resolution. This may be framed as an optimisation problem with the following constraints

1. Resolution of chemistry: the maximum spatial step size that can stably simulate the 25-step reduced chemical kinetic model is $\Delta x_c \approx \delta_L/23$ (as obtained in Figure 6.3).

6.2. Cambridge: freely propagating flames

2. Resolution of turbulence: the maximum spatial step size that can faithfully resolve small-scale turbulent motion is $\Delta x_f = \eta/2.0$ where $\eta = f(L, u')$ (as provided in Equation 3.5). This is directly proportional to L and inversely proportional to u' .
3. Expense of computation: the number of points N used to resolve the above criteria along the smallest dimension L determines the overall computational expense. For an inflow-outflow domain with a relatively longer axial length sL , the total computational expense varies as sN^3 .

The variation of these constraints with domain size is shown in Figure 6.6. Adequate resolution of chemistry imposes a constant constraint on the mesh size (dashed blue line) regardless of the domain size. Resolution of turbulence Kolmogorov scale η , however, imposes a monotonically diminishing constraint (dashed red line). In other words, a larger mesh size Δx may be used to resolve η expected in a domain of larger width L .

The variation of computational expense N^3 corresponding to each of these constraints $N = L/\Delta x$ is shown along side in Figure 6.6 using solid lines. The step size imposed by turbulence $\Delta x_f = \eta/2$ increases as a power $\alpha = 1/4$ of

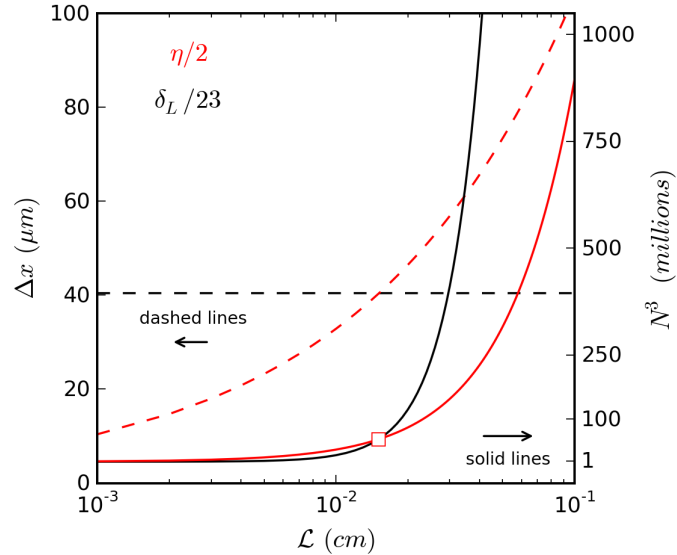


Figure 6.6 Resolution constraints of chemistry (black dashed lines) and turbulence (red dashed line) as well as the corresponding computational expense (black and red solid lines, respectively) as a function of DNS domain size.

6. Towards Validation with the Leeds Experiment

L^α . Hence, the related computational expense (solid red line) varies as $L^{1-\alpha}$. The step size imposed by chemistry $\Delta x_c = \delta_L/23$, however, remains fixed for all L . The number of points required due to this constraint (solid black line) increases, therefore, in direct proportion to L . As a consequence of these varying rates of growth in computational expense, the chemistry constraint becomes more expensive at a critical L (red square in Figure 6.6). In fact, this critical value $L \approx 0.015\text{m}$ corresponds to the largest configuration for which N is determined by the flow resolution constraint Δx_f , and at the same time satisfies the chemical constraint. Hence, this is the domain size chosen in the present simulation.

In principle, this algorithm can be generalised, allowing the *a priori* choice of a few essential physical parameters most relevant to the simulation, such as the regime of combustion. The task of the algorithm would then be to provide the computational parameters such as domain size and integral length scale ℓ_0 . Such algorithms are being investigated presently in order to provide computationally efficient design of DNS studies.

Combustion regime

In order to set abreast the Leeds estimates (Bradley et al., 2013; Bagdanavicius et al., 2015) of the combustion regime, a Karlovitz number is used as follows

$$K = \frac{1}{4} \left(\frac{u'}{s_L} \right)^2 \text{Re}^{-\frac{1}{2}} \quad (6.13)$$

where the Reynolds number $Re \equiv \ell_0 u' / \nu$. The use of this form of Ka is motivated further by its historical use in previous experimental studies (Bradley et al., 2011). The formulation of Equation 6.13 would predict localized flame extinctions to expected to occur for $K \geq 1.0$ in unity Lewis number mixtures. In order to compute the normalised Reynolds number, the kinematic viscosity ν is computed as $\nu \sim \delta_L s_L$, maintaining consistency with experiments (Bagdanavicius et al., 2015).

A regime diagram is presented in Figure 6.7 using the new Karlovitz number definition. The value $K = 1.0$ is taken to separate the flamelet and distributed

6.2. Cambridge: freely propagating flames

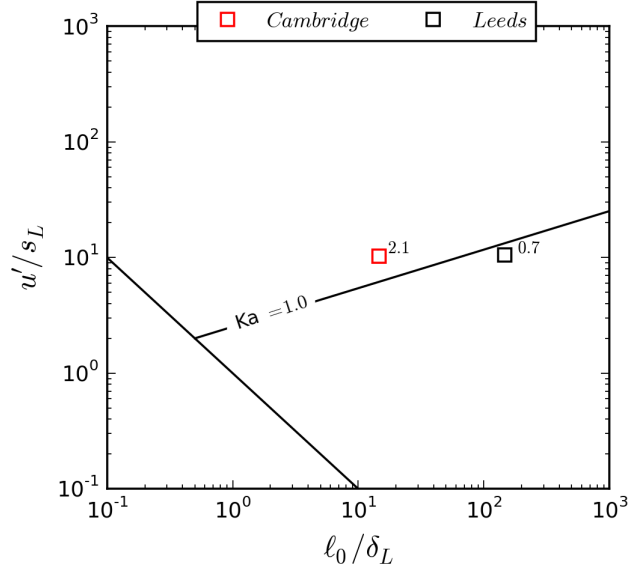


Figure 6.7 Combustion regimes corresponding to the Leeds experiment and the Cambridge DNS in the regime diagram with a modified definition of Ka.

Table 6.1 Input parameters for the Leeds-Cambridge study.

Parameter	Cambridge	Leeds
Ambient pressure, P_a	1 bar	1bar
Inlet temperature, T_u	300K	300K
Kinematic viscosity, ν	$1.585 \times 10^{-5} \text{ m}^2/\text{s}$	$1.62 \times 10^{-5} \text{ m}^2/\text{s}$
Equivalence ratio, ϕ	0.6	0.6
Laminar flame speed, s_L	0.122 ms^{-1}	0.119 ms^{-1}
Laminar flame thickness, δ_L	$1.29 \times 10^{-3} \text{ m}$	$1.36 \times 10^{-3} \text{ m}$
Integral length scale, ℓ_0	0.002m	0.02m
Turbulence intensity, u'	1.25m/s	1.25m/s
Karlovitz number, K	2.1	0.7

regimes of combustion. The normalised turbulence intensity $u'/s_L = 10.0$ for both studies. On the other hand, the Karlovitz numbers are slightly different due to the disparity in integral length scales. Values of these parameters as relevant to the present study have been tabulated in Table 6.1.

6.3 Summary: the ongoing comparative study

Initial comparisons with the Leeds experiment demonstrate a similarity in curvature distributions between two flame surfaces. The ongoing investigation has warranted several modifications of the DNS solver.

Firstly, a 25-step reduced chemical kinetic model is studied and implemented for simulating lean methane-air combustion (Smooke and Giovangigli, 1991). The detailed description of chemical pathways and Lewis number effects in this framework allows for realistic simulations comparable to experiments. Secondly, a modified form (Carroll and Blanquart, 2013) of Lundgren’s forcing strategy is implemented to maintain the intensity of upstream turbulence.

Furthermore, the computational expense of the necessary large-scale detailed simulations are reduced by an improved parameter selection in the adaptive timestep controller (Söderlind and Wang, 2006). Finally, in order to better address the experimental setup, the largest possible domain size is designed. Resolution constraints of turbulence and chemistry are satisfied in a computationally feasible manner using a novel strategy.

It remains to be seen if fully-developed flames of the same turbulence intensity will exhibit similar propagation behaviours as recorded in the preliminary comparisons. As pursued with the previous dataset, Damköhler’s hypotheses will be verified as a starting point.

Chapter 7

Conclusion

This thesis investigates the effects of turbulence intensity u' on flame propagation in gas mixtures. It focuses upon ‘the bending effect’ of turbulent burning velocity $s_T(u')$. A DNS approach is adopted in light of the recent computational advances. In the present DNS approach, governing equations of turbulent reactive flow are solved in compressible form. Using this method, two lines of investigation are pursued.

The first comprises the design, generation and analysis of a parametric DNS dataset that simulates flame propagation in the TRZ regime. The bending effect of $s_T(u')$ is captured upon increasing u' systematically across this regime (see Chapter 3). Subsequently, the validity of Damköhler’s first and second hypotheses is investigated in the dataset generated. Damköhler’s first hypothesis (DH1) is found to be valid throughout the dataset (see Chapter 4). Motivated by this finding, the framework of the FSD approach is used to study the underlying mechanisms governing flame propagation. The bending effect is thereby explained in terms of a competition between components of the FSD source-term. Damköhler’s second hypothesis (DH2) is found to have limited validity in the dataset (see Chapter 5). Minimal conditions for the validity of DH2 are expressed in terms of scalar flux transport regimes.

The second line of investigation aims to verify the explanation proposed for the bending effect so far. Experiments are conducted in the Leeds explosion vessel under conditions of bending informed by the parametric study. In order to facilitate comparisons, a new DNS is designed to simulate flame propagation

7. Conclusion

under appropriate conditions (see Chapter 6). Several modifications are made to the DNS approach adopted previously so as to address comprehensively the goals of this investigation. Upcoming comparative results may help contrast the proposed explanation with the mechanism of bending proposed historically by the Leeds group.

Conclusions drawn from each line of investigation are summarized below.

Parametric study of the bending effect

Firstly, the bending effect of $s_T(u')$ does not depend necessarily upon localized flame quenching as is widely believed (Bradley, 1992). Indeed, the reaction zone may remain intact (see Figure 3.7 and Figure 3.8) even in turbulence with $u' > 10s_L$. The emergent flame propagation may exhibit the bending effect nevertheless (see Figure 3.9).

Secondly, turbulent flame surface area A_T and Flame Surface Density Σ continue to govern s_T (according to DH1) in the bending region (see Figure 4.4). This contrasts with recent experimental measurements in $u' > 10s_L$ (Gülder and Smallwood, 2007; Wabel et al., 2016). The present computations make it plausible that bending occurs as a consequence of the kinematic response of the flame rather than its structural disruption.

Thirdly, the contributions to Σ of local flame surface curvatures h_m do not necessarily ‘even out’ as presumed in previous explanations of the bending effect (Bradley et al., 1992). Indeed, local displacement speed s_d regulates the overall curvature contribution $s_d h_m$ to the source-term of Σ . This contribution is negative and increases in magnitude with u' , whereas the contribution of strain rate a_t remains positive. The overall Σ for any given u' as well as the corresponding s_T emerges from the balance between destructive curvature propagation $s_d h_m < 0$ and extensive tangential strain $a_t > 0$ (see Figure 4.10).

Lastly, the enhancement of s_T due to turbulent diffusion as dictated by DH2 is limited to high-intensity turbulence where gradient transport operates (see Figure 5.7). In low-intensity turbulence corresponding to the Bray number $N_B > 1$, counter-gradient transport prevails, so that $D_T < 0$, and the DH2 expression is invalidated. This suggests that Damköhler’s mechanisms may

neither act ‘always’ nor ‘enhance’ s_T as hypothesized (Damköhler, 1940).

Ongoing comparisons with the experimental measurements in Leeds might help validate these conclusions. Insights gained so far are summarized below.

Comparisons with the Leeds experiment

Initial comparison between the experimentally reconstructed flame surface and the corresponding parametric DNS isosurface show striking similarities (see Figure 6.1 and Figure 6.1b). This suggests that curvature effects may indeed play an important role in overall flame propagation characteristics. Conclusions are reserved at present pending the completion of the ongoing simulation. Design of the corresponding DNS has provided the following conclusions.

Firstly, the detailed 25-step chemical kinetic model (Smooke and Giovangigli, 1991) has a resolution constraint of $\Delta x_c \lesssim \delta_L^{fine}/22.3$ (see Figure 6.3). The lean methane-air flame simulated using this model addresses non-unity Lewis number effects thereby complementing the parametric study.

Secondly, the modified form (Carroll and Blanquart, 2013) of the forcing scheme introduced by Lundgren (2003) maintains turbulent kinetic energy in an HIT simulation (see Figure 6.5a). The upstream region in an inflow-outflow flame configuration may be forced selectively to maintain the regime of combustion (see Figure 6.5b).

Thirdly, adaptive timestep selection based on the PID controller (Kennedy and Carpenter, 2003) used in the parametric investigation is improved using a controller developed by Söderlind and Wang (2006). Not only is the timestep history more stable, but the magnitude of timesteps also increases by nearly two orders of magnitude in the flame simulation (see Figure 6.4).

Lastly, an optimal size of the DNS domain can be obtained by considering various constraints due to resolution requirements on the one hand and computational requirements on the other. On these lines, a basic investigation has provided a relatively large domain configuration with size $L = 0.015\text{m}$ three times the previous parametric study (see Figure 6.6). This optimized domain helps enhance the length scale ratio ℓ_0/δ_L .

Several possibilities for further investigation have emerged. These comprise

7. Conclusion

ongoing work being pursued in collaboration with researchers in the international community as well as proposals for future work.

Ongoing and future work

Firstly, the effect of flame configuration on efficiency factors is being investigated. These include the stretch factor I_0 (seen in Figure 4.5) and efficiency function α (seen in Figure 5.6). DNS datasets of a V-flame and a stagnation flame are being analysed for this purpose in collaboration with Dr. Umair Ahmed (University of Manchester). The objective is to provide insights for flamelet modelling of turbulent premixed flames.

Secondly, the flame response to transient strain is being investigated under the guidance of Dr. Alan Kerstein (Consultant, USA). Correlations between the normal displacement speed s_n and the local strain a_t are being studied (on the lines of Figure 4.6 and Figure 4.9). This may help address the effect of the strain component a_t on the propagation component $s_d h_m$ of the FSD source-term.

Thirdly, a comparison of the present DNS dataset with a similarly obtained dataset (at the University of Lund, Sweden) using an incompressible formulation (Yu et al., 2015) is being pursued. The comparisons are expected to shed light on the role of gas expansion on computed s_T values in the bending effect.

At the same time, recent discussions with Prof. Ö. Gülder and co-workers (University of Toronto) have highlighted similarities recorded in the computed Σ profile (see Figure 4.1b) with experimentally measured profiles. The recent study conducted by Kheirkhah and Gülder (2015) links the increasingly upstream peaking of Σ with a transition to counter-gradient transport (as also presently recorded). This line of investigation is being pursued further.

Furthermore, improvements in adaptive timestep size (see Section 6.2.2) have led to a detailed discussion with Dr. Marc Day (Lawrence Berkeley National Laboratory, USA). Assessment of the solution error and convergence properties is being pursued to formalize the new control procedure.

Finally, the success of the optimization study (see Section 6.2.4) shows

that it is possible to automate the design of a DNS configuration. Algorithms developed for this purpose may also be used in the context of experiments in which an optimized search for design criteria is usually the centre point of all measurements. Indeed, similar algorithms may also be applied to experimental and DNS datasets to reveal critical relationships in the data.

To c or not to c ?

A central issue of turbulent flame propagation modelling is the applicability of the flamelet description under increasingly-intense turbulence. In this regard, the scientific community has been bent on demarcating the regime where flame velocity is inhibited by turbulence due to flame structure disruption, which would thereby invalidate the framework of the progress variable c . The present thesis informs us that inhibition of flame propagation velocity, such as that observed in the bending effect, may occur without flame structure disruption. As opposed to the effect of turbulence on the flame, the effect of the flame on turbulence as well as the self-inhibition of the flame is highlighted. This suggests that we may need to consider all possible interactions between the flame and turbulence in order to address the question: ‘How fast we can burn?’

Appendix A

List of Publications

The contents of this thesis have been published the following communications:

1. Nivarti, G. V. and Cant, R. S. (2015) *Aerodynamic quenching and burning velocity of turbulent premixed methane-air flames*, Proceedings of the ASME Turbo Expo 2015: Turbomachinery Technical Conference and Exposition, GT2015-43416 (Chapter 3).
2. Nivarti, G. V. and Cant, R. S. (2015) *Premixed flame propagation in high-intensity turbulence: investigating the role of detailed chemistry*, Proceedings of the 25th International Colloquium on Dynamics and Explosions of Reactive Systems, paper 028 (Chapter 3)
3. Nivarti, G. V. and Cant, R. S. (2017) *Direct Numerical Simulation of the bending effect in turbulent premixed flames*, Proceedings of the Combustion Institute 36: 1903 – 1910 (Chapter 3 and Chapter 4)
4. Nivarti, G. V. and Cant, R. S. (2017) *Analysis of the bending effect in turbulent burning velocity of premixed flames using Direct Numerical Simulation*, Combustion Theory and Modelling (under review, Chapter 4)
5. Nivarti, G. V. and Cant, R. S. (2017) *Scalar transport and the validity of Damköhler’s second hypothesis in turbulent premixed flames*, Physics of Fluids 29: 085107 (Chapter 5)

Appendix A

6. Ahmed, U., Nivarti, G. V., Prosser, R. and Cant, R. S. (2017) *Flame configuration effects on flamelet modelling in premixed turbulent combustion*, Flow, Turbulence and Combustion (*in preparation*, Chapter 1)

The content has also been presented at the following international conferences:

1. Nivarti, G. V. and Cant, R. S. (2015) *ASME Turbo Expo 2015: Turbo-machinery Technical Conference and Exposition*, Montréal
2. Nivarti, G. V. and Cant, R. S. (2015) *25th International Colloquium on Dynamics and Explosions of Reactive Systems*, Leeds
3. Nivarti, G. V. and Cant, R. S. (2015) *16th International Conference on Numerical Combustion*, Avignon
4. Nivarti, G. V. and Cant, R. S. (2016) *Joint British, Spanish and Portuguese Section Combustion Meeting*, Cambridge
5. Nivarti, G. V., and Cant, R. S. (2016) *36th International Symposium on Combustion*, Seoul
6. Nivarti, G. V., and Cant, R. S. (2017) *17th International Conference on Numerical Combustion*, Orlando
7. Nivarti, G. V., Thorne, B., Cant, R. S., Lawes, M., Bradley, D. (2017) *17th International Conference on Numerical Combustion*, Orlando

The dataset generated in this work is available for investigation upon request.

References

- Abdel-Gayed, R., Bradley, D., and Lawes, M. (1987). Turbulent burning velocities: a general correlation in terms of straining rates. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 414, 389–413.
- Abdel-Gayed, R. G., Al-Khishali, K. J., and Bradley, D. (1984). Turbulent burning velocities and flame straining in explosions. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 391, 393–414.
- Abdel-Gayed, R. G. and Bradley, D. (1977). Dependence of turbulent burning velocity on turbulent Reynolds number and ratio of laminar burning velocity to RMS turbulent velocity. *16th Symposium (International) on Combustion*, 1725–1735.
- Abdel-Gayed, R. G., Bradley, D., Hamid, M. N., and Lawes, M. (1985). Lewis number effects on turbulent burning velocity. *20th Symposium (International) on Combustion*, 505–512.
- Abdel-Gayed, R. G., Bradley, D., and Lung, F.-K. (1989). Combustion regimes and the straining of turbulent premixed flames. *Combustion and Flame*, 76, 213–218.
- Ahmed, U., Nivarti, G. V., Prosser, R., and Cant, R. S. (2017). Effects of flame configuration on flamelet modelling of turbulent premixed flames. *Flow, Turbulence and Combustion*. (in preparation).
- Andrews, G., Bradley, D., and Lwakabamba, S. (1975). Measurement of turbulent burning velocity for large turbulent Reynolds numbers. 655–664.

References

- Aspden, A. J., Bell, J. B., Day, M. S., Woosley, S. E., and Zingale, M. (2008). Turbulence-flame interactions in type Ia supernovae. *The Astrophysical Journal*, 689, 1173–1185.
- Aspden, A. J., Day, M. S., and Bell, J. B. (2011). Turbulence-flame interactions in lean premixed hydrogen: transition to the distributed burning regime. *Journal of Fluid Mechanics*, 680, 287–320.
- Bagdanavicius, A., Bowen, P. J., Bradley, D., Lawes, M., and Mansour, M. S. (2015). Stretch rate effects and Flame Surface Densities in premixed turbulent combustion up to 1.25 MPa. *Combustion and Flame*, 162, 4158–4166.
- Batchelor, G. K. (1952). The effect of homogeneous turbulence on material lines and surfaces. In *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 213, 349–366.
- Batchelor, G. K. and Townsend, A. A. (1948). Decay of Turbulence in the Final Period. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 194, 527–543.
- Bedat, B. and Cheng, R. (1995). Experimental study of premixed flames in intense isotropic turbulence. *Combustion and Flame*, 100, 485–494.
- Bell, J. B., Day, M. S., Grcar, J. F., Lijewski, M. J., Driscoll, J. F., and Filatyev, S. A. (2007). Numerical simulation of a laboratory-scale turbulent slot flame. *Proceedings of the Combustion Institute*, 31, 1299–1307.
- Bell, J. B., Day, M. S., Shepherd, I. G., Johnson, M. R., Cheng, R. K., Grcar, J. F., Beckner, V. E., and Lijewski, M. J. (2005). Numerical simulation of a laboratory-scale turbulent V-flame. *Proceedings of the National Academy of Sciences of the United States of America*, 102, 10006–10011.
- Bilger, R. W., Pope, S. B., Bray, K. N. C., and Driscoll, J. F. (2005). Paradigms in turbulent combustion research. *Proceedings of the Combustion Institute*, 30, 21–42.
- Bird, R. B., Stewart, W. E., and Lightfoot, E. N. (1960). *Transport Phenomena*. John Wiley and Sons, NY.

- Boger, M., Veynante, D., Boughanem, H., and Trouvé, A. (1998). Direct Numerical Simulation analysis of Flame Surface Density concept for Large Eddy Simulation of turbulent premixed combustion. *27th Symposium (International) on Combustion*, 917–925.
- Borghi, R. (1985). On the structure and morphology of turbulent premixed flames. In *Recent Advances in the Aerospace Sciences*, Casci, C. and Bruno, C., editors, 117–138. Springer US.
- Bradley, D. (1992). How fast can we burn? *24th Symposium (International) on Combustion*, 247–262.
- Bradley, D., Lau, A. K. C., and Lawes, M. (1992). Flame stretch rate as a determinant of turbulent burning velocity. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 338, 359–387.
- Bradley, D., Lawes, M., Liu, K., and Mansour, M. S. (2013). Measurements and correlations of turbulent burning velocities over wide ranges of fuels and elevated pressures. *Proceedings of the Combustion Institute*, 34, 1519–1526.
- Bradley, D., Lawes, M., and Mansour, M. S. (2011). The problems of the turbulent burning velocity. *Flow, Turbulence and Combustion*, 87, 191–204.
- Bray, K. N. C. (1980). Turbulent flows with premixed reactants. In *Turbulent Reacting Flows*, Libby, P. A. and Williams, F. A., editors, 44, 115–183. Springer Berlin Heidelberg.
- Bray, K. N. C. (1990). Studies of the turbulent burning velocity. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 431, 315–335.
- Bray, K. N. C. (1995). Turbulent transport in flames. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 451, 231–256.

References

- Bray, K. N. C. and Cant, R. S. (1991). Some applications of Kolmogorov's turbulence research in the field of combustion. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 434, 217–240.
- Bray, K. N. C. and Moss, J. B. (1977). A unified statistical model of the premixed turbulent flame. *Acta Astronautica*, 4, 291–319.
- Buckmaster, J. D. and Ludford, G. S. S. (1982). *Theory of Laminar Flames*. Cambridge University Press.
- Candel, S. M. and Poinso, T. J. (1990). Flame stretch and the balance equation for the flame area. *Combustion Science and Technology*, 70, 1–15.
- Cant, R. S. (2013). SENG2: User guide. Technical Report CUED-THERMO-2012/04 - 2, Cambridge University Engineering Department.
- Cant, R. S. and Mastorakos, E. (2008). *An introduction to turbulent reacting flows*. Imperial College Press.
- Cant, R. S., Pope, S. B., and Bray, K. N. C. (1991). Modelling of flamelet surface-to-volume ratio in turbulent premixed combustion. *23rd Symposium (International) on Combustion*, 809–815.
- Cant, S. (1999). Direct Numerical Simulation of premixed turbulent flames. *Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 357, 3583–3604.
- Carroll, P. L. and Blanquart, G. (2013). A proposed modification to Lundgren's physical space velocity forcing method for isotropic turbulence. *Physics of Fluids*, 25, 105114.
- Chakraborty, N. and Cant, R. S. (2004). Unsteady effects of strain rate and curvature on turbulent premixed flames in an inflow-outflow configuration. *Combustion and Flame*, 137, 129–147.
- Chakraborty, N. and Cant, R. S. (2007). A priori analysis of the curvature and propagation terms of the Flame Surface Density transport equation for large eddy simulation. *Physics of Fluids*, 19, 105101.

- Chakraborty, N. and Cant, R. S. (2009). Effects of Lewis number on scalar transport in turbulent premixed flames. *Physics of Fluids*, 21, 035110.
- Clavin, P. (1985). Dynamic behaviour of premixed flame fronts in laminar and turbulent flows. *Progress in Energy and Combustion Science*, 11, 1–59.
- Clavin, P. and Williams, F. A. (1979). Theory of premixed-flame propagation in large-scale turbulence. *Journal of Fluid Mechanics*, 90, 589–604.
- Damköhler, G. (1940). Der einfluss der turbulenz auf die flammengeschwindigkeit in gasgemischen. *Zeitschrift für Elektrochemie und angewandte physikalische Chemie*, 46, 601–652. (English translation NACA TM 1112, 1947).
- Day, M., Tachibana, S., Bell, J., Lijewski, M., Beckner, V., and Cheng, R. K. (2012). A combined computational and experimental characterisation of lean premixed turbulent low swirl laboratory flames: I. Methane flames. *Combustion and Flame*, 159, 275–290.
- Driscoll, J. F. (2008). Turbulent premixed combustion: Flamelet structure and its effect on turbulent burning velocities. *Progress in Energy and Combustion Science*, 34, 91–134.
- Duclos, J., Veynante, D., and Poinso, T. (1993). A comparison of flamelet models for premixed turbulent combustion. *Combustion and Flame*, 95, 101–117.
- Echekki, T. and Chen, J. H. (1996). Unsteady strain rate and curvature effects in turbulent premixed methane-air flames. *Combustion and Flame*, 106, 184–190.
- Echekki, T. and Chen, J. H. (1998). Structure and propagation of methanol-air triple flames. *Combustion and Flame*, 114, 231–245.
- Eswaran, V. and Pope, S. B. (1988). An examination of forcing in Direct Numerical Simulations of turbulence. *Computers and Fluids*, 16, 257–278.

References

- Filatyeve, S. A., Driscoll, J. F., Carter, C. D., and Donbar, J. M. (2005). Measured properties of turbulent premixed flames for model assessment, including burning velocities, stretch rates, and surface densities. *Combustion and Flame*, 141, 1–21.
- Frisch, U. (2004). *Turbulence*. Cambridge University Press.
- Fru, G., Thévenin, D., and Janiga, G. (2011). Impact of turbulence intensity and equivalence ratio on the burning rate of premixed methane–air flames. *Energies*, 4, 878–893.
- Gillespie, L., Lawes, M., Sheppard, C. G. W., and Woolley, R. (2000). Aspects of laminar and turbulent burning velocity relevant to SI engines. *SAE Technical Paper*, 2000-01-0192.
- Gran, I. R., Echekki, T., and Chen, J. H. (1996). Negative flame speed in an unsteady 2-d premixed flame: A computational study. *26th Symposium (International) on Combustion*, 323–329.
- Griffiths, R. A. C., Chen, J. H., Kolla, H., Cant, R. S., and Kollmann, W. (2015). Three-dimensional topology of turbulent premixed flame interaction. *Proceedings of the Combustion Institute*, 35, 1341–1348.
- Gülder, Ö. L. (1991). Turbulent premixed flame propagation models for different combustion regimes. *23rd Symposium (International) on Combustion*, 743–750.
- Gülder, Ö. L. and Smallwood, G. J. (2007). Flame surface densities in premixed combustion at medium to high turbulence intensities. *Combustion Science and Technology*, 179, 191–206.
- Hamlington, P. E., Poludnenko, A. Y., and Oran, E. S. (2011). Interactions between turbulence and flames in premixed reacting flows. *Physics of Fluids*, 23, 125111.
- Hawkes, E. R., Chatakonda, O., Kolla, H., Kerstein, A. R., and Chen, J. H. (2012). A petascale Direct Numerical Simulation study of the modelling of

- flame wrinkling for Large-eddy Simulations in intense turbulence. *Combustion and Flame*, 159, 2690–2703.
- Haworth, D. C. and Poinso, T. J. (1992). Numerical simulations of Lewis number effects in turbulent premixed flames. *Journal of Fluid Mechanics*, 244, 405–436.
- Ishihara, T., Gotoh, T., and Kaneda, Y. (2009). Study of high-Reynolds number isotropic turbulence by Direct Numerical Simulation. *Annual Review of Fluid Mechanics*, 41, 165–180.
- Jenkins, K. W. and Cant, R. S. (1999). Direct Numerical Simulation of turbulent flame kernels. In *Recent Advances in DNS and LES*, Knight, D. and Sakell, L., editors, 54, 191–202.
- Jones, W. P. and Launder, B. (1972). The prediction of laminarization with a two-equation model of turbulence. *International Journal of Heat and Mass Transfer*, 15, 301–314.
- Karlovitz, B., Denniston, D. W., Knapschaefer, D., and Wells, F. E. (1953). Studies on turbulent flames: A. Flame propagation across velocity gradients B. Turbulence measurement in flames. *4th Symposium (International) on Combustion*, 613–620.
- Karlovitz, B., Denniston Jr, D. W., and Wells, F. E. (1951). Investigation of turbulent flames. *Journal of Chemical Physics*, 19, 541–547.
- Karpov, V. and Severin, E. (1980). Effects of molecular-transport coefficients on the rate of turbulent combustion. *Combustion, Explosion, and Shock Waves*, 16, 41–46.
- Kee, R. J., Dixon-lewis, G., Warnatz, J., Coltrin, M. E., and Miller, J. A. (1986). A Fortran computer code package for the evaluation of gas-phase, multicomponent transport properties. Technical Report SAND86-8246, Sandia National Laboratories.

References

- Kennedy, C. A. and Carpenter, M. H. (2003). Additive Runge-Kutta schemes for convection-diffusion-reaction equations. *Applied Numerical Mathematics*, 44, 139–181.
- Kerstein, A. R. (2002). Turbulence in combustion processes: Modelling challenges. *Proceedings of the Combustion Institute*, 29, 1763–1773.
- Kerstein, A. R., Ashurst, W. T., and Williams, F. A. (1988). Field equation for interface propagation in an unsteady homogeneous flow field. *Physical Review A*, 37, 2728.
- Kheirikhah, S. and Gülder, Ö. L. (2015). Consumption speed and burning velocity in counter-gradient and gradient diffusion regimes of turbulent premixed combustion. *Combustion and Flame*, 162, 1422–1439.
- Kido, H., Kitagawa, T., Nakashima, K., and Kato, K. (1989). An improved model of turbulent mass burning velocity. In *Memoirs of the Faculty of Engineering, Kyushu University*, 49, 229–247.
- Klimov, A. M. (1963). Laminar flame in turbulent flow. *Prikladnoy Mekhaniki i Tekhnicheskoy Fiziki Zhurnal*, 3, 49 – 58. (English translation AD-A200 241 Foreign Technology Division, Air Force Systems Command, 1988).
- Kobayashi, H., Tamura, T., Maruta, K., Niioka, T., and Williams, F. A. (1996). Burning velocity of turbulent premixed flames in a high-pressure environment. *26th Symposium (International) on Combustion*, 389–396.
- Kolmogorov, A. N. (1941). The local structure of turbulence in incompressible viscous fluid for very large Reynolds numbers. *Doklady Akadademii Nauk SSSR*, 30, 301–305.
- Lapointe, S. and Blanquart, G. (2016). Fuel and chemistry effects in high Karlovitz premixed turbulent flames. *Combustion and Flame*, 167, 294–307.
- Lapointe, S., Savard, B., and Blanquart, G. (2015). Differential diffusion effects, distributed burning, and local extinctions in high Karlovitz premixed flames. *Combustion and Flame*, 162, 3341–3355.

- Law, C. K. (1989). Dynamics of stretched flames. *22nd Symposium (International) on Combustion*, 1381–1402.
- Lewis, B. and von Elbe, G. (1934). On the theory of flame propagation. *The Journal of Chemical Physics*, 2, 537–546.
- Libby, P. A. and Bray, K. N. C. (1981). Countergradient diffusion in premixed turbulent flames. *AIAA Journal*, 19, 205–213.
- Libby, P. A., Bray, K. N. C., and Moss, J. B. (1979). Effects of finite reaction rate and molecular transport in premixed turbulent combustion. *Combustion and Flame*, 34, 285–301.
- Lipatnikov, A. and Chomiak, J. (2002). Turbulent flame speed and thickness: phenomenology, evaluation, and application in multi-dimensional simulations. *Progress in Energy and Combustion Science*, 28, 1–74.
- Lipatnikov, A. N., Chomiak, J., Sabelnikov, V. A., Nishiki, S., and Hasegawa, T. (2015). Unburned mixture fingers in premixed turbulent flames. *Proceedings of the Combustion Institute*, 35, 1401–1408.
- Lockermann, G. (1956). The centenary of the bunsen burner. *Journal of Chemical Education*, 33, 20–22.
- Louch, D. S. and Bray, K. N. C. (2001). Vorticity in unsteady premixed flames: vortex pair-premixed flame interactions under imposed body forces and various degrees of heat release and laminar flame thickness. *Combustion and Flame*, 125, 1279–1309.
- Lundgren, T. S. (2003). Linearly forced isotropic turbulence. In *Annual Research Briefs, CTR Stanford*, 461–473.
- Mallard, F. E. and le Chatelier, H. (1883). Recherches expérimentales et théoriques sur le combustion des mélanges gazeux explosifs. *Annales des Mines*, 4, 274–378.
- Markstein, G. H. (1964). *Nonsteady flame propagation*. Pergamon Press.

References

- McBride, B. J. and Gordon, S. (1967). FORTRAN IV program for calculation of thermodynamic data. Technical Report NASA TN D-4097, NASA.
- McMurtry, P. A., Jou, W.-H., Riley, J., and Metcalfe, R. (1986). Direct Numerical Simulations of a reacting mixing layer with chemical heat release. *AIAA Journal*, 24, 962–970.
- Meneveau, C. and Poinso, T. (1991). Stretching and quenching of flamelets in premixed turbulent combustion. *Combustion and Flame*, 332, 311–332.
- Michelson, V. A. (1889). Ueber die normale entzündungsgeschwindigkeit explosiver gasgemischen. *Annalen der Physik*, 273, 1–24.
- Nivarti, G. V. and Cant, R. S. (2015a). Aerodynamic quenching and burning velocity of turbulent premixed methane-air flames. *Proceedings of the ASME Turbo Expo: Turbomachinery Technical Conference and Exposition*, GT2015–43416.
- Nivarti, G. V. and Cant, R. S. (2015b). Premixed flame propagation in high-intensity turbulence: Investigating the role of detailed chemistry. In *25th International Conference for Dynamics of Explosions and Reactive Systems*.
- Nivarti, G. V. and Cant, R. S. (2017). Direct numerical simulation of the bending effect in turbulent premixed flames. *Proceedings of the Combustion Institute*, 36, 1903–1910.
- Nivarti, G. V., Thorne, B., Cant, R. S., Lawes, M., and Bradley, D. (2017). Comparisons of Flame Surface Density measurements with Direct Numerical Simulations of a lean methane-air flame in high-intensity turbulence. In *16th International Conference on Numerical Combustion, Orlando*.
- Peters, N. (1988). Laminar flamelet concepts in turbulent combustion. *21st Symposium (International) on Combustion*, 1231–1250.
- Peters, N. (1999). The turbulent burning velocity for large-scale and small-scale turbulence. *Journal of Fluid Mechanics*, 384, 107–132.
- Peters, N. (2000). *Turbulent combustion*. Cambridge University Press.

- Peters, N., Terhoeven, P., Chen, J. H., and Echehki, T. (1998). Statistics of flame displacement speeds from computations of 2-D unsteady methane-air flames. *27th Symposium (International) on Combustion*, 833–839.
- Peters, N. and Williams, F. A. (1987). The asymptotic structure of stoichiometric methane-air flames. *Combustion and Flame*, 68, 185–207.
- Petersen, M. R. and Livescu, D. (2010). Forcing for statistically stationary compressible isotropic turbulence. *Physics of Fluids*, 22, 116101.
- Poinsot, T. (1996). Using Direct Numerical Simulations to understand premixed turbulent combustion. *26th Symposium (International) on Combustion*, 219–232.
- Poinsot, T., Candel, S., and Trouvé, A. (1995). Applications of Direct Numerical Simulation to premixed turbulent combustion. *Progress in Energy and Combustion Science*, 21, 531–576.
- Poinsot, T. and Lele, S. K. (1992). Boundary conditions for direct simulations of compressible viscous flows. *Journal of Computational Physics*, 101, 104–129.
- Poinsot, T., Veynante, D., and Candel, S. (1991a). Diagrams of premixed turbulent combustion based on direct simulation. *23rd Symposium (International) on Combustion*, 613–619.
- Poinsot, T., Veynante, D., and Candel, S. (1991b). Quenching processes and premixed turbulent combustion diagrams. *Journal of Fluid Mechanics*, 228, 561–606.
- Poludnenko, A. Y. (2015). Pulsating instability and self-acceleration of fast turbulent flames. *Physics of Fluids*, 27, 014106.
- Poludnenko, A. Y. and Oran, E. (2011). The interaction of high-speed turbulence with flames: Turbulent flame speed. *Combustion and Flame*, 158, 301–326.

References

- Pope, S. B. (1988). The evolution of surfaces in turbulence. *International Journal of Engineering Science*, 26, 445–469.
- Pope, S. B. (2001). *Turbulent flows*. Cambridge University Press.
- Pope, S. B., Yeung, P. K., and Girimaji, S. S. (1989). The curvature of material surfaces in isotropic turbulence. *Physics of Fluids A*, 1, 2010–2018.
- Prandtl, L. (1925). Bericht über untersuchungen zur ausgebildeten turbulenz. *Zeitschrift für Angewandte Mathematik und Mechanik*, 5, 136–139. English translation NACA Technical Memorandum 1231, 1949.
- Quadrio, M., Frohnapfel, B., and Hasegawa, Y. (2016). Does the choice of the forcing term affect flow statistics in DNS of turbulent channel flow? *European Journal of Mechanics-B/Fluids*, 55, 286–293.
- Rogallo, R. S. (1981). Numerical experiments in homogeneous turbulence. Technical Report NASA TM 81315, NASA Ames Research Center.
- Rosales, C. and Meneveau, C. (2005). Linear forcing in numerical simulations of isotropic turbulence: Physical space implementations and convergence properties. *Physics of Fluids*, 17, 095106.
- Rudy, D. H. and Strikwerda, J. C. (1980). A nonreflecting outflow boundary condition for subsonic Navier-Stokes calculations. *Journal of Computational Physics*, 36, 55–70.
- Rutland, C. J. and Cant, R. S. (1994). Turbulent transport in premixed flames. In *Proceedings of the Summer Program at the Centre for Turbulence Research, Stanford*, 75–94. NASA Ames/Stanford University.
- Sankaran, R., Hawkes, E. R., Chen, J. H., Lu, T., and Law, C. K. (2007). Structure of a spatially developing turbulent lean methane-air Bunsen flame. *Proceedings of the Combustion Institute*, 31, 1291–1298.
- Savard, B. and Blanquart, G. (2015). Broken reaction zone and differential diffusion effects in high Karlovitz n -C₇H₁₆ premixed turbulent flames. *Combustion and Flame*, 162, 2020–2033.

- Savre, J., Carlsson, H., and Bai, X.-S. (2013). Turbulent methane/air premixed flame structure at high Karlovitz numbers. *Flow, Turbulence and Combustion*, 90, 325–341.
- Schelkin, K. I. (1943). On combustion in a turbulent flow. *Zhurnal Tekhnicheskoi Fiziki*, 13, 520–530. (English translation NACA TM 1112, 1947).
- Shepherd, I., Cheng, R., Plessing, T., Kortschik, C., and Peters, N. (2002). Premixed flame front structure in intense turbulence. *Proceedings of the Combustion Institute*, 29, 1833–1840.
- Shepherd, I. G., Moss, J. B., and Bray, K. N. C. (1982). Turbulent transport in a confined premixed flame. 19th *Symposium (International) on Combustion*, 423–431.
- Shy, S. S., I, W. K., and Lin, M. L. (2000a). A new cruciform burner and its turbulence measurements for premixed turbulent combustion study. *Experimental Thermal and Fluid Science*, 20, 105–114.
- Shy, S. S., Lin, W. J., and Wei, J. C. (2000b). An experimental correlation of turbulent burning velocities for premixed turbulent methane-air combustion. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 456, 1997–2019.
- Smith, G. P., Golden, D. M., Frenklach, M., Moriarty, N. W., Eiteneer, B., Goldenberg, M., Bowman, C. T., Hanson, R. K., Song, S., William C. Gardiner, J., Lissianski, V. V., and Qin, Z. (2017). GRI-MECH 3.0. Available at http://www.me.berkeley.edu/gri_mech/.
- Smooke, M. D. and Giovangigli, V. (1991). Formulation of the premixed and nonpremixed test problems. In *Reduced Kinetic Mechanisms and Asymptotic Approximations for Methane-Air Flames*, Smooke, M. D., editor, 384, 1–28. Springer Berlin Heidelberg.
- Söderlind, G. (2002). Automatic control and adaptive time-stepping. *Numerical Algorithms*, 31, 281–310.

References

- Söderlind, G. and Wang, L. (2006). Adaptive time-stepping and computational stability. *Journal of Computational and Applied Mathematics*, 185, 225–243.
- Steinberg, A. M. and Driscoll, J. F. (2009). Straining and wrinkling processes during turbulence–premixed flame interaction measured using temporally-resolved diagnostics. *Combustion and Flame*, 156, 2285–2306.
- Steinberg, A. M., Driscoll, J. F., and Swaminathan, N. (2012). Statistics and dynamics of turbulence–flame alignment in premixed combustion. *Combustion and Flame*, 159, 2576–2588.
- Sutherland, J. C. and Kennedy, C. A. (2003). Improved boundary conditions for viscous, reacting, compressible flows. *Journal of Computational Physics*, 191, 502–524.
- Trouvé, A. and Poinso, T. (1994). The evolution equation for the Flame Surface Density in turbulent premixed combustion. *Journal of Fluid Mechanics*, 278, 1–31.
- Veynante, D. and Poinso, T. (1997). Effects of pressure gradients on turbulent premixed flames. *Journal of Fluid Mechanics*, 353, 83–114.
- Veynante, D., Trouvé, A., Bray, K. N. C., and Mantel, T. (1997). Gradient and counter-gradient scalar transport in turbulent premixed flames. *Journal of Fluid Mechanics*, 332, 263–293.
- Veynante, D. and Vervisch, L. (2002). Turbulent combustion modeling. *Progress in Energy and Combustion Science*, 28, 193–266.
- Wabel, T. M., Skiba, A. W., and Driscoll, J. F. (2016). Turbulent burning velocity measurements: extended to extreme levels of turbulence. *Proceedings of the Combustion Institute*, 36, 1801–1808.
- Wang, H., Hawkes, E. R., and Chen, J. H. (2016a). Turbulence-flame interactions in DNS of a laboratory high Karlovitz premixed turbulent jet flame. *Physics of Fluids*, 28, 095107.

- Wang, H., Hawkes, E. R., Zhou, B., Chen, J. H., Li, Z., and Aldén, M. (2016b). A comparison between Direct Numerical Simulation and experiment of the turbulent burning velocity-related statistics in a turbulent methane-air premixed jet flame at high Karlovitz number. *Proceedings of the Combustion Institute*, 36, 2045–2053.
- Wenzel, H. and Peters, N. (2000). Direct numerical simulation and modeling of kinematic restoration, dissipation and gas expansion effects of premixed flames in homogeneous turbulence. *Combustion Science and Technology*, 158, 273–297.
- Williams, F. A. (1985). *Combustion Theory*. Westview Press.
- Williams, F. A. (2000). Progress in knowledge of flamelet structure and extinction. *Progress in Energy and Combustion Science*, 26, 657–682.
- Wohl, K., Shore, L., Von Rosenberg, H., and Weil, C. (1953). The burning velocity of turbulent flames. 4th *Symposium (International) on Combustion*, 620–635.
- Yakhot, V. (1988). Propagation velocity of premixed turbulent flames. *Combustion Science and Technology*, 60, 191–214.
- Yu, R., Bai, X.-S., and Lipatnikov, A. N. (2015). A Direct Numerical Simulation study of interface propagation in homogeneous turbulence. *Journal of Fluid Mechanics*, 772, 127–164.
- Yuen, F. T. and Gülder, O. L. (2013). Turbulent premixed flame front dynamics and implications for limits of flamelet hypothesis. *Proceedings of the Combustion Institute*, 34, 1393–1400.
- Zel'dovich, Y. B. and Frank-Kamenetskii, D. A. (1938). Teoriia teplovogo rasprostraneniia plameni. *Zhurnal Fizicheskoi Khimii*, 12, 100–105. (English translation Selected Works of Yakov Borisovich Zeldovich, Volume I, Princeton University Press, 1992.).