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Peer reviewed|Thesis/dissertation

UNIVERSITY OF CALIFORNIA,
IRVINE

A Three-dimensional, Rotational Flamelet Model for Non-premixed Turbulent Reacting
Flows

DISSERTATION

submitted in partial satisfaction of the requirements
for the degree of

DOCTOR OF PHILOSOPHY

in Mechanical and Aerospace Engineering

by

Wes Hellwig

Dissertation Committee:
Distinguished Professor William A. Sirignano, Chair
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DEDICATION

To my mother Mary and father John

TABLE OF CONTENTS

	Page
LIST OF FIGURES	v
LIST OF TABLES	viii
ACKNOWLEDGMENTS	ix
VITA	xii
ABSTRACT OF THE DISSERTATION	xv
1 Introduction	1
1.1 Motivation	1
1.2 Classification and Dimensionless Numbers	3
1.2.1 Turbulent Premixed Combustion	8
1.2.2 Turbulent Non-premixed Combustion	12
2 Combustion Modeling Techniques	18
2.1 A Brief Summary of RANS and Favre Averaging	18
2.2 A Brief Summary of Probability Density Functions	21
2.2.1 Infinitely-Fast Chemistry Models	22
2.3 Models Valid for All Combustion Modes	23
2.3.1 Global Low-Order Kinetics	23
2.3.2 PDF Transport Equation Model	24
2.3.3 Linear Eddy Model	25
2.4 Flamelet Models	26
2.4.1 Classical Premixed Flamelet Formulation	28
2.4.2 Classical Non-premixed Flamelet Formulation	29
2.4.3 Flamelet Models: Advances and Limitations	32
2.5 Summary of Flamelet Modeling and Objectives	43
3 The Rotational Flamelet Model	45
3.1 Geometry	46
3.2 Theoretical Development	51
3.3 Multi-step Chemical Kinetics and Detailed Transport	53
3.3.1 Governing Equations	53

3.3.2	Chemical Kinetics	57
3.3.3	Comparison with Cantera	57
3.3.4	Non-premixed Flames	60
3.3.5	Premixed Flames	71
3.3.6	Partially-premixed Flames	77
3.3.7	Stretched Vortex Layer Hydrocarbon Non-premixed Flames	80
3.3.8	Stretched Vortex Tube Hydrocarbon Non-premixed Flames	87
3.3.9	Summary of Findings for Multi-step Chemical Kinetics with Detailed Transport	89
3.4	Fickian Diffusion and Multi-step Chemical Kinetics: Impact on Scalar Dissipation Rate	91
3.4.1	Governing Equations	92
3.4.2	Scalar Dissipation Rate and Mixture Fraction	95
3.4.3	Chemical Kinetics	96
3.4.4	Equal Transverse Strain Rates ($S_1 = S_2$)	97
3.4.5	Unequal Transverse Strain Rates ($S_1 \neq S_2$) and Non-constant Lewis Numbers	104
3.4.6	Summary of Findings for Multi-step Chemical Kinetics with Fickian Diffusion	106
4	Numerical Methods	109
4.1	Use of Cantera	110
4.2	Necessity for Fast Computations - Hybrid Scheme	111
4.2.1	General Governing Equations	114
4.2.2	Hybrid Scheme: Newton's Method + Backward Euler	118
4.3	Pseudo-arclength Continuation	122
4.3.1	RFM Algorithm	126
4.4	Jacobian Calculation	129
4.4.1	Jacobian Matrix with Perturbation Derivatives	130
4.4.2	Jacobian Matrix with Analytical Derivatives	135
5	Coupling the Flamelet Model to RANS/LES	147
5.1	Mechanical Forward Coupling	149
5.1.1	Vorticity, Enstrophy, and Viscous Dissipation	153
5.1.2	Kinetic Energy	157
5.2	RFM Backward Coupling to RANS or LES	161
5.3	Scalar Coupling	162
5.3.1	Scaling Scalar Gradients	163
5.3.2	Criteria for Practical Scalar Boundary Conditions	168
5.3.3	Cell-averaged Scalar Boundary Conditions	168
5.3.4	Fixed Scalar Boundary Conditions	173
6	Conclusions	177
	Bibliography	180

LIST OF FIGURES

	Page
1.1 S-curve in terms of strain rate S^* . Solid curves indicate stable branches and the dashed curve indicates the unstable branch. The infinitely-fast chemistry limit is shown by the thin, dashed, horizontal line at the top. The ignition point is shown by the red dot in the lower left-hand corner with an upward-point arrow and the extinction point is shown by a central blue dot with a downward-pointing arrow.	8
1.2 Turbulent non-premixed combustion regime diagram adapted from Figure 3.9 (Regimes in nonpremixed turbulent combustion) in Peters, N., <i>Turbulent Combustion</i> [1], Cambridge Monographs on Mechanics, Cambridge University Press, 2000. pp. 192. © 2000 Cambridge University Press. Reproduced with permission of Cambridge University Press through PLSclear. This adaptation features additional annotations and an additional abscissa variable, S_q^*/S^* . An animation of a turbulent jet diffusion flame overlaid onto the graph shows the approximate regimes with respect to changing visual character. The overlaid flame represents a fuel jet injected into a body of quiescent oxidizer. Near the nozzle ($S_q^*/S^* < 1$), the residence time is too short for combustion to occur. As oxidizer is entrained downstream and the residence time increases (strain rate decreases), the mixture becomes flammable; however, the mixture fraction variance is still large (<i>separated flamelets regime</i>). Further entrainment and mixing reduce the strain rate and the mixture fraction variance (below the horizontal line at $Z'_{st}/(\Delta Z)_F = 1$) and the jet enters the <i>connected flame zones regime</i> . The downward-sloping line for $Z'_{st}/(\Delta Z)_r = 1$ separates the <i>connected flamelets regime</i> from the <i>connected reaction zones regime</i>	15
3.1 Deformation of a square volume under shear strain.	47
3.2 Transformation from the Newtonian (black) to the non-Newtonian reference frame and alignment of strain rates and vorticity. $x \rightarrow \xi$ and $y \rightarrow \chi$; i.e., the $\xi - \chi$ plane rotates about z at $d\theta/dt = \omega/2$	51
3.3 Orientation of RFM in the stretched vortex layer and tube configurations. The reader should interpret the figures as snapshots in time as the counterflow structure rotates about the z (ω and S_2) axis as time progresses. Non-premixed oxidizer side (blue); non-premixed fuel side (red).	52
3.4 Comparison between the RFM and Cantera's counterflow diffusion flame. (a) Axial velocity; (b) Temperature; (c) H_2O and H_2 mass fractions; (d) O_2 and N_2 mass fractions. The maximum strain rate for matched curves is $S_{max}^* = 1,654,000$ 1/s and the transverse strain rates in the RFM are equal, i.e., $S_1 = S_2 = 0.5$ or $S_1^* = S_2^* = 500,000$ (1/s), to achieve axisymmetry.	58

3.5	Extinction curves (S-curves) of counterflow non-premixed flames with varying strain rate and vorticity magnitudes. Sub-figures (a), (b), and (c) are plotted against ambient strain rate (S^*) while sub-figures (d), (e), and (f) are plotted against the local maximum strain rate at the stagnation point (S_{max}^*).	61
3.6	Non-premixed flame. (a) Axial (inflow) velocity u_χ ; (b) Similarity variable f ; (c) Transverse outflow velocity normal to vorticity vector divided by length (u_ξ/ξ); (d) Transverse outflow velocity parallel to vorticity vector divided by length (w/z). $S_1 = S_2 = 0.5$, $S^* = 1,000,000$ 1/s.	63
3.7	Non-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$, $S_2 = 0.5$, $S^* = 1,000,000$ 1/s.	65
3.8	Non-premixed flame. (a) Axial (inflow) velocity u_χ ; (b) Similarity variable f . $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$, $\omega = 0.0, 1.0$, $S^* = 1,000,000$ 1/s. The three curves on each sub-figure for $\omega = 0.0$ are coincident with the solid red curve.	66
3.9	Non-premixed flame. (a) Absolute temperature; (b) Major species mass fractions; (c) Dimensional axial velocity (u_χ); Similarity variable f . $S_1 = S_2 = 0.50$, $\omega = 0.0, 1.3$, $T_{max} = 2010K$	67
3.10	Non-premixed flame. (a) u_ξ/ξ , $\omega = 0.0$; (b) u_ξ/ξ , $\omega = 1.0$; (c) w/z , $\omega = 0.0$; (d) w/z , $\omega = 1.0$. $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$. $S^* = 1,000,000$ 1/s.	68
3.11	Non-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$. $\omega = 0.0, 1.0$, $S^* = 1,000,000$ 1/s.	69
3.12	S-curves of premixed twin flames with varying strain rate and vorticity magnitudes.	71
3.13	Premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse mass efflux normal to vorticity vector divided by length ($\rho u_\xi/\xi$); (d) Transverse mass efflux parallel to vorticity vector divided by length ($\rho w/z$). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 1,000,000$ 1/s.	72
3.14	Premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 1,000,000$ 1/s.	73
3.15	Premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.45, 0.50, 0.75$; $S_2 = 0.55, 0.50, 0.25$; $\omega = 0.0, 1.0$; $S^* = 2,000,000$ 1/s.	75
3.16	Premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse mass efflux normal to vorticity vector divided by length ($\rho u_\xi/\xi$); (d) Transverse mass efflux parallel to vorticity vector divided by length ($\rho w/z$). $S_1 = 0.45, 0.50, 0.75$; $S_2 = 0.55, 0.50, 0.25$; $\omega = 0.0, 1.0$; $S^* = 2,000,000$ 1/s.	76
3.17	Extinction curves (S-curves) of partially-premixed flames with varying vorticity magnitudes plotted against ambient strain rate (S^*).	77
3.18	Partially-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) H_2O reaction rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 30,000$ 1/s.	78
3.19	Partially-premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse outflow velocity normal to vorticity vector divided by length (u_ξ/ξ); (d) Transverse outflow velocity parallel to vorticity vector divided by length (w/z). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 30,000$ 1/s.	79

3.20	JP-5/Air non-premixed stretched vortex layer flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω	82
3.21	CH ₄ /O ₂ non-premixed stretched vortex layer flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω	82
3.22	Stretched vortex layer flamelet streamlines in the non-Newtonian reference frame. Horizontal planes show surfaces of constant scalar properties. Solid and dashed lines indicate streamlines originating on the near and far sides of the inflows, respectively.	84
3.23	JP-5/Air non-premixed stretched vortex tube flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω	87
3.24	CH ₄ /O ₂ non-premixed stretched vortex tube flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω	88
3.25	(a) Extinction curves in terms of maximum temperature; (b) Extinction curves in terms of heat release rate. Both sub-figures are plotted versus: maximum scalar dissipation rate, χ_{max} (red); ambient strain rate, S^* (black); maximum local strain rate, S^*_{local} (blue). . .	97
3.26	Temperature versus integrated H ₂ O burning rate.	98
3.27	SDR versus Ambient Strain Rate.	98
3.28	(a) Temperature versus mixture fraction; (b) Axial velocity versus mixture fraction; (c) Scalar dissipation rate versus mixture fraction. Stable branch (navy); unstable branch (orange). $S^* = 903, 500$ 1/s.	102
3.29	(a) Three-dimensional extinction surface; (b) Three-dimensional SDR surface. Sub-figure (a) temperature color-code from coldest to hottest (dark red $\rightarrow$ red $\rightarrow$ orange $\rightarrow$ yellow); Sub-figure (b) stable/unstable branch color code (stable: red; unstable: blue).	103
3.30	S-curves using multicomponent diffusion with transverse ambient strain rate variation. . .	104
3.31	(a) Extinction curves in terms of maximum temperature; (b) Extinction curves in terms of heat release rate. Both sub-figures are plotted versus: maximum scalar dissipation rate, χ_{max} ; ambient strain rate, S^* ; maximum local strain rate, S^*_{local} . Vorticity is constant at $\omega = 1$ for all curves. $S_1 = 1/2, 1/3$, $S_2 = 1/2, 2/3$	105
4.1	Example of Cantera usage in the RFM through the MATLAB interface.	110
4.2	Pictorial representation of the hybrid method; explicit pseudo-time (blue) to Newton's method (red) in residual-iteration number space. Explicit marching occurs until a set pseudo-time is reached, after which Newton's method quickly iterates the solution until the convergence criteria is satisfied.	114
4.3	Log of residual magnitudes, $\ R\ _2$, versus log of iteration number, n , (base 10) for a lightly-strained diffusion flamelet. Residuals 1-5 pertain to f'_1 , f'_2 , h , α , and β , respectively. . . .	145
5.1	Transformation from the Newtonian reference frame (x, y, z) to the rotating non-Newtonian reference frame (ξ, χ, z)	151
5.2	Integrated heat release rate (HRR or $-\dot{Q}''_{\kappa}$) as a function of CFD cell fuel and oxidizer mass fractions, $Y_{F,I}$ and $Y_{O,I}$	172
5.3	Integrated heat release rate (HRR or $-\dot{Q}''_{\kappa}$) and maximum temperature as a function of CFD cell temperature, T_I	174
5.4	Integrated species production and consumption rates (SPR or $\pm\dot{\omega}''_{m,\kappa}$) as a function of CFD cell temperature, T_I	175

LIST OF TABLES

	Page
2.1 Two general interpretations of flamelet models	42
3.1 Normalizations for dependent variables	54
3.2 Percentage increase in flammability limits between $\omega = 0 \rightarrow 1$	85
3.3 Percentage increase in flammability limits between $\omega = 0 \rightarrow 1$	88
3.4 Output variables at constant transverse strain rates, S_1^*	106
4.1 Normalizations for dependent variables	116
5.1 Mass Fraction Boundary Conditions	169
5.2 Temperature Boundary Conditions	170

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Portions of the text, figures, and tables of Chapter 3, Sections 3.1-3.2 and 3.3.1-3.3.6 of this dissertation are an adaptation of the material as it appears in Hellwig, W., Shi, X., and Sirignano, W. A., Three-dimensional vorticity effects on extinction behaviour of laminar flamelets, *Combustion Theory and Modelling*, Vol. 29, No. 1, 2025, pp. 62-92., used with permission from Taylor & Francis. The coauthors listed in this publication are Wes Hellwig, Xian Shi, and William A. Sirignano. William A. Sirignano directed and supervised research which forms the basis for the dissertation.

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- Hellwig, W., Shi, X., and Sirignano, W. A., Vortex stretching of non-premixed, diluted hydrogen/oxygen flamelets, *Combustion and Flame*, Vol. 273, 2025, pp. 113900. 2025
- Hellwig, W., Shi, X., and Sirignano, W. A., “Three-dimensional vorticity effects on extinction behaviour of laminar flamelets,” *Combustion Theory and Modelling*, Vol. 29, No. 1, 2025, pp. 62–92. 2024

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- Hellwig, W., Vortex Stretching on Non-premixed, Diluted Hydrogen/Oxygen Flamelets, *17th Southern California Flow Physics Symposium*, Irvine, California, April 2024 2024
- Hellwig, W., Shi, X., and Sirignano, W. A., “Three-dimensional Vorticity Effects on the Extinction Behavior of JP-5 - Air Laminar Flamelets,” *2023 Fall Technical Meeting of the Western States Section of The Combustion Institute*, Northridge, California, October 2023. 2023
- Hellwig, W., Shi, X., and Sirignano, W. A., “Three-dimensional Rotational Flamelet with Detailed Chemistry and Transport Models” *13th U.S. National Combustion Meeting*, Central States Section of the Combustion Institute, College Station, Texas, March 2023. 2023

SOFTWARE

Matlab <https://www.mathworks.com/products/matlab.html>

Cantera <https://cantera.org/>
Chemical kinetics and transport software package.

ABSTRACT OF THE DISSERTATION

A Three-dimensional, Rotational Flamelet Model for Non-premixed Turbulent Reacting
Flows

By

Wes Hellwig

Doctor of Philosophy in Mechanical and Aerospace Engineering

University of California, Irvine, 2026

Distinguished Professor William A. Sirignano, Chair

Turbulent combustion modeling within Reynolds-Averaged Navier-Stokes (RANS) and Large Eddy Simulations (LES) is a critical aspect of aerospace design, particularly for jet and rocket combustors and ground-based gas turbines. One common approach for modeling turbulent combustion is the flamelet model. While there has been substantial improvement to flamelet theory over its near 50-year history, there are still areas where models fail to include and predict critical physics. This work aims to address two of these areas. First, among other assumptions, existing flamelet models do not incorporate the three-dimensional effects of vortex stretching on the sub-grid fluid-chemical structure through a solution to the momentum equations. Including three-dimensional vortex stretching in the flamelet model produces a centrifugal effect which substantially increases the flammability limit predicted for the reacting mixture. This effect is explored in detail and incorporated into a new flamelet model, called the Rotational Flamelet Model (RFM). Second, a new coupling procedure is developed between the flamelet model and the larger CFD program. This coupling procedure is two-fold as it addresses mechanical coupling; i.e., the influence of turbulent straining and rotation on the flamelet model, and scalar coupling; i.e., how the thermodynamic state in a given CFD cell informs the scalar boundary conditions of the counterflow flamelet. Most flamelet models operate under the modeling assumption that *the turbulent flame samples*

the internal structure of a single canonical counterflow diffusion flame under various strain rates. Under this assumption, flame-local quantities, i.e. parameters defined in the center of the flamelet reaction zone, are used to couple the flamelet to the CFD program. These include scalar dissipation rate (SDR) or flamelet progress variable (FPV) for the mechanical constraint, and mixture fraction for the scalar constraint. Unfortunately, turbulence cascade theory does not present a clear manner of relating or scaling a quantity from RANS or LES to a quantity in the center of a flame that occurs below the mean in RANS or on a much smaller scale in LES, due to the complicated physics that determine the qualities of the reaction zone. Instead, this work adopts the view that turbulent cascade theory better relates the mean or resolved-scale quantities to velocity gradients far removed from the center of the flamelet. The flame-local qualities are then determined through a solution to the sub-grid governing equations, including vortex stretching and density variation in the momentum equations. It is shown that the inclusion of three-dimensional momentum equations with varying levels of vorticity and asymmetric strain rates yields substantially different heat release rates and species production rates compared to an irrotational, symmetric flamelet. Furthermore, by exploring various scalar boundary conditions for the flamelet model, many flamelet families are produced, i.e., flamelets with different scalar boundary conditions, which show further differences in heat release rates and species production rates. For situations in which the flamelet inflows mirror the global fuel and oxidizer inflows (both in composition and enthalpy, which is the practice in the classical flamelet approach), the RFM reproduces classical flamelet behavior such as S-curves, extinction/flammability limits, stable and unstable branches, etc., albeit with the modifications of three-dimensional vortex stretching. The classical behavior is reproduced because the inflows in these situations do not contain high active radical concentrations nor high enthalpy; thus, the flame must provide enough heat to self-sustain or else it extinguishes. However, in situations where the flamelet inflows have high enthalpy, the behavior is substantially different from that of classical flamelets because the inflows themselves may provide enough heat to sustain reactions. It is shown that vary-

ing inflow enthalpies substantially alters flammability limits, an effect that is not included in most flamelet libraries. In summary, by including new sub-scale physics and boundary conditions that follow established turbulent scaling laws, a flamelet model is developed to better-predict non-premixed turbulent combustion.

Chapter 1

Introduction

1.1 Motivation

Combustion is the primary method of energy conversion in systems involving high thrust and high mass flow rates, such as jet and rocket combustors. These flows are usually characterized by high Reynolds numbers (Re), making them turbulent in the absence of chemical reactions. Turbulence enhances the mixing of fuels and oxidizers, which leads to more complete combustion in a reacting flow. Exothermic reactions release heat, which in turn causes flow instabilities in the form of buoyancy and expansion, further enhancing turbulence. This cyclic nature makes nearly all practical combustor flows turbulent. As engineers strive for engines with higher thrust, higher efficiency, reduced emissions, and a host of other technical improvements, simulations of turbulent reacting flows are needed to evaluate the impact of varying design parameters prior to constructing prototypes.

Three general methods exist for simulating turbulent flows. Conceptually, the most straightforward of the three methods, which directly solves the Navier-Stokes equations producing an exact solution to the continuum equations, is called a Direct Numerical Simulation (DNS).

DNS resolves all length and time scales and is thus extremely costly, both from a financial and computational perspective. As the computational cost increases as Re^3 according to Pope [2], DNS is unfeasible for simulations of practical combustors, precipitating the need for simplified classes of simulations. The second class of simulations, in decreasing order of computational cost, are Large-Eddy Simulations (LES), which resolve only the larger turbulent structures in the inertial subrange. Small-scale turbulent motions, the impact of which is confined to the residual stress tensor in the LES equations, are left to simplified eddy-viscosity models, e.g., the Smagorinsky model, or other sub-grid-scale (SGS) models [2]. In many flows of practical interest, it is the large-scale, unsteady motion that is dependent on system geometry, which thus becomes the natural arbiter of engineering design decisions and must be resolved. The small-scale turbulent motions, on the other hand, are to a degree, independent of the system geometry, allowing closure of the LES equations by simpler models. The result is a simulation that attempts to sufficiently resolve those quantities important to system design, without wasting computational resources explicitly solving the small-scale motions as is done in DNS. The last of the three simulation classes are Reynolds-Averaged Navier-Stokes (RANS), which are actually models rather than simulations because they solve for mean flow quantities, typically averaged in time. Here again, a turbulent viscosity model is necessary to close the unknown Reynolds stress, in similar fashion to the residual stress tensor in the LES equations. In some engineering applications, a mean velocity or scalar field may be all that is necessary to facilitate system design, and thus further computational resources are saved by employing RANS. The primary difference between RANS modeling and the other two simulation classes is that RANS does not resolve turbulence of any scale; all fluctuations from the mean are modeled.

In both LES and RANS, unknown terms appear in the global CFD equations which must be quantified or “closed” to arrive at a numerical solution. The models for such terms are referred to as “closure models” and account for the unknown behavior occurring on a scale smaller than the filtered scale in LES and fluctuations from the mean quantities in RANS. In

a non-reacting flow, it is the Reynolds stress (RANS) and residual stress (LES), accounting for the rate at which kinetic energy is dissipated by viscosity and turned into heat, that must be modeled. This is already a daunting task, but the problem is compounded when the turbulent fluid is a reacting mixture. In this case, there are unclosed chemical source terms in addition to the unclosed viscous dissipation terms. This introduces the need for a second class of closure models pertaining to chemistry, one of which is developed and employed in this dissertation, namely, the Rotational Flamelet Model.

1.2 Classification and Dimensionless Numbers

Before discussing modeling techniques, knowledge of the fundamental physical process is necessary, as there is no “one-size-fits-all” approach that gives sufficiently accurate results. There are two limiting combustion modes in both laminar and turbulent reacting flows: premixed combustion and non-premixed combustion [3]. Although some elements of the combustion process are the same for laminar and turbulent flows, this section deals only with globally-turbulent reacting flows. Later, it will be seen that laminar flames are a fundamental building block of turbulent combustion models. In reality, almost all real-world flows lie somewhere between the premixed and non-premixed limits, yet many of the turbulent combustion models developed over the past four decades are strictly valid for only one mode. In purely premixed turbulent combustion, fuel and oxidizer are fully mixed prior to ignition, and once ignited, the flame propagates into the unburnt mixture, leaving behind a zone of burnt gas. While there will be some discussion of premixed flames, this dissertation is primarily concerned with non-premixed turbulent combustion as this is the primary mode in aerospace propulsion systems. In idealized turbulent non-premixed combustion, fuel and oxidizer are not mixed prior to ignition, which causes flames to occur in relatively narrow interfaces where diffusion has produced a flammable mixture. However, in the real

turbulent non-premixed case, some degree of premixing occurs such that many flames are better classified as partially-premixed flames; reactants may be mixed without combusting because there is no ignition source or because the local strain rate is too high. Similarly, in real premixed turbulent combustion, it is virtually impossible to perfectly mix fuels and oxidizers, especially in short periods of time such as one would find in a high RPM internal combustion engine, also leading to partially-premixed flames. Partially-premixed flames are also relevant to jet and rocket combustors because recirculation of high-temperature burnt gases impacts flame holding, auto-ignition, quenching, and re-ignition [4–6]. This situation contains a central diffusion flame fed by inflowing mixtures comprised of high-temperature reactants diluted by products, that is, a diffusion flame fed by one or two non-stoichiometric premixed flames. Whatever the case, it is useful to consider the magnitudes of various non-dimensional numbers to gain insight as to the degree and manner by which turbulence will affect combustion.

Some important dimensionless quantities in turbulent combustion are the Reynolds number (Re), Prandtl number (Pr), Schmidt number (Sc), Lewis number (Le), Damköhler number (Da), and Karlovitz number (Ka). These quantities can be defined for various cases, depending on the reference values chosen, but a general overview is presented first. We focus on gas-phase properties. The Reynolds number is generally defined as $Re \equiv \frac{\rho UL}{\mu} = \frac{UL}{\nu}$ and quantifies the relative magnitudes of inertial forces to viscous forces. In the preceding definition, the quantities ρ and μ or ν , U , and L are generic representations of density, dynamic viscosity, kinematic viscosity, velocity scale, and length scale, respectively. The precise choice of these parameters for various situations will change in accordance with the objective of the discussion. In the following paragraphs, the Reynolds number is defined as $Re = \frac{u' \delta_t}{\nu}$ where u' is the root mean square (RMS) of the velocity fluctuations, δ_t is the turbulence integral length scale, and ν is the kinematic viscosity. If $Re \leq 1$, the viscous forces match or dominate the inertial forces and the flow is laminar (viscosity successfully damps out instabilities). If $Re > 1$ (moderately), unstable instabilities (coherent structures) form,

but are not so powerful that the flow is fully turbulent; here the flow is in a transitional state from laminar to turbulent flow. If $Re \gg 1$, the inertial forces dominate the viscous forces; i.e., viscosity cannot damp out flow instabilities and the flow is turbulent. Of course, the transitional Reynolds number depends on the flow configuration, so Re alone is not enough to classify the flow. This dissertation is concerned with the flows of practical jet and rocket combustors in which the global Reynolds number $Re \gg 1$.

The Prandtl number is the ratio of momentum diffusivity to thermal diffusivity and can be defined for both laminar flow (molecular) as $Pr = \nu/\alpha = c_p\mu/\lambda$ and turbulent flow as $Pr_t = \nu_t/\alpha_t$ flow. Here ν is the molecular kinematic viscosity, α is the molecular thermal diffusivity, c_p is the specific heat at constant pressure, μ is the molecular dynamic viscosity, λ is the molecular thermal conductivity, ν_t is the eddy viscosity, and α_t is the thermal eddy diffusivity. The molecular and turbulent Prandtl numbers are both $O(1)$ for hydrogen and hydrocarbon combustion, with common values for both falling in the range $0.7 - 0.9$. The Schmidt number is the ratio of momentum diffusivity to mass diffusivity and generally follows suit with the Prandtl number. The molecular and turbulent Schmidt numbers are defined as $Sc = \nu/D = \mu/\rho D$ and $Sc_t = \nu_t/D_t$ with D being the molecular mass diffusivity and D_t being the mass transfer eddy diffusivity. The Schmidt numbers are also generally $O(1)$. The Lewis number is the ratio of thermal diffusivity to mass diffusivity $Le = \alpha/D = Sc/Pr$ and is also usually $O(1)$.

Turbulent flows are characterized by numerous eddies of various sizes or length scales. Assuming the turbulence is homogeneous (statistics are independent of position) and isotropic (statistics are direction-invariant), Kolmogorov's eddy cascade hypothesis [7] states that turbulence kinetic energy (TKE) $k = (\overline{u' \cdot u'})/2 = 3\overline{u'^2}/2$ is steadily transferred from the large scales to the smallest scales (Kolmogorov scale), where it is finally dissipated by viscous action and turned into heat. The dissipation rate of TKE, ϵ , then must be equal to the rate of energy transfer between scales to avoid a pile-up of TKE at the bottom of the cascade. The

transfer rate is therefore scale-invariant within the *inertial sub-range* which extends from the so-called *integral scale*, δ_t , to the Kolmogorov scale, δ_κ . The integral scale contains the majority of turbulence kinetic energy.

Arguments are made in this chapter involving quantities at various scales. At the integral scale, the root mean square (RMS) velocity fluctuation is u' ; the length scale is δ_t , and the eddy turnover time, which is also thought of as the turbulent transport time scale, is τ_t . At the Kolmogorov scale, the reference quantities are related to ϵ as: length scale $\delta_\kappa = (\nu^3/\epsilon)^{1/4}$, velocity scale $u_\kappa = (\nu\epsilon)^{1/4}$, and time scale $t_\kappa = (\nu/\epsilon)^{1/2}$ according to Pope [2].

The turbulent Damköhler number is the ratio of the turbulent transport time scale to the chemical time scale $Da_t \equiv \frac{\tau_t}{\tau_c}$. When $Da_t \ll 1$, chemical changes occur over much longer periods than convection and diffusion of mass, meaning that reactions do not adapt to quickly-changing mixtures or temperatures. This leads to significant reactant mixing, which is enhanced by turbulence, prior to combustion. In the limit, called a “perfectly-stirred reactor”, reactants are fully mixed before combustion occurs. This situation is uncharacteristic of the present systems of interest because fuel oxidation happens very quickly and will thus not be discussed further. When $Da_t \gg 1$, the chemical changes occur rapidly relative to fluid mixing, allowing combustion to quickly alter local thermodynamic states in response to convection and diffusion. This results in thin reaction zones that move and deform with the fluid, broadly termed the *thin reaction zone regime*. As the reaction zones are thin in the high Damköhler limit, the internal flame structure is not severely affected by turbulence and the local flame may be regarded as a laminar flame or “flamelet” [1, 4, 8, 9]. In this case, the effect of turbulence is to wrinkle (twist or rotate) and strain the flamelets [4]. In the interior of real jet and rocket combustors, or in the entirety of an adiabatic combustor, the Damköhler number is of medium ($Da_t > 1$) to high ($Da_t \gg 1$) magnitude, supporting the notion of thin, highly sheared, diffusive-reactive zones as described by Peters [1]. Moura et al. [10] reports non-premixed turbulent combustion in a Mach 10 scramjet approximately occurring

for Damköhler numbers between $5 < Da_t < 600,000$ and premixed turbulent combustion for $5 < Da_t < 25,000$ with more than half, but not a dominant amount, of the combustion occurring in the non-premixed mode. Near non-adiabatic boundaries, efflux of heat away from the reactive fluid can cause locally lower Damköhler numbers as the Arrhenius rates drop due to lower temperatures. Generally, fuel oxidation occurs for $Da_t \gg 1$ (fast chemistry) while NOx production and the production of other pollutants occurs for lower Damköhler numbers [4, 9].

The Damköhler number or strain rate, S^* , can be used to define the “S-shaped curve” or “S-curve” for the combustion process at a given location within a combustor. The S-curve illustrates how the flow time scale, relative to the chemical time scale, influences combustion stability. When the local flow time scale is long relative to the chemical time scale (high Damköhler number, low strain rate), the flame is stable at that location and the temperature is high. In the inverse scenario with a low Damköhler number or high strain rate, the flame’s fuel-oxidation kinetics cannot keep up with the short time scale of the fluid, causing local extinction. This may result in local premixing without reaction. The pocket of fluid may be convected to a different location with a higher Damköhler number or lower strain rate where a flame can keep up with the flow time scale, leading to reignition. In either mode, the temperature of the initial location decreases as the Damköhler number decreases (strain rate increases). A qualitative depiction of an S-shaped curve in terms of S^* is shown in Fig. 1.1. An S-shaped curve in terms of Damköhler number may be found in Peters [1, p. 4].

The upper solid portion of the curve represents stable burning states; this is often called the “stable branch”. The lower solid portion represents stable non-burning states and is referred to as the “non-reacting branch”. Here, the fluid only experiences convection and diffusion; there is substantive no reaction. The middle dashed portion represents unstable situations where there is a rapid transition from a non-burning to a burning state; this region is called the “unstable branch”. The transitions of an initially non-burning state through

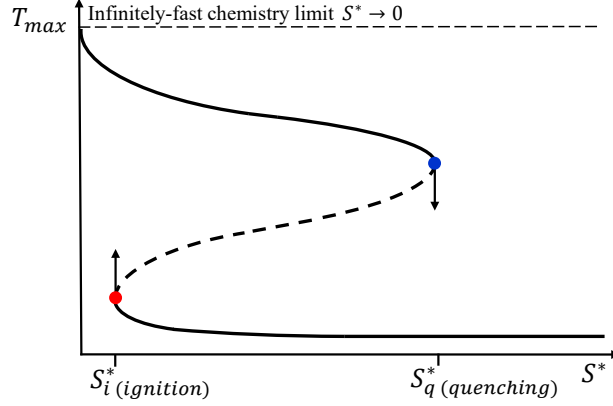


Figure 1.1: S-curve in terms of strain rate S^* . Solid curves indicate stable branches and the dashed curve indicates the unstable branch. The infinitely-fast chemistry limit is shown by the thin, dashed, horizontal line at the top. The ignition point is shown by the red dot in the lower left-hand corner with an upward-point arrow and the extinction point is shown by a central blue dot with a downward-pointing arrow.

the process of ignition, burning, and extinction back to a non-burning state can be traced on the S-curve starting from the point of lowest maximum temperature (right-most point in terms of strain rate). If the residence time increases, moving the state to the red marker, a rapid unsteady transition to a burning state occurs. If the residence time remains long enough, a stable flame will occupy the zone corresponding to the solid black upper branch. However, if the residence time were to decrease enough to bring the state to the blue marker, perhaps due to turbulent fluctuations, the flame will extinguish, moving back to the non-reacting stable branch. The strong temperature sensitivity of fuel-oxidation kinetics makes it overwhelmingly likely that the realization of any thermodynamic state will be on one of the two stable branches; realizations on the unstable branch are very uncommon [1, 11]. Reactions occurring on the reacting stable branch are usually fast relative even to the fastest turbulent flow time scale, τ_κ , and thus occur in thin layers smaller than δ_κ .

1.2.1 Turbulent Premixed Combustion

Many practical combustors, namely the gasoline internal combustion engine (ICE) for automobiles and other small vehicles, utilize premixed turbulent combustion. Fuel is typically

injected upstream of the combustion chamber in a Venturi, where it atomizes and mixes with air prior to compression and ignition in the cylinder. Although not the dominant mode, jet engines also have some degree of premixed combustion resulting from mixing under excessively high strain rates and recirculation. As reactants are already mixed prior to combustion, the chemical reaction rate is the rate-controlling process in this case.

The following equations and associated text, up to the beginning of Sec. 1.2.2, are an adapted and modified summary of the premixed flamelet regime formulation presented in Borghi [12], Peters [13], Peters [1, p. 78-80] and later reviewed by Veynante and Vervisch [4]. Assuming a unity Schmidt number $Sc = \nu/D = 1$ for the premixed case, the flame thickness is $\delta_F = D/S_L$ and the flame time scale is $\tau_F = D/S_L^2 = \tau_c$. S_L is the laminar flame speed. The turbulent Damköhler number may then be written as Eq. 1.1.

$$Da_t \equiv \frac{\tau_t}{\tau_c} = \frac{\delta_t/u'}{\delta_F/S_L} \quad (1.1)$$

In the premixed mode, it is also useful to define the turbulent Karlovitz number as the ratio of the flame or chemical time scale to the Kolmogorov time scale.

$$Ka_t \equiv \frac{\tau_F}{\tau_\kappa} = \frac{\delta_F/S_L}{\delta_\kappa/u_\kappa} \quad (1.2)$$

Taking the unity Kolmogorov Reynolds number as

$$Re_\kappa = \frac{u_\kappa \delta_\kappa}{\nu} = \frac{u_\kappa \delta_\kappa}{D} = \frac{u_\kappa \delta_\kappa}{S_L \delta_F} = 1 \quad (1.3)$$

the Karlovitz number can also be written as Eq. 1.4.

$$Ka_t = \frac{\delta_F^2}{\delta_k^2} = \frac{u_k^2}{S_L^2} \quad (1.4)$$

For the sake of brevity, I will use Ka to indicate Ka_t . If $Ka < 1$, combustion is said to occur in the *thin flamelet regime*. This is the classical regime where premixed laminar flamelet models are thought to be valid. Within this regime, a further delineation is introduced by the ratio of the RMS turbulent velocity fluctuation to the laminar flame speed, i.e., u'/S_L [13]. $Ka = 1$ is colloquially termed the *Klimov-Williams Criterion* and separates the *thin flamelet regime* ($Ka < 1$) from a general regime called the *thin reaction zone regime* or *thickened wrinkled flamelet regime* $1 < Ka \lesssim 100$ in which the flame is significantly influenced by turbulent eddies but the reaction zone is unbroken [14]. Interestingly, Klimov believed that thin reaction zones could still be the most prominent even when $\tau_c u' / \delta_{Taylor} \gg 1$, where δ_{Taylor} is the Taylor microscale [15], and expressed in private letters that he did not approve of the term “Klimov-Williams criterion” [16]. Veynante and Vervisch [4] argue that the smallest turbulent eddies have only moderate effects on combustion because viscous dissipation causes these eddies to be short-lived despite classical theory suggesting they produce leading order effects. Poinso, Veynante, and Candel [17] introduced a method for turbulent premixed combustion whereby knowledge of the turbulence integral scale and turbulent kinetic energy can determine whether the flow will feature classical flamelets, pockets, or distributed reaction zones, suggesting extended applicability of flamelet modeling beyond classical theoretical regime limits. Newer experimental [18–21] and numerical results [22–28] and review papers [16, 29, 30] have shown that Klimov was correct and the flamelet regime extends beyond $Ka = 1$, yet the term remains widely used in the premixed turbulent combustion community. When $Ka > 1$, following the work of Peters [1, 13] it becomes useful to define a second Karlovitz number based on the reaction zone thickness in relation to the Kolmogorov scale,

$$Ka_r = \left(\frac{\delta_r}{\delta_\kappa} \right)^2 = \left(\frac{\delta_r}{\delta_F} \right)^2 Ka \quad (1.5)$$

to classify whether or not the reaction zone is thick enough to contain, or be broken by,

Kolmogorov eddies. Various premixed regimes in terms of the two Karlovitz numbers have been proposed and elaborated on [1, 4, 13] and are summarized in the bulleted list below. The regimes can also be viewed graphically in premixed flamelet regime diagrams such as that originally conceived by Borghi [31] and later modified by Peters [1, 13]. Other turbulent premixed regime diagrams also exist [18, 32, 33].

- $Ka < 1$ & $u'/S_L < 1$: Turbulent fluctuations are slower than the flame speed, leading mainly to laminar flame characteristics with mild distortion or “wrinkling”. Hence, this situation is called the *wrinkled flamelet regime*. This regime is not of practical interest because u' , even for large eddies, is so low that the laminar flame speed dominates the combustion process. This is an unrealistic case for jet combustors and was shown by Moura et al. [10] to be unreachable in a scramjet combustor as well.
- $Ka < 1$ & $u'/S_L > 1$: Turbulent fluctuations are faster than the flame speed, although Kolmogorov eddies are still larger than the flame thickness, and thus the diffusive-reactive layers are entirely embedded within Kolmogorov eddies. Pockets are created, rather than wrinkles, due to the higher value of u' ; however, the reaction zone is still thin and unbroken, and the flow is quasi-laminar and quasi-steady. Essentially, the turnover velocity of large eddies is greater than S_L ; therefore, these fluctuations will distort the flame causing corrugation; however, small eddies having a lower turnover velocity than S_L will not corrugate, nor even wrinkle the flame. This regime is called the *corrugated flamelet regime*.
- $Ka > 1$ & $Ka_r < 1$: Turbulent motion affects the flame as small eddies may lie within the preheat zone, but the reaction zone is still too narrow to contain or be affected by Kolmogorov eddies. The reaction zone thickness $\delta_r \approx 0.1\delta_F$, which in an order of magnitude sense agrees with DNS studies of Poinso et al. [17, 33], suggests that the flamelet regime extends to $Ka_r = 1$. This regime falls within the *thin reaction zone regime* [1, 9, 13] and is also termed the *thickened wrinkled flamelet regime* [4]. This is

the upper limit where flamelet modeling is theoretically valid, and generally requires *thickened flamelet models* as opposed to the standard premixed *laminar flamelet model*.

- $Ka > 1$ & $Ka_r > 1$: Kolmogorov eddies are smaller than, and can exist within the reaction zone; thus, there is no semblance of a premixed laminar flame and the situation is referred to as the *broken reaction zone regime*. The interaction of Kolmogorov eddies within the reaction zone causes enhanced heat loss and a decrease in radicals, ultimately leading to extinction. A diffusion layer results where mixing occurs at lower temperatures [1, p. 85].

1.2.2 Turbulent Non-premixed Combustion

Many other practical combustors do not mix fuel and oxidizer upstream of the combustor. This results in mixing, aided by turbulence, and combustion happening simultaneously in the combustion chamber. Diesel engines, rocket engines, turbojet and turbofan engines, ramjets, and scramjets constitute the bulk of non-premixed turbulent combustion engines. As the author is principally interested in high-performance aerospace vehicles, this dissertation focuses on combustion modeling tailored to non-premixed combustors. Although, as alluded to at the beginning of Section 1.2, premixed and partially-premixed combustion play a role in non-premixed combustors, hence their earlier inclusion.

Compared to premixed combustion, non-premixed combustion with a high Damköhler number is temporally limited by the rate at which fuel and oxidizer mix to create a flammable mixture, not by the much faster chemical reaction rate. That is to say, convection and diffusion, both aspects of turbulent mixing, often occur over a longer period than do chemical reactions. For this reason, the assumption of infinitely fast chemistry (local chemical equilibrium) seems valid, at least more so than for a premixed combustion mode. In an ideal world, the assumption of infinitely fast chemistry would accurately describe, and greatly simplify,

the problem as all finite-rate effects could be neglected. However, in flows where the fluid experiences a high degree of straining and shearing, i.e., high Reynolds number turbulent flows, the local mixing time scale decreases and can become commensurate with the chemical reaction time scale, leading to local flame extinction, lift-off, and in extreme cases, blow-off. Thus, it is important to note here that, while the flow looks like a high Damköhler number flow globally, it is not homogeneously of high a Damköhler number; at certain locations and at certain times, the Damköhler number can decrease to Da_q as shown in Fig. 1.1. Accumulation of extinction events will alter global engine performance metrics; thus, it is desirable to accurately quantify these phenomena. Finite-rate effects are also important in predicting pollutant formation, which has become more important in recent decades.

The following equations and associated text, up to the beginning of Chap. 2, is an adapted and modified summary of the non-premixed flamelet regime formulation presented in Peters [1, p. 190-193]. The time scale associated with non-premixed flamelets, as defined by Peters [1], is based on the axial velocity gradient originating in the oxidizer stream $a = -\frac{\partial v_\infty}{\partial y}$. The asymptotic strain rate in the fuel stream, S^* , which is the primary parameterizing strain rate in the Rotational Flamelet Model (RFM) developed in this dissertation, could also be used. The reciprocal of the strain rate gives a characteristic time scale and can be used in conjunction with the stoichiometric diffusivity, D_{st} , to define a characteristic diffusion layer thickness $\delta_D = \sqrt{\frac{D_{st}}{a}}$. For a binary inflow counterflow, the mixture fraction Z is defined as the ratio of mass originating in the fuel stream to the total mass originating in both streams and will vary from $0 \leq Z \leq 1$ between the oxidizer and fuel streams, respectively. We will see later that this creates a problem for partially-premixed flames, i.e., situations in which some fuel originates from the oxidizer stream or visa versa, and when a multi-component diffusion formulation is used, resulting in counter-gradient diffusion. The mixture fraction is assumed to follow a transport equation, Eq. 2.19, where the diffusivity of the mixture fraction is set equal to thermal diffusivity or the assumed uniform diffusivity of all species.

The reaction zone is located where the mixture fraction equals its stoichiometric value, $Z = Z_{st}$, and its gradient can be related to the physical length scale to define a diffusion thickness in mixture fraction space $(\Delta Z)_F = |\nabla Z|_{st} \delta_D$. The scalar dissipation rate is defined as $\chi = 2D|\nabla Z|^2$ and in the reaction zone, has a value $\chi_{st} = 2D_{st}|\nabla Z|_{st}^2$. The mixture fraction diffusion thickness is then rewritten as $(\Delta Z)_F = \sqrt{\frac{\chi_{st}}{2a}}$ which includes the reaction zone and the surrounding diffusion layer. The thickness of the reaction zone is less than the thickness of the diffusion layer, thus $(\Delta Z)_r < (\Delta Z)_F$. As the strain rate (and thus scalar dissipation rate) increases, the diffusion flame will eventually extinguish. The strain rate and scalar dissipation rate at extinction are denoted a_q and χ_q , respectively; q for “quenching”. Extinction begins when the local mixing time scale decreases to the point that it becomes equal in magnitude to the chemical time scale τ_c . This condition can be written in terms of a local Damköhler number $Da_q = \frac{a_q^{-1}}{\tau_c}$.

To define turbulent non-premixed combustion regimes, Peters [1] states that the characteristic diffusion layer and reaction layer thicknesses in mixture fraction space, $(\Delta Z)_F$ and $(\Delta Z)_r$, must be compared with the stoichiometric RMS mixture fraction variance $Z'_{st} = (\widetilde{Z''^2})_{st}^{1/2}$ and considered for various values of $\chi_q/\widetilde{\chi}_{st}$, where $\widetilde{\chi}_{st}$ is the conditional Favre mean stoichiometric scalar dissipation rate. In layman’s terms, Peters defined regimes by comparing the diffusion layer and reaction zone thicknesses to the “lengths” over which the mixture fraction varies, and then further delineated cases by how close a particular region is to extinction. The regimes are illustrated in Fig. 1.2 (which is an adaptation of Fig. 3.9 in [1, p. 192]) and discussed in the following list.

- $Z'_{st} > (\Delta Z)_F$: This region is characterized by large fluctuations of mixture fraction that range from very lean to very rich such that diffusion layers and their internal reaction zones are separated from other diffusion layers and reaction zones elsewhere in the flow. This is the *separated flamelets regime*. The flamelet model is valid in this regime because the reaction zone is much smaller than the smallest turbulent scales.

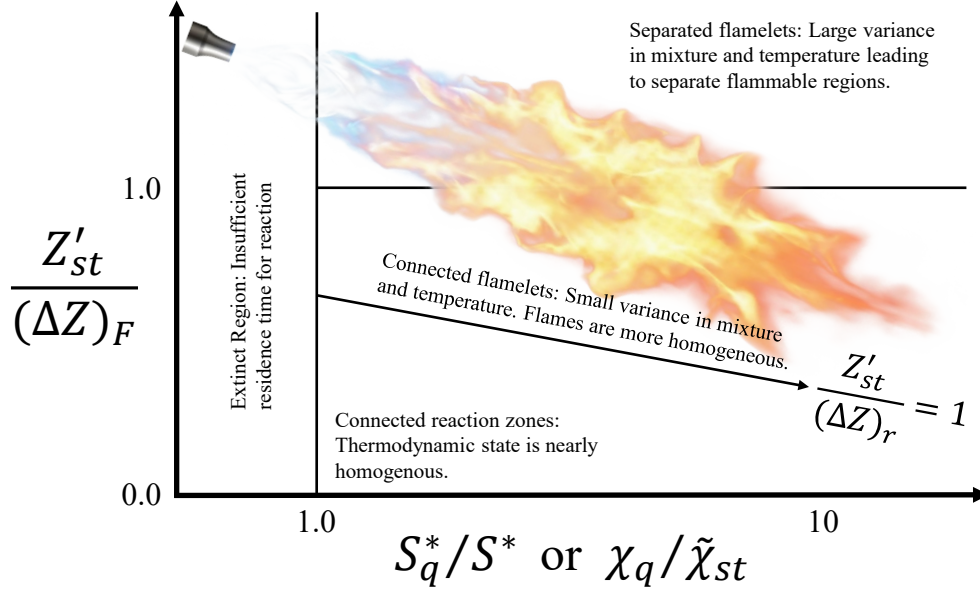


Figure 1.2: Turbulent non-premixed combustion regime diagram adapted from Figure 3.9 (Regimes in nonpremixed turbulent combustion) in Peters, N., *Turbulent Combustion* [1], Cambridge Monographs on Mechanics, Cambridge University Press, 2000. pp. 192. © 2000 Cambridge University Press. Reproduced with permission of Cambridge University Press through PLSclear. This adaptation features additional annotations and an additional abscissa variable, S_q^*/S^* . An animation of a turbulent jet diffusion flame overlaid onto the graph shows the approximate regimes with respect to changing visual character. The overlaid flame represents a fuel jet injected into a body of quiescent oxidizer. Near the nozzle ($S_q^*/S^* < 1$), the residence time is too short for combustion to occur. As oxidizer is entrained downstream and the residence time increases (strain rate decreases), the mixture becomes flammable; however, the mixture fraction variance is still large (*separated flamelets regime*). Further entrainment and mixing reduce the strain rate and the mixture fraction variance (below the horizontal line at $Z'_{st}/(\Delta Z)_F = 1$) and the jet enters the *connected flame zones regime*. The downward-sloping line for $Z'_{st}/(\Delta Z)_r = 1$ separates the *connected flamelets regime* from the *connected reaction zones regime*.

- $Z'_{st} < (\Delta Z)_F$ & $Z'_{st} > (\Delta Z)_r$: This region is characterized by small fluctuations of mixture fraction which may occur when significant turbulent mixing has decreased scalar variance or the fluid was already partially-premixed. Small eddies may have a time scale too fast for reaction, and thus a premixed gas may be created that reacts after mixing. In this case, individual diffusion layers are not clearly separated from one another and the situation is termed the *connected flame zone regime*. The flamelet model is valid in this regime because the reaction zone is still smaller than the smallest turbulent scales, even though the flame thickness is comparable.
- $Z'_{st} < (\Delta Z)_F$ & $Z'_{st} < (\Delta Z)_r$: This case is an extension of the former in which the

turbulent mixing is so intense that neither the diffusion layers nor reactions zones are separated. This is the *connected reaction zones regime*. The flamelet model is not valid in this regime because the Kolmogorov eddies, and perhaps larger eddies, are smaller than the reaction zone.

The vertical line at $\chi_q/\tilde{\chi}_{st} = 1$ separates extinguished mixtures from burning mixtures in terms of residence time. The horizontal line $Z'_{st} = (\Delta Z)_F$ in Fig. 1.2 distinguishes the *separated flamelets regime* from the *connected flame zones regime* and the negatively sloped line $Z'_{st} = (\Delta Z)_r$ distinguishes the latter from the *connected reaction zones regime*. Although not stated by Peters, it appears these three regimes parallel, at least in part, the turbulent premixed combustion regimes delineated by Ka and u'/S_L , although the analogy is imperfect. Specifically, $Z'_{st} > (\Delta Z)_F$ parallels the premixed case of $Ka < 1$ and $u'/S_L < 1$ (*wrinkled flamelet regime*) in which the smallest eddies are much too large to affect the flame; in the non-premixed case, this appears as large fluctuations in mixture fraction leading to the *separated flamelets regime*. $Z'_{st} < (\Delta Z)_F$ & $Z'_{st} > (\Delta Z)_r$ parallels the premixed case of $Ka < 1$ and $u'/S_L > 1$ (*corrugated flamelet regime*) where the smallest eddies begin to alter the flame zone but not the reaction zone; in the non-premixed case, this manifests as smaller fluctuations in mixture fraction leading to the *connected flame zones regime*. Lastly, $Z'_{st} < (\Delta Z)_F$ & $Z'_{st} < (\Delta Z)_r$ parallels the premixed case of $Ka_r > 1$ where the reaction zone is significantly affected by Kolmogorov eddies; in the non-premixed case, this situation appears as very small fluctuations in mixture fraction leading to the *connected reaction zones regime*. Bilger [34] notes that this later situation, where the reaction zone is larger than Kolmogorov eddies, is found in most high Damköhler number, non-premixed, jet flames and recirculating combustors studied in the article. In such cases, it was found that χ varies strongly within the reaction zone which prevents the flame from being characterized by a single χ_{st} and thus the flamelet concept is invalidated. Note that combustion regime diagrams are often defined with simplifying assumptions including equal

diffusivities, assumed probability density functions, and constant Schmidt, Prandtl, and Lewis numbers, among others, and are therefore crude. It can be noted that the simplified concepts used to describe regimes are based on the consideration of only one length scale in the wide range that actually exist in a turbulent combustor. These diagrams give a general understanding of behavior but are quantitatively inaccurate.

Chapter 2

Combustion Modeling Techniques

The primary goal of turbulent combustion models is to quantify the mean heat release rate and net production and consumption rates of chemical species tracked on the resolved scale (LES) or time-averaged mean flow level (RANS). Models should perform these two objectives with minimum computational overhead and should provide closure to the global CFD equations using known quantities, e.g., mean or filtered values. A closure model that itself is unclosed is useless in a practical sense. Models have various ranges of applicability governed by their assumptions; so, this section presents a non-exhaustive overview of turbulent combustion modeling techniques and their strengths and limitations.

2.1 A Brief Summary of RANS and Favre Averaging

The typical Reynolds decomposition of some variable a into its mean $\bar{a}$ and fluctuating component a' is known as Reynolds averaging, with the average of the fluctuation being zero; $\overline{a'} = 0$. When applied to the Navier-Stokes equations, the Reynolds-Averaged Navier-Stokes (RANS) equations are obtained which are commonly used to solve for the mean fields

in incompressible or low-Mach number flows. Unclosed terms result from the averaging process, such as $\overline{u'a'}$, which must be modeled.

In the case of reacting flows, large variations in density are prevalent as a result of heat release. In these cases, Reynolds averaging produces additional unclosed correlations between density and the other flow variables; so, it is beneficial to use a density-weighted average called a Favre average; $a = \tilde{a} + a''$. The Favre mean of a is $\tilde{a} = \overline{\rho a} / \bar{\rho}$ and the Favre mean of the fluctuation is $\tilde{a}'' = \overline{\rho(a - \tilde{a})} / \bar{\rho} = 0$. Over-bars $\bar{a}$ indicate a Reynolds average and over-tildes $\tilde{a}$ indicate a Favre average. The governing equations can be Favre-averaged, producing a set of equations that are more useful for variable density flows. The flow variables, including reactive scalars, ψ_i , such as species mass fractions Y_m or sensible enthalpy h , are split into their Favre means and variances according to Eq. 2.1. The Favre-averaged conservation equations for mass, momentum, energy, and species are given by Eqs. 2.2-2.5 according to Poinot and Veynante [35, p. 142]. Equation 2.4 is written in terms of sensible enthalpy $h_m = \int_{T_{ref}}^T c_{p,m} dT'$ and $h = \sum_{m=1}^{n_{sp}} h_m Y_m$ where $c_{p,m}$ is the specific heat of species m and λ is the thermal conductivity. The viscous stress tensor and species diffusion velocities are τ_{ij} (second equation in Eq. 4.2) and $v_{m,j}$ (Eq. 4.10), respectively.

$$\psi_i = \tilde{\psi}_i + \psi_i'' \quad ; \quad \tilde{\psi}_i'' = 0 \quad (2.1)$$

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_j) = 0 \quad (2.2)$$

$$\frac{\partial (\bar{\rho} \tilde{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{u}_i \tilde{u}_j) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\bar{\tau}_{ij} - \overline{\rho u_i'' u_j''} \right) \quad (2.3)$$

$$\begin{aligned} \frac{\partial (\bar{\rho} \tilde{h})}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\rho} \tilde{h} \tilde{u}_j) &= \frac{\partial \bar{p}}{\partial t} + \overline{u_i \frac{\partial p}{\partial x_i}} + \frac{\partial}{\partial x_j} \left(\overline{\lambda \frac{\partial T}{\partial x_j}} - \overline{\rho u_j'' h''} \right) + \overline{\tau_{ij} \frac{\partial u_i}{\partial x_j}} \\ &\quad - \frac{\partial}{\partial x_j} \left(\overline{\rho \sum_{m=1}^{n_{sp}} v_{m,j} Y_m h_m} \right) + \bar{\dot{Q}} \quad (2.4) \end{aligned}$$

$$\frac{\partial(\bar{\rho}\tilde{Y}_m)}{\partial t} + \frac{\partial}{\partial x_j} \left(\bar{\rho}\tilde{Y}_m\tilde{u}_j \right) = -\frac{\partial}{\partial x_j} \left(\overline{v_{m,j}Y_m} + \bar{\rho}\widetilde{u_j''Y_m''} \right) + \bar{\omega}_m \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (2.5)$$

Equations 2.3-2.5 contain unclosed terms that turbulence closure models attempt to quantify. Various unclosed terms employ different types of closure models. The Reynolds stress $\widetilde{u_i''u_j''}$ is usually closed via eddy viscosity models such as the $k-\epsilon$, $k-\omega$, or $k-\omega$ SST models. Laminar diffusive fluxes $\overline{v_{m,n}Y_m}$ and $\overline{\lambda \frac{\partial T}{\partial x_j}}$ are often neglected as they are small in magnitude compared to turbulent fluxes in high Reynolds number flows. Enthalpy and species turbulent fluxes, $\widetilde{u_j''h''}$ and $\widetilde{u_j''Y_m''}$, respectively, are often closed via gradient transport assumptions in which a turbulent scalar diffusivity is modeled similarly to an eddy-viscosity; however, this assumption is strictly valid only for non-reacting scalars. The gradient transport assumption, otherwise known as the eddy-viscosity or eddy-diffusivity hypothesis, postulates that turbulent fluxes are equal to an eddy-viscosity or diffusivity multiplied by the mean gradient. This is a qualitatively reasonable postulate if the transported quantity is non-reacting, e.g., velocity or mixture fraction, because these quantities are only convected and diffused, which makes their gradients rather smooth, non-intermittent, and relatively isotropic (away from walls). Thus, local mean gradients represent their fluxes well. However, a reacting scalar is not only convected and diffused, but also created and destroyed by the chemical source and sink terms, $\bar{Q}$ and $\bar{\omega}_m$. This introduces anisotropy and intermittency; e.g., flame-normal gradients will typically be of much higher magnitude than flame-tangential gradients and high-magnitude scalar pockets may exist immediately adjacent to low-magnitude pockets. This distribution is not captured by a mean gradient. Furthermore, the source and sink terms typically have much faster time scales than do the convection and diffusion terms, which means that the mean gradient is temporally insensitive to fast chemistry. As such, other closures have been proposed [1, 36, 37], some of which include two or more source/sink terms which respond to different time scales. This is an ongoing area of work in the field of turbulence. However, turbulent transport terms are not the subject of this document; instead, the focus lies entirely on modeling the chemical source terms, $\bar{Q}$ and $\bar{\omega}_m$.

2.2 A Brief Summary of Probability Density Functions

The cumulative distribution function $F(Z; \vec{x}, t)$ gives the total probability that the random variable ζ (defined in the sample space Z) will take a value $\zeta \leq Z$. The probability density function (PDF), $P(Z; \vec{x}, t)$, is the differential rate at which the probability of a particular realization of ζ changes with respect to the sample space variable, i.e., $P(Z; \vec{x}, t) = dF(Z; \vec{x}, t)/dZ$. Consequently, the probability of finding a value ζ within the differential range $[Z, Z + dZ]$ is $P(Z; \vec{x}, t)dZ$, and the total probability of finding ζ over the entire possible range $[Z_{min}, Z_{max}]$ (or $[0, 1]$ if Z is mixture fraction) is unity, as in Eq. 2.6.

$$\int_{Z_{min}}^{Z_{max}} P(Z; \vec{x}, t)dZ = \int_0^1 P(Z; \vec{x}, t)dZ = 1 \quad (2.6)$$

The average value of Z is obtained by Eq. 2.7 and the average value of a function $f(Z)$ is similarly obtained by Eq. 2.8. These are “first moments” of the PDF because the exponent on Z and $f(Z)$ in the integral kernel is one. Central moments (where the mean is subtracted from Z in the kernel) and higher moments (where the exponent is > 1) can also be defined, for example the mixture fraction variance $\overline{Z'^2}$, as shown in Eq. 2.9.

$$\overline{Z}(\vec{x}, t) = \int_0^1 ZP(Z; \vec{x}, t)dZ \quad (2.7)$$

$$\overline{f}(\vec{x}, t) = \int_0^1 f(Z)P(Z; \vec{x}, t)dZ \quad (2.8)$$

$$\overline{Z'^2} = \int_0^1 (Z - \overline{Z})^2 P(Z; \vec{x}, t)dZ \quad (2.9)$$

The following notation is adopted for PDFs, $P(\sim; \sim)$: variables inside the parentheses to the left of the semicolon define the space of the PDF, e.g. Z space, and the $\vec{x}$ and t to the right of the semicolon indicate the PDF’s functional dependence on space and time.

Note that in homogeneous turbulence, PDF's are not functions of position and in stationary turbulence PDF's are not functions of time. The above equations are PDFs using a Reynolds decomposition. If a Favre average is used, the Favre PDF is denoted $\tilde{P}(\sim; \sim)$ and is defined by Eq. 2.10 in relation to the standard PDF used above.

$$\tilde{P}(Z; \vec{x}, t) = \frac{\rho(Z)P(Z; \vec{x}, t)}{\bar{\rho}} \quad (2.10)$$

The Favre PDF has the following properties in parallel to Eqs. 2.6-2.9.

$$\int_0^1 \tilde{P}(Z; \vec{x}, t) dZ = 1 \quad (2.11)$$

Favre mean of Z :

$$\tilde{Z}(\vec{x}, t) = \int_0^1 Z \tilde{P}(Z; \vec{x}, t) dZ \quad (2.12)$$

Favre mean of $f(Z)$:

$$\tilde{f}(\vec{x}, t) = \int_0^1 f(Z) \tilde{P}(Z; \vec{x}, t) dZ \quad (2.13)$$

Favre variance of Z :

$$\widetilde{Z'^2} = \int_0^1 (Z - \tilde{Z})^2 \tilde{P}(Z; \vec{x}, t) dZ \quad (2.14)$$

2.2.1 Infinitely-Fast Chemistry Models

Non-premixed flames are typically described by the mixture fraction Z whose Favre mean $\tilde{Z}$ and variance $\widetilde{Z'^2}$ are calculated in global CFD transport equations. These quantities can be used to parameterize a probability density function for Z which is well represented by, and

often assumed to be, a β -PDF [38], $\tilde{P}(Z; \vec{x}, t)$. If infinitely-fast chemistry is assumed with a one-step reaction, the flame properties are known as functions of Z and the mean properties on the global scale can be obtained through convolution with the β -PDF as shown in Eq. 2.15, where $\tilde{\psi}_i$ is a Favre mean reactive scalar such as mass fraction, temperature.

$$\tilde{\psi}_i = \int_0^1 \psi_i(Z) \tilde{P}(Z; \vec{x}, t) dZ \quad (2.15)$$

Once $\tilde{\psi}_i$ are known, the heat release rate can be quantified using the heats of formation. The infinitely-fast chemistry assumption is strictly valid only when the Damköhler number is infinite and thus represents an upper bound for perfect combustion but is realistically impossible. Obviously, the extinction events described in Sec. 1.2.2 pertaining to a decrease in the Damköhler number are neglected, as are any other effects associated with finite-rate chemistry. Other models assuming infinitely-fast chemistry for the premixed combustion mode are the Eddy-Break-Up (EBU) model by Spalding [39], the Eddy-Dissipation Model (EDM) by Magnussen and Hjertager [40] (which is a derivative of the EDU model), the Bray-Moss-Libby Model [41], and Coherent Flame Models [42]. Non-premixed combustion models in the infinitely fast chemistry limit include a derivative of the EDU/EDM model by Bilger [43] and the Conserved Scalar Equilibrium model which uses a presumed PDF to couple Burke-Schumann solutions [44] to the mean and variance of mixture fraction.

2.3 Models Valid for All Combustion Modes

2.3.1 Global Low-Order Kinetics

The simplest finite-rate turbulent combustion model is obtained by assuming a one-step (or few-step) global reaction on the resolved or integral scale. This method will generally capture, at least in a qualitative sense, the conversion of chemical energy to thermal and

kinetic energy, including the effects of buoyancy and gas expansion, but will otherwise poorly emulate the physical process and will certainly be quantitatively inaccurate. There are three main reasons why this approach is inaccurate. First, reactions happen over small length and time scales as discussed earlier with the Damköhler and Karlovitz number arguments. On these small scales, velocity gradients and scalar gradients are larger in magnitude than their mean or filtered-scale counterparts because their fluctuations increase faster than the length scale decreases. Thus, flames occurring on these scales are subject to scalar quantities and velocity gradients that differ substantially from their global values. Secondly, unsteady effects happening over smaller time scales are either filtered or averaged out by employing LES or RANS. Lastly, the assumed one-step or few-step global reactions neglect the formation, conversion, disappearance, and general existence of short-lived radicals; any effects of elementary reactions are entirely neglected. The accumulation of these assumptions results in inaccurate predictions of the heat release rate and major species production rates, including the ability to model pollutant formation. Xiong et al. [45] and Zhan et al. [6] found that the heat release rate and species production rates are over predicted by global low-order kinetics, citing unmodeled sub-grid turbulence-flame interactions, unmodeled multi-modal combustion, and overly-simple kinetics as likely culprits.

2.3.2 PDF Transport Equation Model

One method of modeling chemistry is to obtain a joint probability density function [46] for the velocity, viscous dissipation, and reactive scalars as proposed by Pope [47–49] or velocity, velocity gradients, reactive scalars, and reactive scalar gradients as proposed by Dopazo [50]. Peters [1] notes that the latter has the advantage of closing terms that describe straining and rotation of scalar gradients in addition to convection and chemical source terms. A transport equation for the joint PDF is then derived, which contains some unclosed terms (depending on which of the aforementioned PDFs is chosen); however, the chemical source

terms are closed. The quality of the solution obtained with PDF methods then depends on the quality of the models for the unclosed terms. In flows with low Damköhler numbers, PDF methods tend to work well because the molecular mixing terms and the chemical source terms are temporally unrelated to each other. However, with high Damköhler number flows, these terms are of commensurate order and higher errors are incurred as a result. PDF methods are attractive because they are widely applicable to all combustion modes, turbulent fluctuations of all quantities are fully represented by the PDF, and complex chemical mechanisms are treated exactly. However, in addition to the difficulty with high Damköhler number flows, PDF methods are also not readily applied to common CFD solvers because of their high dimensionality, making Monte Carlo simulations the preferred solution technique. In order to achieve numerical accuracy with Monte Carlo simulations, many particles are needed within each CFD cell, which when compounded, creates a huge computational burden given how many cells are required to simulate something like a full-scale jet engine combustor.

2.3.3 Linear Eddy Model

The Linear Eddy Model, originally developed for non-reacting flows by Kerstein [51–55] who later extended it to reacting flows [56, 57], models turbulence-chemistry interactions via stochastic rearrangements of diffusive-reactive balances. Time-dependent transport equations, including diffusion and source/sink reaction terms, are solved along a 1D domain for reactive scalars Y_m and T , producing a scalar filament. A succession of eddy “rearrangement events” is then performed, which mimic how an individual eddy modifies the reactive scalar filament. Eddy rearrangement events are described by a triplet map in which a randomly selected interval in the 1D domain is compressed, folded, and rearranged (looking like the italicized capital letter N), simulating stretching and rotation by turbulence. In other words, the monotonic scalar profile is rearranged via compression and flipping, increasing scalar gradients and removing monotonicity. Momentum equations are not solved and convective terms

are not included in the transport equations. The eddy sizes are determined stochastically using PDFs, and the location of the eddy within the domain is determined at random from a uniform distribution. Both the transport equation and the rearrangement events take place on the smallest turbulent scales, making the LEM very computationally expensive relative to tabulated chemistry models, though still much cheaper than fully-resolved DNS.

2.4 Flamelet Models

Flamelet modeling dates back to Williams’ seminal work [58] who first proposed that turbulent non-premixed flames may be thought of as an ensemble of thin, highly sheared, diffusive reactive zones or “flamelets” which move and deform with the fluid. Liew et al. [59] built on Williams idea suggesting that each microscopic flame element in the ensemble could be represented as an individual laminar diffusion flamelet. The consequential assumption at the root of traditional non-premixed flamelet modeling can be summarized as *the turbulent flame samples the internal structure of a single canonical counterflow diffusion flame under various strain rates*. Using mixture fraction as the independent variable for non-premixed combustion, Peters [8] and Kuznetsov [60] separately derived 1D laminar flamelet equations for the reactive scalar fields in Z space. Peters [61] states that the laminar flamelet treatment of turbulent combustion is valid in a regime in which chemical reactions occur faster than transport processes. This condition confines flames and reaction zones to asymptotically thin layers, called flamelets, embedded within the turbulent fluid. This is a general statement for premixed and non-premixed turbulent reacting flows and the condition of applicability is true for most practical combustors, including internal combustion engines, rocket engines, and gas turbine engines. Consequently, the majority of flamelet models assume Peters’ conditions of applicability. If the turbulence intensity increases such that Kolmogorov eddies are smaller than the reaction zone, the laminar structure is broken down and unsteady effects

emerge leading to flame extinction, or in the converse scenario, flame ignition. It is generally believed that these situations involving rapid ignition and extinction transients are best described by unsteady flamelet analysis [1, 62–64] due to rapid changes of the strain rate and low temperature (lower chemical rate) combustion which does not confine the reaction zone to thin layers [65].

In most flamelet models for premixed and non-premixed combustion, the location of the reaction zone is defined by a scalar iso-surface for which a field equation can be derived. In premixed combustion, that scalar is typically the non-reacting scalar G or the reacting scalar “progress variable” C , which both vary from the burnt gas behind the premixed flame to the unburnt gas ahead, allowing the flame to be fixed to a specific realization of G or C . In non-premixed combustion, the mixture fraction Z is commonly used for the scalar. The mixture fraction is a nonreactive (conserved) scalar that varies from $0 \leq Z \leq 1$ between the oxidizer and fuel streams, respectively. The flame is then located at the stoichiometric mixture fraction Z_{st} . Once the statistical distributions of the scalar are known, and the reactive scalar fields normal to the scalar iso-surface are solved with the appropriate flamelet equations, the statistical moments of the reactive scalars can be obtained through convolution with the scalar PDF as summarized in Sec. 2.2. The advantage of using non-reacting scalars G or Z , as opposed to C is that their field equations do not have a source term and thus classical turbulent modeling assumptions for non-reactive scalars are valid.

The flamelet equations govern the reactive scalar field in the reaction zone and surrounding diffusion layer. Peters’ derivations [1, 8] for steady and unsteady non-premixed flamelets employ a transformation from 3D physical space to 3D mixture fraction space, after which it is argued through asymptotic analysis that derivatives of reactive scalars tangential to the flame surface are small compared to derivatives in the normal direction and the field may be treated as 1D (boundary layer approximation). More recent works [66–68] have argued that curvature effects are important in situations where the thin layer approximation

is unjustified, leading to much more complicated flamelet equations in 3D Z space which often have their own unclosed terms requiring grandiose assumptions for closure.

2.4.1 Classical Premixed Flamelet Formulation

Assuming a premixed flame is viewed as a thin interface between burnt and unburnt gases, an equation can be developed for the propagation of the scalar iso-surface. The scalar G is defined by a field equation; so, the actual flame front is located at a specific realization of $G(\vec{x}, t) = G_0$; this is called the “level set approach” as developed by Sethian [69]. The G equation was originally introduced by Williams [70] for the *corrugated flamelet regime* where the premixed laminar flame speed is defined. Modifications to S_L can be made to include the effects of stretch and curvature [71, 72] and the G equation can be further altered to apply it in the *thin reaction zones regime*, where the flame propagation speed is better represented by a turbulent burning velocity.

$$\frac{\partial G}{\partial t} + u_j \frac{\partial G}{\partial x_j} = S_L \left| \frac{\partial G}{\partial x_j} \right| \quad (2.16)$$

Using Eq. 2.16, flamelet equations can be derived in terms of G that govern the reactive scalar fields near G_0 . The premixed case will not be discussed in detail as this work is concerned with globally non-premixed flows, but we will see in Sec. 2.4.2 that parallel logic is used to derive non-premixed flamelet equations in terms of Z , given the mixture fraction transport equation, Eq. 2.19. The steady laminar flamelet equations obtained by Peters [1] in terms of G are Eq. 2.17 where ψ_i is a reactive scalar.

$$\rho S_L \left| \frac{\partial G}{\partial x_j} \right| \frac{d\psi_i}{dG} = \frac{d}{dG} \left(\rho D_i \left| \frac{\partial G}{\partial x_j} \right|^2 \frac{d\psi_i}{dG} \right) + \dot{\omega}_i \quad (2.17)$$

The global flow quantities can then be obtained by convolution with a PDF parameterized by the mean and variance of G . If this PDF is presumed, then the coupling procedure is

termed the *presumed PDF approach*. Alternatively, the PDF could be obtained from a PDF transport equation; however, this is not the usual practice.

Premixed flamelets can also be cast in terms of the progress variable C , which is defined as a normalized temperature or weighted sum of product mass fractions. As such, the transport equation for the progress variable, unlike Eq. 2.16 for G and Eq. 2.19 for Z , has a source term. Neglecting molecular diffusion, the transport equation for the progress variable C is written as Eq. 2.18.

$$\bar{\rho} \frac{\partial \tilde{C}}{\partial t} + \bar{\rho} u_j \frac{\partial \tilde{C}}{\partial x_j} + \frac{\partial}{\partial x_j} \left(\widetilde{\bar{\rho} u_j'' C''} \right) - \bar{\dot{\omega}}_C = 0 \quad (2.18)$$

In this equation, the turbulent flux term $\widetilde{\bar{\rho} u_j'' C''}$ must be modeled in addition to the progress variable source term. The turbulent flux term is not well-modeled using the gradient transport assumption because C is a reacting scalar (see comments in Sec. 2.1 and Peters [1, p. 50]); however, this assumption is often used because of its simplicity.

2.4.2 Classical Non-premixed Flamelet Formulation

As discussed in the prior section, non-premixed flamelets commonly employ the mixture fraction Z as the independent variable. In this section, it is assumed that diffusion follows a Fickian formulation, the thermal diffusivity $\alpha = \lambda / \rho c_p$, and the Lewis numbers $Le_i = \alpha / D_i$ are constant, where D_i is the binary mass diffusivity of species i w.r.t. an abundant species. If it is also assumed that the diffusivities of all reactive scalars are the same and equal to the mixture fraction diffusivity, i.e., $\alpha = D_i = D_Z = D$, then the field equation for the mixture fraction takes the form of Eq. 2.19 and the flame surface is located at $Z(\vec{x}, t) = Z_{st}$. The following derivation and associated text, up to Sec. 2.4.3, is an annotated summary of the classical non-premixed, steady, laminar flamelet equations originally conceived by V.R. Kuznetsov [60] and shortly thereafter, independently derived by Peters [8, 61].

$$\rho \frac{\partial Z}{\partial t} + \rho u_j \frac{\partial Z}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Z}{\partial x_j} \right) \quad (2.19)$$

Using a steady, axisymmetric counterflow, with one-dimensional variation of scalar properties for the flowfield in the vicinity of Z_{st} , with x as the coordinate normal to the counterflow axis, y as the coordinate along the counterflow axis, assumed potential flow velocity gradients in the x and z directions of $du/dx = dw/dz = U$, and an assumed axial velocity gradient in the oxidizer stream of $\partial v_\infty / \partial y = -a$, the governing equations for mass, momentum, mixture fraction, and the reactive scalars are given by Eqs. 2.20-2.23. Later, it will be shown that the RFM does not require this geometry or equality of transverse strain rates.

$$\frac{d\rho v}{dy} + 2\rho U = 0 \quad (2.20)$$

$$\rho v \frac{dU}{dy} = -\rho U^2 + \rho_\infty a^2 + \frac{d}{dy} \left(\mu \frac{dU}{dy} \right) \quad (2.21)$$

$$\rho v \frac{dZ}{dy} = \frac{d}{dy} \left(\rho D \frac{dZ}{dy} \right) \quad (2.22)$$

$$\rho v \frac{d\psi_i}{dy} = \frac{d}{dy} \left(\rho D_i \frac{d\psi_i}{dy} \right) \quad (2.23)$$

Equations 2.20-2.23 can be converted to mixture fraction space using the transformation Eq. 2.24 which gives the steady flamelet equation, Eq. 2.25, for the reactive scalars in terms of the scalar dissipation rate defined by Eq. 2.26.

$$\frac{d}{dy} = \frac{dZ}{dy} \frac{d}{dZ} \quad (2.24)$$

$$\frac{\rho \chi}{2Le_i} \frac{d^2 \psi_i}{dZ^2} + \dot{\omega}_i = 0 \quad (2.25)$$

$$\chi = 2D \left(\frac{dZ}{dy} \right)^2 \quad (2.26)$$

The flamelet equations can now be solved in Z -space assuming the profile $\chi(Z)$ is known. To be exact, this functional dependence would come from a solution to all of the governing equations (mass, momentum, energy, species); however, if these equations were solved, the reactive scalar profiles would also be solved, making the flamelet equation, Eq. 2.25, which gives reactive scalars as a function of Z , redundant. Instead, Peters [8] used an integral solution assuming constant density in the momentum equation and $\rho^2 D = \text{const.}$ (Chapman's approximation) to obtain Eq. 2.27 for $\chi(Z)$ where erfc^{-1} is the inverse complementary error function. This functional form gives Gaussian dependence for $\chi(Z)$ and is commonly used in many applications of non-premixed flamelet models despite the strong assumptions involved.

$$\chi(Z) = \frac{2a}{\pi} \exp \left(-2 [\text{erfc}^{-1}(2Z)]^2 \right) \quad (2.27)$$

Later, Kim and Williams [73] developed an approximate solution for $\chi(Z)$ considering variable density while making other simplifying assumptions such as $\rho h = \text{const.}$, $\rho D = \text{const.}$, and $Le = 1$, while acknowledging variable Lewis number, temperature-dependent transport properties, and varying chemical composition are all areas of necessary investigation. A more general form of the flamelet equations, including unsteady effects and Lewis numbers which differ from one species to another, can also be derived (Eq. 2.28); however, the diffusion formulation is still Fickian.

$$\rho \frac{\partial \psi_i}{\partial t} = \frac{\rho \chi}{2Le_i} \frac{d^2 \psi_i}{dZ^2} + \dot{\omega}_i = 0 \quad (2.28)$$

At the flame, the scalar dissipation rate is $\chi_{st} = 2D_{st}(dZ/dy|_{st})^2$ and represents the inverse of the diffusion time scale. The steady flamelet equations (Eq. 2.25) are valid for burning states having a thin fuel oxidation layer corresponding to high temperature, high radical

locations (upper stable branches in Fig. 1.1) and non-burning states (lower stable branches in Fig. 1.1). During ignition and extinction transients, the unsteady flamelet equations (Eq. 2.28) better capture the phenomena.

The coupling method of the steady laminar flamelet solutions to the global turbulent field is to know or presume a joint PDF of Z and χ_{st} , i.e., $\tilde{P}(Z, \chi_{st}; \vec{x}, t)$. Then the Favre means of the reactive scalars can be obtained through convolution with the PDF, Eq. 2.29.

$$\tilde{\psi}_i(\vec{x}, t) = \int_0^1 \int_0^\infty \psi_i(Z, \chi_{st}) \tilde{P}(Z, \chi_{st}; \vec{x}, t) d\chi_{st} dZ \quad (2.29)$$

However, the joint PDF is often too computationally expensive or even impossible to obtain without other simplifying assumptions, so many practical CFD codes, such as ANSYS Fluent, default to the convenient, but not strictly physical, assumption that fluctuations in Z and χ_{st} are statistically independent [74, p. 322]. Typically, a β PDF is used for the marginal PDF of Z and delta function is used for the marginal PDF of χ_{st} . The latter ignores fluctuations in χ_{st} and the established observation that Kolmogorov-scale velocity gradients are higher in magnitude than those on larger scales; however, this imprecision may be overshadowed by errors incurred from the closure of the Reynolds stress via eddy viscosity hypotheses. Another coupling method, where unsteady effects are more important, is to average the flamelet equations over χ_{st} and then replace the marginal PDF for χ_{st} in Eq. 2.29 by a delta function centered at the conditional Favre mean scalar dissipation rate [1].

2.4.3 Flamelet Models: Advances and Limitations

Many improvements have been made to flamelet theory since its inception nearly 50 years ago. The derivation of Eqs. 2.25 and 2.28 involve neglecting diffusion tangential to the Z_{st} iso-surface. This assumption was adopted in part due to convenience and was classically justified with a few sub-assumptions. First, a high Damköhler number or low Karlovitz

number is assumed, making the flame thin relative to the smallest eddies. In this case, the radius of curvature is very large relative to the flame thickness, and thus the flame appears flat from the view point of an eddy. For premixed flamelets, a low Karlovitz number also implies that the laminar flame speed is fast relative to the Kolmogorov velocity fluctuation, which means that the propagation of the flame front is insensitive to fluctuating flow velocity and can thus remain relatively flat. These conditions are frequently found in practical combustors, e.g., at moderate injector nozzle standoff distances in a turbulent jet flame, but there are also numerous situations in which the thin flame assumption is invalid, e.g., close to the nozzle and very far from the nozzle in the same turbulent jet flame. The thin flame assumption weakens or is invalid in the *thin reaction zone* and *broken reaction zone* regimes (premixed mode) and the *connected flame zones* and *connected reaction zones* regime (non-premixed mode) discussed in Sec. 1.2.1-1.2.2.

Second, a unity Lewis number is generally assumed under the argument that molecular diffusion is insignificant compared to turbulent diffusion [1, 8, 75–77], which independently nullifies the effects of stretch and curvature. This is certainly true globally, and for larger scales when the Reynolds number is high, but is not true within laminar flamelets. Barlow et al. [78] point out the transition from molecular to turbulent diffusion through mean scalar profiles of Sandia Flames A-F, noting that those with a high Reynolds number show little evidence of differential diffusion. This observation is used to justify the unity Lewis number assumption, presumably for the overall turbulent flame, not individual laminar flamelets. Specific fuel-oxidizer combinations with large differences in molecular weight, e.g., H_2 burning with any oxidizer or heavy hydrocarbons burning with light oxidizers, are particularly susceptible to preferential and differential diffusion and are poorly simulated with a unity Lewis number approximation [79–82].

The many instances in which these two assumptions are not experimentally-observed motivated the inclusion of non-unity Lewis numbers, curvature effects, and tangential diffusion in

flamelet models. Non-premixed flamelet formulations, including differential diffusion, were introduced by Pitsch and Peters [83] and were followed by an unstable formulation by Pitsch [84]. Pitsch and Peters introduced differential diffusion effects via a re-definition of mixture fraction whereby Z is no longer a weighted sum of reactive scalars. Instead, they define Z via a conservation equation and state that taking the mixture fraction diffusivity equal to the thermal diffusivity produces a sufficiently accurate flame structure; however, it has been shown that this model over-predicts differential diffusion effects in turbulent jet flames since it does not factor in Reynolds number dependence [84, 85]. The equations they obtain via a transformation from physical space to mixture fraction space are exact with respect to the pre-transformed equations if $\chi(Z)$ is known. Herein lies one of the recurring problems which the work of this dissertation seeks to address; one cannot know $\chi(Z)$ without solving the momentum equations with vorticity, variable density, and in the absence of other simplifications. In their conclusion, Pitsch and Peters clearly state that an exact flamelet formulation using $\chi(Z)$ requires the solution of the complete set of fluid dynamic equations rather than an assumed profile for $\chi(Z)$ [83].

Differential diffusion effects have also been included in premixed flamelets [86] and addressed in the context of curvature effects [67]. Wang [85] identifies the influence of Reynolds number on differential diffusion showing analytically that molecular diffusion is dominant at low Reynolds numbers while turbulent diffusion is dominant at high Reynolds numbers. Consequently, Wang introduces the ratio of molecular to turbulent diffusion as an explicit parameter used to blend Peters' [8] equal diffusivity model with Pitsch and Peters [83] differential diffusion model which has been shown to better approximate flame structures as compared to unity Lewis number and variable Lewis number models; however, results still showed deviation from experiments [82, 85]. In a later work, Han and Wang [87] identified the importance of unsteady effects and the influence of various scalar dissipation rate profiles on correctly modeling differential diffusion. Following the work of Wang and Gierth et al., Jiang et al. [88] proposed the species-weighted flamelet (SWF) model, based on the

FPV model, which, while similar to [82, 85], uses detailed molecular diffusion in addition to the Lewis number dependence on Reynolds number. The SWF model includes unity Lewis number (ULF) ($R_e \rightarrow \infty$) and variable Lewis number (VLF) ($R_e \rightarrow 0$) databases which are combined in a weighted average to approximate the effects of differential molecular diffusion. They found that differential diffusion notably alters profiles of temperature and species with LES results differing from experimental results [89] by less than 6%. The SWF model better captures the inter-related physics of combustion intensity, turbulence intensity, mixture fraction, and differential diffusion.

Curvature effects, which were not present in classical theories [1, 8, 77, 83], have been added to flamelet models over the last two decades. As the name suggests, curvature effects describe the implications of a curved flame front as opposed to the flat flame fronts originally considered. In a turbulent environment, it is certainly conceivable that a flame could be distorted by an eddy, depending on the size of that eddy, and that the mathematical framework based on a flat flame would then break down. Following Peters' [1, 8] transformation from 3D physical space to 3D mixture fraction space ($x_1, x_2, x_3 \rightarrow Z_1, Z_2, Z_3$), Xuan et al., [67] derived a mathematical framework for three-dimensional (in mixture fraction space) flamelets considering curvature and differential diffusion. They found that curvature effects must be considered "when the radius of curvature is comparable [to] or smaller than the local flame thickness" [67] where flame thickness is defined as $l_F = (\Delta Z)_F / |\nabla Z|_{st}$. This is an important addition to flamelet theory and one that helps steer the analysis in this dissertation. While curvature should be addressed in the future, the existing development of the RFM adopts the formalism that curvature effects may be neglected on the basis that no fluid structures with length smaller than the Kolmogorov scale exist in the flow and thus the radius of curvature is larger than the flame thickness.

Xuan et al. [67] also found that curvature effects do not affect transport physics if the Lewis number is assumed to be unity but do affect transport physics if differential diffusion

effects are considered. The development of the RFM presented in later sections is not limited to constant or unitary Lewis numbers; however, these conditions can be imposed if desired. A brief note on curvature and vorticity is also important. The curvature effects for flamelets and scalar iso-surfaces [68, 90–93] are fundamentally different from the vorticity effect we incorporate in the RFM [64, 94–98] (to be discussed later). Curvature effects describe distortion of the mixing layer and flame which produce scalar transport in directions tangential to the counterflow axis. They do not include a centrifugal term in the momentum equations as we have done. While flow vorticity can contribute to the degree of curvature of a scalar iso-surface in turbulence, the inclusion of curvature terms in the flamelet equations is not a substitute for the solution of the momentum equation with vorticity. For example, Dopazo et al. [90] in their Eq. 38 show that the time rate of change of the unit normal vector to the iso-scalar surface depends on both strain rate and vorticity. They correctly make no claim that curvature is thereby a surrogate for vorticity since the equation only relates the rate of change, not the magnitude of the normal vector, to vorticity. In a steady state formulation, Dopazo’s equation can be interpreted to relate curvature to the gradient of vorticity. However, the RFM focuses on the core of the eddy, taking the peak value of vorticity to be uniform through the flamelet. Thereby, the gradient of vorticity is zero and curvature, which involves higher order derivatives, has negligible effect in the domain of study. Some numerical results [99, 100] and experimental work [101] illustrates the history dependence (temporal derivatives) of scalar gradients (curvature) on vorticity in premixed flames, further supporting the conclusion that curvature is not a substitute nor surrogate for vorticity, especially under the quasi-steady assumption.

In the non-premixed progress variable approach (FPV), upon which many recent flamelet models are based, Pierce and Moin [77, 102] object to Peters [1, 8] practice of prescribing axial counterflow velocity via a fixed strain rate a as $v(y) = -ay$ which is not valid across the entire domain as it violates the continuity equation, ignoring important dilatation effects. Pierce and Moin adopt zero advection in place of a counterflow ($v(y) = 0$, $\chi(Z) \approx \text{const}$),

making the flamelet equations a purely diffusive-reactive balance in physical space, and apply Dirichlet boundary conditions to species and enthalpy at a finite separation distance L in lieu of solving the momentum equations. This simulates counterflow streams by capping the diffusive domain, creating scalar gradients from which the mixture fraction can be defined, assuming $Z(y)$ is monotonic. In the FPV approach, the flamelet equations are solved in physical space giving $\psi_i(y)$, after which mixture fraction is calculated and the profiles of reactive scalars are recast as functions of the mixture fraction, that is, $\psi_i(Z)$. One set of $\psi_i(Z)$ exists for a given value of L , which is essentially the flamelet length scale. In order to include the unstable branch of the S-curve, Pierce and Moin adopt a mapping procedure such that the reactive scalar dependence on L is cast in terms of a monotonic variable that can be tracked on the LES resolved scale; this variable is a weighted sum of product mass fractions called the “progress variable” C which has its own “contrived” resolved scale governing equation. Reactive scalars are then parameterized by mixture fraction and progress variable, instead of mixture fraction and scalar dissipation rate. Favre-filtered reactive scalars are then obtained with the presumed PDF approach except here, the PDF is conditioned on Z and C rather than Z and χ .

The FPV approach offers two primary benefits over the classical flamelet approach. Classical flamelet approaches are only capable of returning reactive scalar solutions along the stable non-reacting and stable reacting branches of the S-curve because χ and S^* are multi-valued for $S^* < S_q^*$ (Fig. 1.1). In the FPV approach, the monotonic behavior of C allows the entire S-curve to be called from the resolved scale, not just the stable non-reacting and reacting branches. Pierce and Moin acknowledge that the inclusion of the unstable branch through the FPV approach is technically incorrect because the branch is physically unsteady, and thus including it through a contrived steady formulation is a departure from the true unsteady physics. However, the imperfect inclusion of the unstable branch is still a large improvement over complete neglect of the branch. The results Pierce and Moin obtained with the FPV approach for a coaxial jet combustor agree much better with experimental

data than the fast chemistry and classical steady-flamelet approaches. In particular, the FPV approach predicts the experimentally-observed [103] lifted flame behavior, whereas the other approaches predict attached flames [77]. The FPV approach has also been used by Ihme et al. [104], Nguyen et al. [105], and Nguyen and Sirignano [106, 107] where it was again found in [106] to agree better with the experimental data due to the inclusion of the unstable branch. For this reason, the RFM program developed in this dissertation includes the ability to calculate the unstable branch, and the novel RFM coupling procedure respects its importance.

Two issues pertain to the use of scalar dissipation rate as the mechanical constraint parameter. First, the assumption of a functional form for the scalar dissipation rate $\chi(Z)$ leads to some error. As discussed previously, the scalar dissipation rate, defined by Eq. 2.26, is a function of the local diffusivity and the mixture fraction gradient, which in turn are functions of the reactive scalars themselves. To solve the flamelet equations 2.25 and 2.28 which give the reactive scalars $\psi_i(Z)$, the profile $\chi(Z)$ must be known. Thus, the reactive scalar distribution is solved from a profile that implicitly assumes the reactive scalar distribution is already known, leading to a technical contradiction. In defense of proponents of the existing model, this assumption is fairly good in certain situations; nonetheless, there is some error. The classical assumption where $\chi(Z)$ is assumed through a constant density solution to the momentum equations has been relaxed [73] as previously mentioned. More recent studies have identified discrepancies between presumed and computed profiles. Ameen et al. [108] conducted an evaluation between simulations using a Gaussian profile for scalar dissipation rate and DNS solutions for scalar dissipation rate, finding that the Gaussian shape fails to emulate the scalar evolution in igniting flames. Temperature and thermal expansion alter scalar dissipation rate significantly; these effects cannot be captured with assumptions of equal diffusivities, unity Lewis numbers, or a fixed functional dependence of $\chi(Z)$. Ameen et al. note that using the $\chi(Z)$ profile obtained from DNS drastically reduces the error. Hellwig et al. [97] showed that inclusion of three-dimensional strain fields and vorticity also

changes the scalar dissipation rate profile and Sirignano et al. [109] showed that the peak of the $\chi(Z)$ curve shifts toward the inflowing stream with higher thermal diffusivity. Other sources also cite issues with assumed profiles. In light of these findings, it is evident that the universal Gaussian assumption for SDR as a function of mixture fraction is not entirely adequate. To address this, a coupling procedure will be developed in Sec. 5.1 under the hypothesis that scaling resolved flow velocity derivatives to ambient values relative to the flame, and then determining flame structure via sub-scale physics subject to these ambient boundary conditions, including vorticity and three-dimensional strain rates, may better mimic the physical process.

The second issue pertaining to the typical usage of scalar dissipation rate concerns scale separation. There is no reason to believe that the resolved or mean value of scalar dissipation rate, $\tilde{\chi}$, is equal to the sub-grid laminar flamelet value, χ . In fact, cascade theory indicates the opposite; larger gradients occur on smaller scales which means $\chi \gg \tilde{\chi}$. However, if the common practice of using a delta function as the marginal PDF for χ in the presumed PDF coupling procedure is retained, scale separation of the flamelet and the resolved or mean flow is ignored. This is done as follows. The Favre-averaged scalar dissipation rate is often given through the linear relaxation model, Eq. 2.30

$$\tilde{\chi} = \frac{\widetilde{Z''^2}}{k/\epsilon} \quad (2.30)$$

and the joint PDF $\tilde{P}(Z, \chi_{st}, \vec{x}, t)$ is decomposed into the conditional PDF $\tilde{P}(Z|\chi_{st}, \vec{x}, t)$ multiplied by the marginal PDF $\tilde{P}(\chi_{st}, \vec{x}, t)$. Furthermore, if Z and χ are assumed to be statistically independent, then the conditional PDF reduces to a marginal PDF for Z which is assumed to be a β -PDF. Using a Dirac delta function for the marginal PDF of χ as $\tilde{P}(\chi_{st}, \vec{x}, t) = \delta(\tilde{\chi}_{st})$ is a mathematical way of stating $\chi = \tilde{\chi}$ (Peters [1, p. 212]), which is not physically true. A better approximation is obtained by using a log-normal distribution for $\tilde{P}(\chi_{st}, \vec{x}, t)$ [8, 76]; however, Peters notes that this is very costly for steady-state flamelets

and, for all intents and purposes, impossible for unsteady flamelets [1, pp. 215-216]. The author suspects that the assumption $\chi = \tilde{\chi}$ is even worse if unsteady effects are considered and the unstable branch is used because the Favre mean SDR, $\tilde{\chi}$, will average out the instantaneous large-magnitude fluctuations that exist for χ on the flamelet scale.

Another shortcoming of many flamelet models frequently used today stems from the geometric assumption of a 2D planar or axisymmetric flow field with only normal, and often equal, imposed strain rates. These assumptions simplify the mathematics but neglect anisotropy of velocity gradients in turbulence; that is, the potential for a 3D strain field including both unequal normal strain rates and shear strain rates. In fact, these tenets of existing flamelet models are in disagreement with the LES results obtained using the models. Specifically, the flamelet geometry has normal strain rates but no shear strain, while LES results using the flamelet model [6, 62, 110–114] and DNS results using infinitely-fast chemistry [115–117] and one-step Arrhenius kinetics [118] indicate that flames embedded in turbulent flows are subject to substantial normal and shear straining. Through a transformation to a non-Newtonian reference frame, these flames experience normal strain rates and a centrifugal effect due to the rotation of the Lagrangian reference frame. To the best of the author’s knowledge, these qualities have not been included in any flamelet formulation prior to Sirignano [94]. Inclusion of rotation or vortex stretching requires a 3D treatment which is rarely used except in those models which include tangential diffusion and curvature effects (discussed previously) which retain three dimensions in mixture fraction space. However, in similar fashion to Eq. 2.25-2.28, these models also do not solve momentum equations which means the effects of variable transverse strain rates and centrifugal force from vorticity are neglected through an assumed profile for $\chi(Z)$. Theoretically, $\chi(Z)$ could be obtained from a full solution of all the governing equations but this has not been done and leads to the redundancy discussed in the text following Eq. 2.26.

Another issue with existing models relates to the fixed scalar boundary conditions applied

to the flamelet counterflow. Scalar quantities, namely mixture and temperature, obviously vary throughout the combustor domain. Thus, each RANS or LES computational cell has its own thermodynamic state determined by local composition, temperature, and pressure. When the flamelet model is viewed as a subgrid model, the expectation is that the inflows to the counterflow would vary in accordance with the local resolved scale state as determined by scaling relations connecting the resolved scale to the flamelet scale. However, every non-premixed flamelet model known to the author assumes that the two inflows of the counterflow have fixed mixtures: oxidizer on one side and fuel on the other, such that $0 \leq Z \leq 1$, and that both inflow streams are at a fixed temperature. The fuel and oxidizer inflow mixtures and temperatures are classically chosen to be the same as the global inflows; e.g., equal to the fuel and oxidizer conditions at the injector face. This means that irrespective of the thermodynamic state of a resolved flow computational cell, the flamelet applied in that cell has the same scalar boundary conditions as every other flamelet in every other cell. This is obviously non-physical if the entirety of the flamelet counterflow is assumed to exist within each cell, as is the view adopted in this dissertation using the flamelet as a “sub-grid model”. However, classical flamelet models do not seem to adopt this viewpoint. Instead, they use the modeling assumption that *the turbulent flame samples the internal structure of a single canonical counterflow diffusion flame under various strain rates*, which in practice, significantly reduces the error compared to if the entire counterflow structure were placed uniformly within the resolved-scale cell without varying the scalar boundary conditions. The classical coupling procedure uses the mean and variance of the mixture fraction in the given cell to weight and confine the flamelet reactive scalar profile to a thin range of mixture fraction space, i.e., $\psi_i(\Delta Z_{chosen}) \in \psi_i(0 \leq Z \leq 1)$ to reflect the statistical Z -values that are likely to occur based on the resolved-scale state. In doing so, the fixed scalar boundary conditions are somewhat avoided and the flamelet model becomes less of a subgrid model and more of a tabulation technique for fluid-chemistry interaction. In other words, there appear to be two fundamental interpretations of what a flamelet model is; see Table 2.1.

Table 2.1: Two general interpretations of flamelet models

Subgrid Model
The flamelet counterflow is a solvable flow geometry to approximate the sub-grid fluid-chemistry interaction, involving a fluid-dynamic calculation of the behavior within a finite volume CFD cell as determined by conservation of mass, momentum, energy, and species, while the boundary conditions for the counterflow depend on the properties within the larger CFD cell. The counterflow, being on the order of the Kolmogorov scale, is much smaller than the cell, thus many counterflows exist within the cell and an average counterflow is used to represent the net effect of many individual counterflows. In this case, the boundary conditions of the average counterflow are subject to both mechanical and scalar constraints imposed by the mean flow or resolved-scale velocity and scalar fields. In this way, the entirety of a particular flamelet counterflow is placed within the CFD cell.
Tabulated Fluid-Chemistry Model
The flamelet counterflow is used as a convenient flow field in order to quantify the interaction between compressive strain rate (i.e., scalar dissipation rate, residence time, or progress variable) and reaction rate. By solving a counterflow that varies from global fuel injection conditions to global oxidizer injection conditions ($0 \leq Z \leq 1$) with fixed boundary temperatures for a variety of scalar dissipation rates (progress variables), reactive scalars are quantified in terms of one mixture parameter (Z) and one mechanical constraint (χ or C). Then, the averaged reactive scalar returned to the CFD cell is obtained by convoluting the laminar flamelet reactive scalar profile with the joint PDF. The convolution “smudges” the laminar flamelet reactive scalar profile based on turbulence intensity, which is intended to simulate the scaling mechanism between the flamelet scale and resolved scale, and weights the profile based on the resolved scale mixture. Thus, if the resolved-scale $\tilde{Z}$ is close to Z_{st} and the variance $\tilde{Z}''^2$ is low, then the portion of the laminar flamelet profile used will be heavily weighted to a narrow section around Z_{st}. Conversely, if $\tilde{Z}$ is away from stoichiometry and/or $\tilde{Z}''^2$ is high, the portion of the laminar profile used will be weighted away from Z_{st} where little to no reaction occurs. In this way, the “geometry” represented in each resolved-scale cell by the flamelet model is a weighted, thin section in $Z - \chi$ or $Z - C$ space; i.e., the entire counterflow geometry is not uniformly placed within the cell.

In in Chap. 5 of this dissertation, a new coupling procedure is developed whereby resolved or mean flow velocity gradients and scalar fields are used in conjunction with cascade theory scaling laws to obtain approximate Kolmogorov-scale conditions for the average flamelet belonging in the given cell. These conditions are viewed as asymptotic or far-field conditions relative to the Kolmogorov scale. It is hypothesized that this manner of obtaining sub-grid conditions, in conjunction with other improvements to the flamelet model itself, will lead to

better experimental agreement. The second of the two interpretations of flamelet models in Table 2.1 will not suit this coupling procedure as the boundary conditions are fixed and the entire counterflow is not represented, which is a necessary condition for the vorticity and transverse strain rate effects to be included in the model. Instead, we will view RFM the as a “sub-grid model” according to the first interpretation in Table 2.1.

2.5 Summary of Flamelet Modeling and Objectives

Flamelet modeling is an attractive turbulence-chemistry approximation technique which allows inclusion of arbitrarily complex chemical kinetics mechanisms and their associated finite-rate chemistry effects without the added cost of solving highly nonlinear, coupled reactions in global CFD computations. Flamelet models can be applied to premixed, partially-premixed, and non-premixed combustion modes and represent the influence of turbulence on combustion reasonably well when used in valid combustion regimes. Quasi-steady laminar flamelet models assume that chemical time scales are faster than turbulent time scales, and therefore the reaction zone is thin relative to the smallest turbulent length scales. These models have been improved over the years to the point where modern versions include differential diffusion, variable thermo-physical properties, and stable and unstable branches. However, flamelet models still invoke some limiting assumptions, which the work in this dissertation seeks to improve upon. The broad goals of this work are summarized in the list below.

1. The fundamental goal of the Rotational Flamelet Model (RFM) is to include rotation (vorticity) and three-dimensional, asymmetric and symmetric strain rates in the counterflow flamelet structure. These qualities have not been explicitly included in any other flamelet model to the best of the author’s knowledge despite there being prolific evidence that vortices and three-dimensionality are critical aspects of turbulence. As the RFM is tailored to non-premixed combustion where diffusion and mixing are the

rate-limiting physics, and the fastest diffusion rates occur on the smallest scales, it is assumed that the leading-order heat release rate and reaction rates can be determined from flamelets on the small scales. Thus, the RFM is a Kolmogorov-scale flamelet model, subject to the approximate mechanical dynamics of the small-scales.

2. Due to the physical scale and thus boundary conditions of item 1., knowledge of approximate Kolmogorov-scale velocity gradients and flamelet scalar boundary conditions are required to couple the RFM solutions to the resolved-scale computation. Therefore, a new coupling procedure is employed which links the turbulence kinetic energy dissipation rate to the flamelet mechanical constraints through turbulence cascade theory. This new mechanical coupling procedure replaces the progress variable or scalar dissipation rate PDFs in former models which are less-substantiated by turbulence theory. A simple scalar argument is used for mixture and enthalpy coupling.
3. Many classical flamelet models simplify molecular transport with a Fickian diffusion approximation for use of scalar dissipation rate as a parameterizing variable. However, Fickian diffusion is less accurate than multicomponent diffusion, especially in the laminar environment of Kolmogorov and sub-Kolmogorov scales. Many existing models worsen the approximation by using fixed or unity Lewis numbers which neglect differential and preferential diffusion. Because the RFM is developed without scalar dissipation rate, full multicomponent diffusion may be used, and no assumptions or approximations regarding thermo-physical properties are necessary. Of course, if desired, mixture-averaged or Fickian diffusion, as well as other assumptions, can still be employed to make direct comparisons with other models, but the RFM does not require these simplifications.

Chapter 3

The Rotational Flamelet Model

The Rotational Flamelet Model was first proposed by Sirignano [94] to relax several assumptions of existing flamelet models. The first was the assumption of constant density across the flamelet. Density is obviously variable through the flamelet because heat released in the reaction zone will elevate the local temperature far beyond that of the inflows. The second was the assumption of a 2D planar or axisymmetric counterflow. While mathematically convenient, there is no guarantee that velocity derivatives in small-scale turbulent structures produce either of these symmetries; a more general geometry allows the three normal strain rates to take independent magnitudes. Third, shear strain or vorticity was classically neglected despite its high magnitude on the Kolmogorov scale and can be included by adding a centrifugal term to the momentum equations. Lastly, the combustion mode in most flamelet models is prescribed (premixed or non-premixed) while numerous studies show multiple modes are accessed in the same combustor. Relaxing these assumptions introduces momentum equations which must be solved in addition to the equations for the reactive scalars; i.e., the prior practice of assuming a solution to a simplified momentum equation and only explicitly solving the reactive scalar equations 2.25 or 2.28 is no longer possible.

3.1 Geometry

Via appropriate scaling for turbulent flows, estimates for the Kolmogorov scales for velocity, length, time, strain rates and vorticity can be obtained. Strained non-premixed flames (i.e., counterflow diffusion flames) will not occur at smaller scales because higher strain rates than the Kolmogorov scale are not possible. Flames with thickness much smaller than an eddy size would be wrinkled flames propagating through the eddies rather than flamelets held in capture by an eddy. Premixed flames with size larger than some eddies would rely on turbulent diffusion to assist propagation. These flames might be large enough to describe well at the resolved scale. The focus is on flamelets captured by the small eddies. Therefore, the physics of the flamelet can be approached through laminar modeling. We expect the diffusive-convective balance for these flamelets at approximately the Kolmogorov scales, having the shortest characteristic length and time, such that the quasi-steady assumption can be made. The reader may question whether Kolmogorov eddies, having similar characteristic times to the flamelet diffusion time, would cause unsteadiness. Here, the quasi-steady assumption weakens, suggesting the need for unsteady flamelet analysis; however, important physical insights can still be gleaned with the quasi-steady assumption.

On these small turbulent scales both normal and shear strain rates are important. Shear strain can be decomposed into the combined effects of normal strain plus rotation where the rotation rate (angular velocity) is half the vorticity magnitude. For example, consider in 2D, an initially square shape subjected to shear strain; it will deform, becoming a parallelogram. When viewed from the principal directions (see Fig. 3.1), one diagonal is stretched (tensile normal strain) and one diagonal is compressed (compressive normal strain). Both diagonals are rotated. Notice the angle $\theta(t_0) > \theta(t_0 + \Delta t)$ and mathematically, $d\theta/dt = \omega/2$.

The combined influences of strain and rotation are especially important on the small scales where chemical reactions occur. As is well known, the magnitudes of velocity gradients

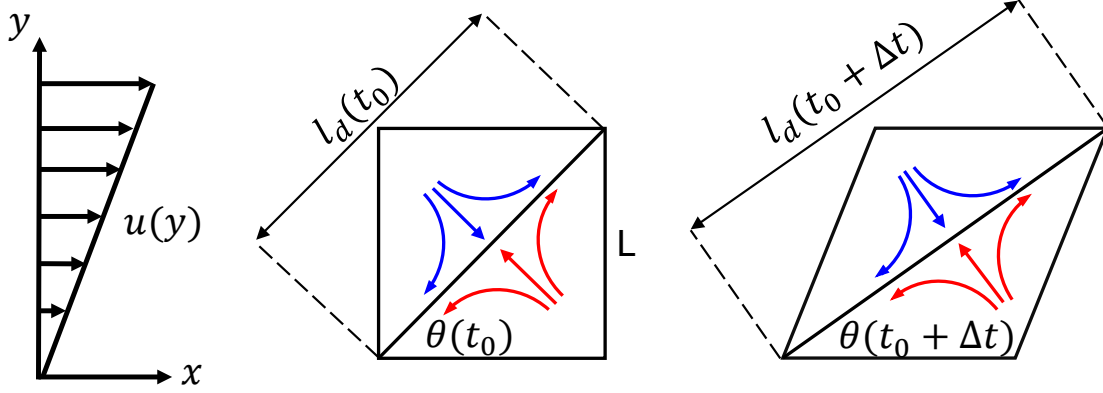


Figure 3.1: Deformation of a square volume under shear strain.

increase as the turbulent length scale or eddy size decreases. This causes velocity gradients to maximize on the Kolmogorov scale, which thus becomes the scale experiencing the strongest influence from velocity gradients. In keeping with this physical reality, the work of this dissertation aims to create a flamelet model embedded in a three-dimensional, rotational strain field approximating Kolmogorov-scale mechanical influences.

For flames which are mixing-controlled, we hypothesize that the fastest heat release rate, that is, the leading-order addition of heat to the flow from chemical reactions, will occur on the scales of fastest mixing; i.e., the Kolmogorov scale having maximal velocity gradients. Thus, the present flamelet model is a Kolmogorov scale model. Final molecular mixing and chemical reactions occur on a scale even smaller than the Kolmogorov scale where the diffusion layer is held in capture by a Kolmogorov eddy. The diffusion layer and reaction zone are then subject to far-field shear and normal strain rates imposed by the small scales. Diffusion flame time scales, Damköhler numbers, and ignition/extinction behavior are controlled by Kolmogorov velocity gradients through residence time. Due to the inherent three-dimensional nature of turbulent flows, we argue that the magnitudes of all velocity gradients must impact the fluid-chemistry interaction on the smallest scales; not only the compressive strain rate. In their 1992 paper, Nomura and Elghobashi state “The strain rate and vorticity fields dominate the behavior of the scalar field and thus the reactive interface” furthermore, “...the magnitude of vorticity affects that of the scalar gradient through strain rate amplification by vortex

stretching” [115]. Two-dimensional planar and axisymmetric configurations without vorticity included in the momentum equations cannot explicitly capture these effects.

When velocity gradients are viewed from the principal axes, one strain rate will be tensile ($\alpha > 0$), one will be compressive ($\gamma < 0$), and the third may be either tensile ($\beta > 0$), compressive ($\beta < 0$), or zero ($\beta = 0$) with $\alpha > \beta > \gamma$, while all axes rotate according to the vorticity magnitude. The statistical alignment and magnitudes of these strain rates relative to one another are important to turbulent combustion modeling because fluid-chemistry modification by vortex stretching significantly influences flamelet extinction limits and heat release rates [94–98]. Direct numerical simulations of constant density (non-reacting) homogeneous, isotropic turbulence and homogeneous, shear turbulence, indicate that the vorticity vector most often aligns with the axis of intermediate strain and is perpendicular to the axes of major tensile and major compressive strain [115, 119, 120]. Furthermore, Ashurst [119] and Nomura and Elghobashi [115] report that at 75% of the sample points, the intermediate strain rate is tensile and the major tensile strain rate is nearly as high in magnitude as the major compressive strain rate. Kerr [120] also reports a likelihood that the intermediate strain component is tensile and that this likelihood increases in regions with high dissipation. Thus, stretched vortex sheets or layers ($\alpha > \beta > 0 > \gamma$), rather than stretched vortex tubes ($\alpha > 0 > \beta > \gamma$), are found to be the primary dissipative structures. Sources agree that the compressive strain rate has the highest magnitude with the major tensile strain rate being a close second, and that the intermediate strain rate, be it tensile or compressive, is much lower in magnitude, with a common proportionality given by Eq. 3.1 [115, 119, 120].

$$|\alpha| : |\beta| : |\gamma| \propto 3 : 1 : 4 \tag{3.1}$$

Lastly, Ashurst [119] and Nomura and Elghobashi [115] found that scalar gradients are aligned with the major compressive axis supporting Kerr’s finding that the dot product between vorticity and the scalar gradients tends toward zero. More recently, Hamlington

et al. [121] and Fiscaletti et al. [122] reproduced the preferred alignment of small-scale vorticity with the small-scale intermediate tensile strain rate in non-reacting turbulence. Fiscaletti et al. also confirmed an additional alignment between the small-scale vorticity and the large-scale tensile strain rate originally observed by Hamlington et al. [121].

The alignment characteristics change somewhat when a reacting turbulent flow of variable density is considered. Exothermic energy release causes strong density variation throughout the flow, thus the sum of the principal strain rates is non-zero. Nomura and Elghobashi [116] performed DNS on a non-premixed reacting flow with initially homogeneous isotropic turbulence, later developing inhomogeneity due to dilatation. They found that at early times when scalar gradients are high, the major tensile strain rate α tends to have the highest magnitude while the intermediate strain rate is almost always positive ($\beta > 0$), making stretched vortex layers the most likely geometric configuration. The third strain rate γ retains its negative probability, but is shifted closer to zero and, in extreme cases of expansion, may become positive. For the flamelet concept to exist, γ must be negative, otherwise the counterflow is destroyed, preventing fuel and the oxidizer from combining. At later times, after considerable mixing and reaction, the flow more closely resembles that of the constant density incompressible cases discussed previously. In the reactive, variable density case, Nomura and Elghobashi [116] found that vorticity is more likely to align with the most extensional strain axis α in regions with the greatest extent of chemical reaction (where the mixture fraction is near stoichiometric) and is more likely to align with β in unmixed and unreacted regions of the flow and in regions with high enstrophy. In general, the vorticity intensity is reduced relative to the non-reacting case and tube-like structures are less likely to occur [116]. Later, Boratav et al. [117, 118] performed DNS for non-premixed non-buoyant and buoyant turbulent flames and in both cases found considerable alignment of the vorticity vector with the α -strain rate. For the non-buoyant case, vorticity alignment with the α -strain rate was preferred and in the buoyant case, vorticity was nearly as likely to align with the α -strain rate as with the β -strain rate.

In a counterflow configuration, the diffusion plane is normal to the principal compressive axis and scalar gradients are aligned with the principal compressive axis [115–119]. Betchov [123] showed that a tensile intermediate principal strain rate is most critical for the generation of vorticity and cascade of energy to smaller scales and that the normal compressive strain rate is of the same order of magnitude as vorticity across all length scales. This equivalency serves as the basis for choosing vorticity values on the same order of magnitude as the asymptotic compressive strain rate, S^* , for computations later in this manuscript.

These various DNS results indicate two major points with regard to non-premixed flamelet models: 1) the flamelet geometry and flowfield is not axisymmetric, and 2) the magnitude of vorticity likely impacts the fluid-chemistry interaction through density variation. As flamelet models prior to Sirignano [94], [95] and Hellwig et al. [97] [98] did not address these two points, the present authors developed a new flamelet model which has four mechanical inputs, three strain rates S_1^* , S_2^* , S^* , and vorticity ω^* . The major compressive strain rate $-S^*$ is negative and its magnitude, S^* , is used to non-dimensionalize the transverse strain rates and vorticity as shown in Eq. 3.2. In non-dimensional form, $\omega \approx O(1)$ according to DNS findings and theoretical analysis, while the transverse strain rates S_1 and S_2 may approximately vary through the proportionality shown in Eq. 3.1 [123–125]; however, further analysis of DNS non-premixed turbulent flames is necessary to fine-tune these values. Note, flamelet models which do not include vorticity and three-dimensional strain rate variation have implicitly set 2D-planar ($S_1 = \text{const}$, $S_2 = 0$) or axisymmetric ($S_1 = 0.5$, $S_2 = 0.5$) velocity gradients with $\omega = 0$.

$$S_1 = \frac{S_1^*}{S^*} \quad S_2 = \frac{S_2^*}{S^*} \quad \omega = \frac{\omega^*}{S^*} \quad (3.2)$$

3.2 Theoretical Development

Based on the statistical and geometric findings of Betchov[123], Ashurst [119], Nomura and Elghobashi [115, 116], and Boratav and Elghobashi [117, 118], Sirignano [94, 95] developed the Rotation Flamelet Model (RFM) using a transformation to a non-Newtonian reference frame rotating with the vorticity vector. The counterflow configuration is subject to three independent principal strain rates in the three non-Newtonian coordinate directions with a rotational effect included where the vorticity vector is aligned with the S_2 principal strain rate direction. The scalar gradients are aligned with the compressive strain rate. The transformation and 3D geometry are shown in Fig. 3.2-3.3 along with the orientation of mechanical constraints and scalar gradients.

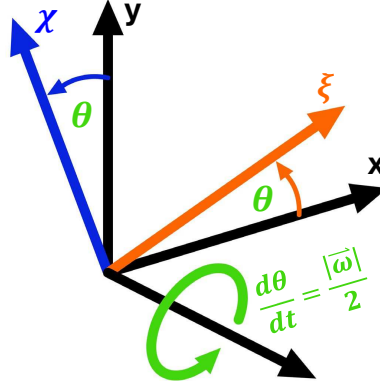
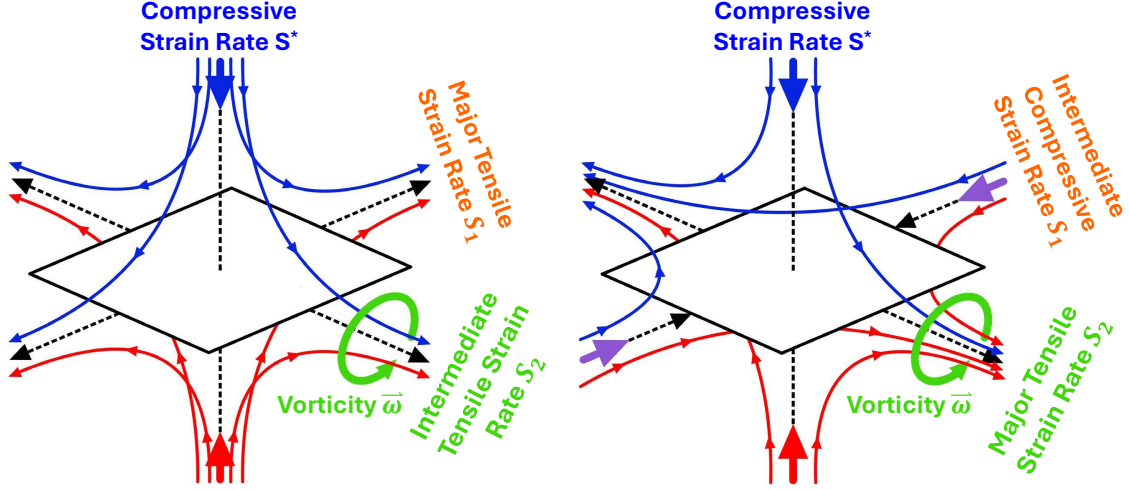


Figure 3.2: Transformation from the Newtonian (black) to the non-Newtonian reference frame and alignment of strain rates and vorticity. $x \rightarrow \xi$ and $y \rightarrow \chi$; i.e., the $\xi - \chi$ plane rotates about z at $d\theta/dt = \omega/2$.

Using Fickian diffusion and one-step propane/oxygen kinetics, Sirignano [94] showed that the 3D governing equations could be mathematically reduced to functions of only the axial coordinate through a similarity solution. The centrifugal effect due to vorticity decreases mass flux through the counterflow which increases the residence time, thereby allowing diffusion flames that would otherwise extinguish at a given strain rate to survive until a higher strain rate is applied. The reduction in mass flux also decreases the burning rate. A common residence time (between premixed and non-premixed flames) was used in constructing the



(a) Stretched vortex layer counterflow in the non-Newtonian reference frame. $S_1 > 0$, $S_2 > 0$. (b) Stretched vortex tube counterflow in the non-Newtonian reference frame. $S_1 < 0$, $S_2 > 0$.

Figure 3.3: Orientation of RFM in the stretched vortex layer and tube configurations. The reader should interpret the figures as snapshots in time as the counterflow structure rotates about the z (ω and S_2) axis as time progresses. Non-premixed oxidizer side (blue); non-premixed fuel side (red).

Damköhler number which reflects the Kolmogorov time scale. This time scale is the natural time scale for non-premixed flames but not for premixed flames. Separated premixed flames, i.e., those with large standoff distance, are found to exist at much higher Damköhler numbers (lower strain rates) than diffusion flames and partially-premixed flames, owing to the relatively constant laminar flame speed with strain rate. This means the inflow velocity must be low for a premixed flame to propagate away from the stagnation point diffusion layer. Therefore, it is expected that in a highly strained turbulent flow, separated premixed flames are unlikely to appear, and the premixed flames that do occur will likely be merged with the diffusion layer, resulting in partially-premixed flames. Although the DNS results show a likelihood of the intermediate principal strain rate being tensile, this is not always the case. Therefore, Sirignano extended the RFM to include inward swirling geometry [95] and stretched tubular vortex structures [96]. Sirignano also introduced unsteady effects [64]. These earlier studies with the RFM employed a Fickian diffusion formulation and used unity Lewis numbers and one-step kinetics. For all cases, the effect of vorticity is to decrease the extinction Damköhler number.

3.3 Multi-step Chemical Kinetics and Detailed Transport

Sirignano’s initial demonstrations of the RFM used Fickian diffusion with unity Lewis numbers and a one-step kinetics model, originally developed for premixed propane-oxygen combustion [126]. As a primary benefit of flamelet modeling is the inclusion of detailed chemistry, a natural improvement was the inclusion of arbitrarily complex chemical kinetic mechanisms. For an accurate description of these multi-component mixtures, the transport formulation was also upgraded from a Fickian diffusion formulation to a multi-component form with variable thermo-physical properties.

3.3.1 Governing Equations

The governing equations for unsteady 3D flow, shown below, retain the non-Newtonian reference frame used by Sirignano; the vorticity vector aligns with the z -axis while the ξ and χ axes (which respectively, are the x and y axes in Fig. 3.2) rotate about z at a constant angular speed, $d\theta/dt = \omega/2$ where ω is the Kolmogorov vorticity. Again, note that the following text uses ξ as the non-Newtonian x coordinate and χ as the non-Newtonian y coordinate; i.e., χ is not scalar dissipation rate in this section. Inflows to the counterflow enter along the χ axis. Velocity components and spatial variables in this rotating frame are $u_i = u_\xi, u_\chi, w$ and $x_i = \xi, \chi, z$ respectively. The centrifugal acceleration is $a_i = \langle \xi\omega^2/4, \chi\omega^2/4, 0 \rangle$. See Sirignano [94] for the coordinate transformation relations.

$$P = \rho R_{sp} T \tag{3.3}$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0 \tag{3.4}$$

$$\rho \frac{\partial u_i}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho a_i \quad ; \quad \tau_{ij} = -\frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (3.5)$$

$$\begin{aligned} \frac{\partial(\rho h)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j h) + \frac{\partial}{\partial x_j} \sum_{m=1}^{n_{sp}} \rho v_{m,j} Y_m h_m - \frac{\partial p}{\partial t} - u_j \frac{\partial p}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) \\ - \rho \sum_{m=1}^{n_{sp}} h_{f,m} \dot{\omega}_m + \tau_{ij} \frac{\partial u_i}{\partial x_j} \end{aligned} \quad (3.6)$$

$$\frac{\partial(\rho Y_m)}{\partial t} + \frac{\partial}{\partial x_j} (\rho Y_m u_j) + \frac{\partial}{\partial x_j} (\rho Y_m v_{m,j}) = \rho \dot{\omega}_m \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.7)$$

The quantities ρ , p , T , h , h_m , v_m , Y_m , λ , c_p , c_{p_m} , $h_{f,m}$, and $\dot{\omega}_m$ are density, pressure, temperature, mixture specific enthalpy, specific enthalpy of species m , diffusion velocity of species m , mass fraction of species m , mixture thermal conductivity, mixture specific heat, specific heat of species m , heat of formation of species m , and reaction rate of species m , respectively. The analysis will use the low-Mach number approximation; i.e., terms on the order of kinetic energy per unit mass are small compared to thermal energy and therefore are negligible. This applies to the last terms on the left and right hand sides of Eq. 3.6. Additionally, viscous dissipation terms are assumed to be negligible except for cases with extremely large strain rates which are not the subject of this work and will not be analyzed here, though, they should be addressed in the future.

Table 3.1: Normalizations for dependent variables

Variable(s)	u_j, v_m	t	x_i	ρ	$h, h_m, h_{f,m}$	p
Normalization	$\sqrt{\frac{S^* \mu_\infty}{\rho_\infty}}$	S^{*-1}	$\sqrt{\frac{\mu_\infty}{\rho_\infty S^*}}$	ρ_∞	$c_{p_\infty} T_{\text{ref}}$	$S^* \mu_\infty$
Variable(s)	$\dot{\omega}_m$	μ	λ	c_p, c_{p_m}	ω	T
Normalization	S^*	μ_∞	$\mu_\infty c_{p_\infty}$	c_{p_∞}	S^*	T_∞

While the boundary conditions are presented for the similar form in the following paragraphs,

we will briefly discuss what they would be for Eqs. 3.3-3.7. The energy and species conservation equations use Dirichlet boundary conditions for temperature and mass fractions and are the same in both the Newtonian and non-Newtonian reference frames. The velocities use Neumann boundary conditions to specify imposed strain rates in the three coordinate directions. In this rotating frame, the effect of the vorticity in the original reference frame now appears through a centrifugal acceleration.

The non-dimensional forms of the governing equations remain identical to Eqs. 3.3-3.7 when specific normalization factors are chosen. See Table 3.1 for details. Note, dimensional normal strain rates imposed on the ξ and z axes are respectively S_1^* and S_2^* and are each normalized by the principal strain rate at $\chi = \infty$, $S^* \equiv S_1^* + S_2^*$, forming non-dimensional strain rates S_1 and S_2 . This relation requires $S_1 + S_2 = 1$ so that the velocity field is divergence-free in the far-field. Total specific enthalpy is defined as $h_m^0 \equiv h_m + h_{f,m}$ and is normalized according to Table 3.1. The similarity solution derived by Sirignano is used to reduce the 3D governing equations to a set of ODEs employing the density-weighted Illingworth transformation $\eta \equiv \int_0^\chi \rho(\chi') d\chi'$. In the similar form, $u_\xi = S_1 \xi(df_1/d\eta)$, $w = S_2 z(df_2/d\eta)$, and $u_\chi = -f/\rho$ with $f \equiv S_1 f_1 + S_2 f_2$. The several mixed second derivatives of pressure are zero, thereby allowing the simplification of the momentum equations for the ξ and z directions and the formation of the similar form of those equations. The final forms of the governing equations with boundary conditions are presented below. Note, the centrifugal effect is incorporated in the last term of Eq. 3.8 and in the corresponding boundary condition at $\eta = -\infty$ in Eq. 3.15. The physical problem remains three-dimensional in space. The diffusion formulation can be either the multicomponent form, shown in Eqs. 3.12-3.13, or a mixture-averaged form not shown. The full multicomponent form ensures mass conservation while the mixture-averaged form does not; however, the later can be solved for $n_{sp} - 1$ species where the final species is $Y_{n_{sp}} = 1 - \sum_{m=1}^{n_{sp}-1} Y_m$ which is asymptotically correct when species n_{sp} is a trace compound. Soret effects can be included in either form and can be important when large temperature gradients exist for a flow with a large variation in species molecular weights.

$$\rho\mu f_1''' + f_1''(\rho\mu)' + f f_1'' + S_1 \left(\frac{1}{\rho} - (f_1')^2 \right) + \frac{\omega^2}{4S_1} \left(1 - \frac{1}{\rho} \right) = 0 \quad (3.8)$$

$$\rho\mu f_2''' + f_2''(\rho\mu)' + f f_2'' + S_2 \left(\frac{1}{\rho} - (f_2')^2 \right) = 0 \quad (3.9)$$

$$fT' + \frac{1}{c_p}(\rho\lambda T')' - \frac{1}{c_p}T' \sum_{m=1}^{n_{sp}} J_m c_{p_m} - \frac{1}{c_p} \sum_{m=1}^{n_{sp}} h_m^0 \dot{\omega}_m = 0 \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.10)$$

$$fY'_m - J'_m + \dot{\omega}_m = 0 \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.11)$$

The multicomponent species diffusion flux and diffusion velocity are shown by Eqs. 3.12-3.13, respectively. Useful conversions are given in Eq. 3.14. Note that the Soret effect can be included as shown in Eqs. 3.12-3.13; however, it is omitted here as it is a secondary effect that mainly impacts light species, such as H radicals, which are not the subject of this work. Boundary conditions are shown by Eqs. 3.15-3.17.

$$J_m \equiv \rho Y_m v_{m,\eta} = \frac{\rho^2 W_m}{\bar{W}_{mix}^2} \sum_{n=1}^{n_{sp}} W_n D_{mn} X'_n - \frac{\rho D_m^T}{T} T' \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.12)$$

$$v_{m,\eta} = \frac{\rho W_m}{\bar{W}_{mix} Y_m} \sum_{n=1}^{n_{sp}} W_n D_{mn} X'_n - \frac{D_m^T}{Y_m T} T' \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.13)$$

$$X_m = \frac{\bar{W}_{mix}}{W_m} Y_m \quad ; \quad \bar{W}_{mix} \equiv \sum_{n=1}^{n_{sp}} X_n W_n \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.14)$$

$$f'_1(\infty) = 1 \quad ; \quad f'_1(-\infty) = \sqrt{\frac{1}{\rho_{-\infty}} + \left(\frac{\omega}{2S_1} \right)^2 \left(1 - \frac{1}{\rho_{-\infty}} \right)} \quad ; \quad f_1(0) = 0 \quad (3.15)$$

$$f'_2(\infty) = 1 \quad ; \quad f'_2(-\infty) = \frac{1}{\sqrt{\rho_{-\infty}}} \quad ; \quad f_2(0) = 0 \quad (3.16)$$

$$T(\infty) = 1 \quad ; \quad T(-\infty) = T_{-\infty} \quad ; \quad Y_m(\infty) = Y_{m,\infty} \quad ; \quad Y_m(-\infty) = Y_{m,-\infty} \quad (3.17)$$

3.3.2 Chemical Kinetics

Sections 3.3.3-3.3.6 cover $\text{H}_2\text{-O}_2$ flamelets diluted with N_2 and will use the $\text{H}_2\text{-O}_2$ subset of the Foundational Fuel Chemistry Model 1.0 (FFCM-1) [127]. This reduced model considers 25 reactions among nine species. Hydrocarbons, namely CH_4 and JP-5 are also explored in Sec. 3.3.7-3.3.8. JP-5 flamelets combusting with air will use a skeletal version of the HyChem chemical kinetics model including 41 species among 202 reactions [128, 129] while $\text{CH}_4\text{-O}_2$ combustion will use a reduced version of FFCM-1 [127], tailored to methane-oxygen combustion in liquid rocket engines. This version of FFCM-1 has 39 reactions among 12 species. NO_x formation is not considered in any of the chemical kinetics mechanisms.

3.3.3 Comparison with Cantera

Computations from the RFM were compared with axisymmetric counterflow non-premixed flames from Cantera to validate proper qualitative flame zone behavior. Here, the case of a nitrogen-diluted hydrogen-oxygen counterflow non-premixed flame is presented. The oxidizer stream is pure O_2 at 300 K, while the fuel stream is an equimolar mixture of H_2 and N_2 at 300 K. Nitrogen was added to the fuel to shift the location of minimum density into the flame zone. During development, it was noted that the centrifugal effect is most prominent when the location of minimum density coincides with the location of maximum (or near-maximum) temperature. Because the centrifugal effect is the core aspect this study seeks to demonstrate, the minimum-density/maximum-temperature coincidence was imposed to make the centrifugal effect more prominent. Additionally, most fuel-oxidizer combinations in use today have this coincidence; so, it is believed that this arrangement also helps demonstrate the ubiquity of the centrifugal effect. It was found that approximately 50% N_2 by mole fraction in the fuel stream was sufficient to coincidentally locate minimum density and maximum temperature; so, an equimolar $\text{H}_2\text{-N}_2$ fuel was chosen for the ease

of round numbers. The pressure is set at 10 atmospheres (atm) to achieve a compromise between actual engineering applications which often operate above 10 atm and validation data, both for the chemical kinetics model and laboratory flames, which are predominantly at 1 atm. Soret effects were negligible for the $\text{H}_2\text{-N}_2\text{-O}_2$ flames and thus were not included.

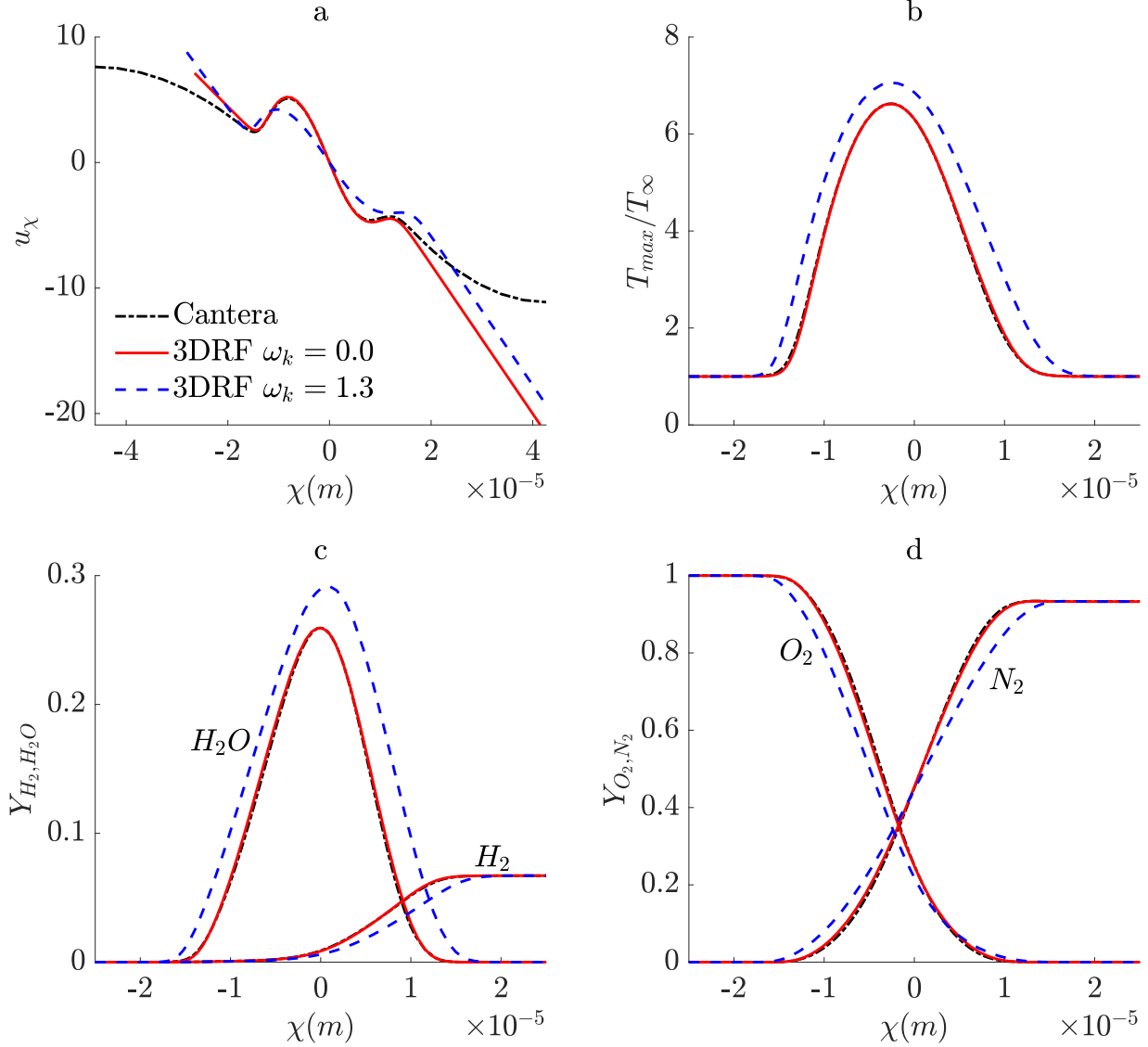


Figure 3.4: Comparison between the RFM and Cantera's counterflow diffusion flame. (a) Axial velocity; (b) Temperature; (c) H_2O and H_2 mass fractions; (d) O_2 and N_2 mass fractions. The maximum strain rate for matched curves is $S_{max}^* = 1,654,000$ 1/s and the transverse strain rates in the RFM are equal, i.e., $S_1 = S_2 = 0.5$ or $S_1^* = S_2^* = 500,000$ (1/s), to achieve axisymmetry.

A maximum local strain rate $S_{max}^* = 1,654,000$ (1/s) is maintained in the flame zone corresponding to $S^* = 1,000,000$ (1/s). Equal strain rates along the ξ and z directions, i.e.,

$S_1 = S_2 = 0.5$ or $S_1^* = S_2^* = 500,000$ (1/s), were considered in the RFM to match the axisymmetry of Cantera. Axial velocity, temperature, and mass fraction profiles are compared and shown in Fig. 3.4. There is excellent agreement in the various profiles within the diffusion layer. This is expected because the local maximum strain rates are the same by design (less than 0.16% error). Equivalency of the local strain rate, combined with the central stagnation point in the flame zone requires axial velocity profiles to closely match. Since the diffusion formulation is identical, as is the transport model, it follows that the advective-diffusive-chemical balance is the same, resulting in excellent agreement of scalar curves. Outside the diffusion layer, there are notable differences in velocity resulting from the mathematical framework the two codes are based on.

Cantera is based on a nozzle counterflow where the fuel and oxidizer streams issue from nozzles at a fixed and finite separation distance. This forces the axial velocity gradient to zero at the boundaries as is seen in Fig. 3.4a. The incoming streams for the RFM are instead based on a far-field potential counterflow in which the axial strain rate is non-zero at the computational boundary. In these regions outside the flame zone, the RFM should not be compared with a nozzle-based counterflow flame. The axial strain rate is constant in the far-field, thereby better describing sub-grid turbulent-flow conditions. A viscous layer exists in the interfacial region of the flamelet. The excellent agreement in the flame zones between the RFM and Cantera demonstrates the thermo-physical computational validity of the RFM. Also shown in Fig. 3.4 are profiles for $\omega = 1.3$ to demonstrate the vorticity effect plotted in physical space. A full discussion of vorticity effects is given in Sec. 3.3.4.

In the example shown in Fig. 3.4, the ambient strain rate is $S^* = 1,000,000$ (1/s), the flame thickness dimension (region of elevated temperature) is approximately $30 \mu m$, the reaction zone is approximately $15 \mu m$, and the viscous layer thickness is $\delta = (\nu/S^*)^{1/2} \approx 3 \mu m$ with kinematic viscosity $\nu = O(\times 10^{-5} m^2/s)$. The viscous layer thickness is based on the local $Re = O(1)$ which makes it the same order as the Kolmogorov scale if the flamelet were

embedded in a turbulent field. A situation with these conditions would occur on the smallest scale of the turbulent flow if the integral scale had a shear flow with a velocity variation of $O(100 \text{ m/s})$ across a shear layer with transverse dimension $O(10 \text{ cm})$, which produces $Re = 10^6$ and a strain rate of $O(1000 \text{ 1/s})$ on the integral scale. The strain rate, velocity, and length sizes would scale as $Re^{1/2}$, $Re^{-1/4}$, and $Re^{-3/4}$, respectively [2, 125, 130, 131], as we move from the integral scale to the Kolmogorov scale. Eddies that are an order of magnitude larger than the Kolmogorov scale are unlikely to distort or affect the flamelet with unsteady behavior because these larger eddies would have longer time scales; however, this is a proper issue for future study. In the following section on non-premixed flames, note that the flame thickness is several times, up to one order of magnitude, larger than the viscous Kolmogorov scale, even near the extinction strain rate. Thus, the flame thickness tends to exceed the Kolmogorov scale with our detailed transport treatment, while the reaction zone is on the order of the Kolmogorov scale. Comparison of Fig. 3.4a with Fig. 3.4b, 3.4c, and 3.4d indicates that the layer for viscous stress has a thickness comparable with the layer thickness for the scalar variables. Thus, it is suggested that our scaling estimate, which does not neglect the temperature effect on kinematic viscosity, actually underestimates the Kolmogorov scale for reacting flows.

3.3.4 Non-premixed Flames

The non-premixed flame case discussed in the prior section is further examined here for impacts of vorticity and transverse strain rates. The axial strain rate is gradually increased to obtain extinction curves. In addition, three combinations of non-dimensional far-field ξ and z strain rates are used, $(S_1 = 0.75, S_2 = 0.25)$, $(S_1 = 0.50, S_2 = 0.50)$, and $(S_1 = 0.33, S_2 = 0.67)$, and three values of non-dimensional vorticity are applied ($\omega = 0.0, 1.0, 1.3$).

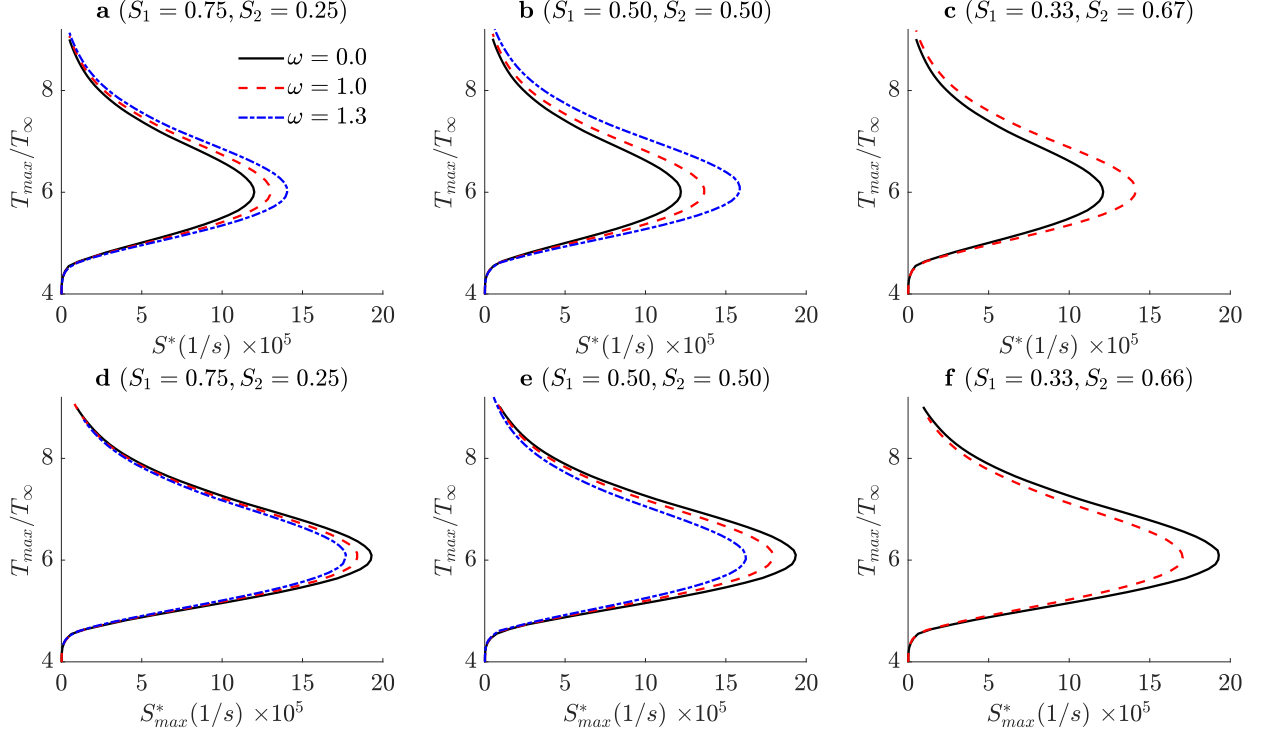


Figure 3.5: Extinction curves (S-curves) of counterflow non-premixed flames with varying strain rate and vorticity magnitudes. Sub-figures (a), (b), and (c) are plotted against ambient strain rate (S^*) while sub-figures (d), (e), and (f) are plotted against the local maximum strain rate at the stagnation point (S_{max}^*).

Figure 3.5 shows the extinction curves or S-curves of the N_2 -diluted H_2 - O_2 non-premixed flamelet for various combinations of S_1 , S_2 , and ω . Figure 3.5a, 3.5b, and 3.5c clearly demonstrate that imposing vorticity on the counterflow domain extends the flammability limit in terms of S^* . When $S_1 = 0.75$, $S_2 = 0.25$, there is a 17.0% increase in the ambient extinction strain rate S_q^* between vorticity values of $\omega = 0.0$ and $\omega = 1.3$. When $S_1 = S_2 = 0.5$, there is a 30.0% increase in S_q^* for the same vorticity range. When $S_1 = 0.33$, $S_2 = 0.67$, there is a 16.8% increase in S_q^* between $\omega = 0.0$ and $\omega = 1.0$. Note that ω^* changes with S^* due to normalization. Thus, the extinction points for $\omega = 1.0$ and $\omega = 1.3$ have different dimensional values of vorticity applied. Differences in S-curve behavior based on magnitudes of S_1 and S_2 are a result of flame stability dependence on mass efflux rates in the ξ and z directions. S_1 and S_2 are indicative of the percentages of outflow leaving the domain along the ξ and z axes, respectively. However, they only give exactly the outflow percentage if $\omega = 0.0$. Note that ξ lies in the plane in which centrifugal force acts on the

flow while z is normal to this plane and does not align with a centrifugal force. Thus, when $S_1 > S_2$, a higher percentage of flow exits along the ξ -axis and is accelerated by the centrifugal force, reducing residence time and leading to earlier extinction as compared to $S_1 = S_2 = 0.5$. Conversely, when $S_1 < S_2$, a higher percentage of flow exits along the z -axis and is not accelerated by centrifugal force. In this case, the residence time is not reduced and may increase depending on the relative magnitudes of S_1 and S_2 . Regardless of the S_1 - S_2 combination, a case with non-zero vorticity extinguishes at higher strain rate than the same case without vorticity.

Figure 3.5d, 3.5e, and 3.5f show the same S-curves plotted against the local maximum strain rate at the stagnation point, S_{max}^* . Opposite behavior, with respect to vorticity, is observed here because the primary function of vorticity is to reduce the strain rate in the flame zone. Thus, at the same maximum temperature, a flame with vorticity has a lower S_{max}^* . Figure 3.5a, 3.5b, and 3.5c may be thought of as plots of output (ordinate) versus input (abscissa) while Fig. 3.5d, 3.5e, and 3.5f may be thought of as output versus output. Analysis of local strain rate is further developed in Fig. 3.9c and the accompanying text.

Figure 3.6a-d shows the three velocity components as well as the similarity variable f , indicative of the axial mass flux, for the axisymmetric case $S_1 = S_2 = 0.5$, and $S^* = 1,000,000$ 1/s. However, the flow is only axisymmetric if $\omega = 0$. All plots are non-dimensional unless stated otherwise. Velocity profiles in the ξ and z directions, i.e., u_ξ and w , are divided by their respective spatial variables. Inspection of the slopes of the u_χ velocity profiles (Fig. 3.6a) in the diffusion layer ($-5 \leq \eta \leq 5$) reveals the cause of the increased ambient extinction limits noted in Fig. 3.5. Although the imposed far-field strain rates are the same for all values of vorticity, the strain rate (slope) in the flame zone is reduced as vorticity increases. This essentially allows a flame with vorticity that is highly strained in the far-field to behave like a flame without vorticity that is moderately strained in the far-field. These effects are most prevalent when the location of minimum density coincides with the location of peak

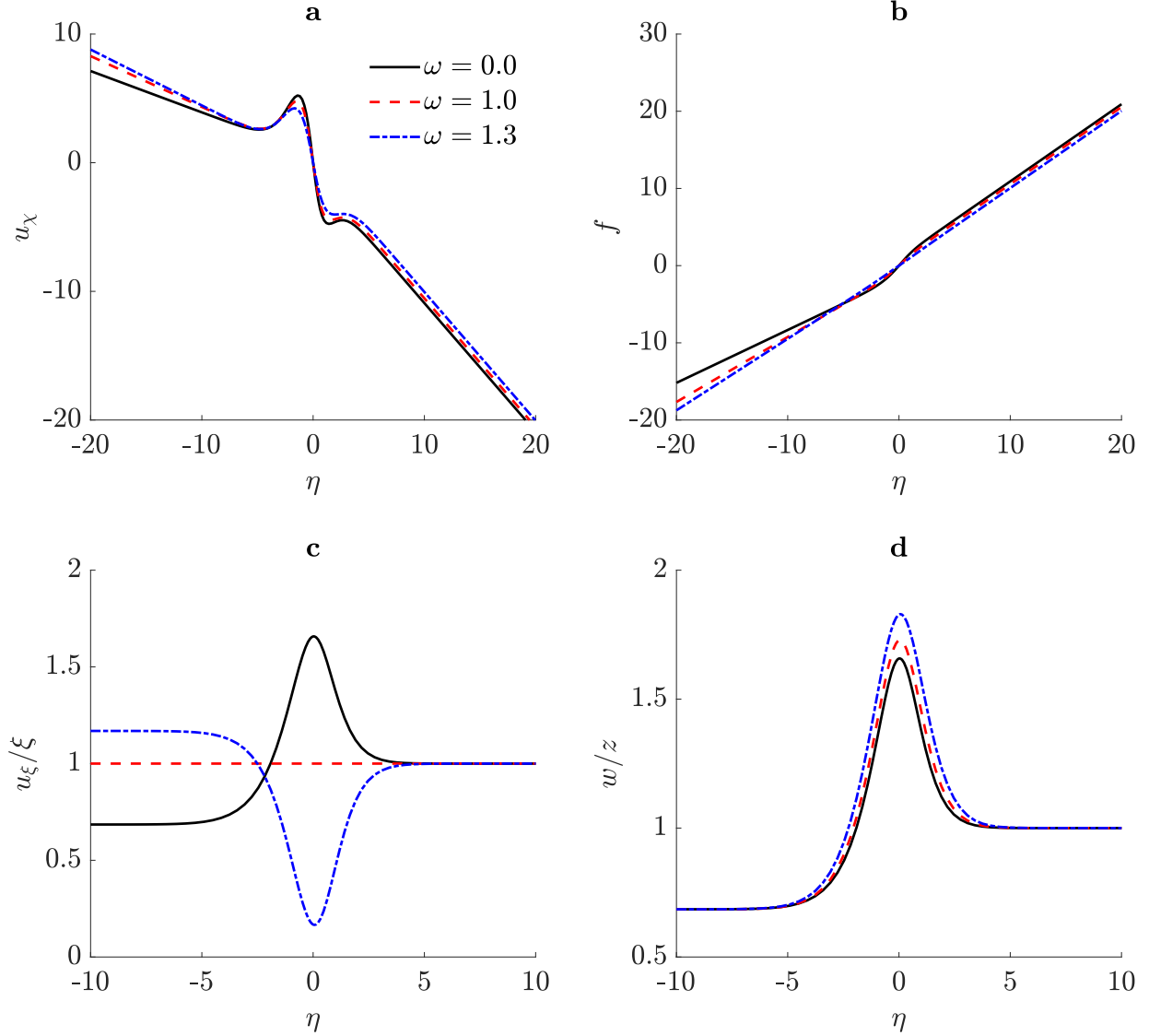


Figure 3.6: Non-premixed flame. (a) Axial (inflow) velocity u_χ ; (b) Similarity variable f ; (c) Transverse outflow velocity normal to vorticity vector divided by length (u_ξ/ξ); (d) Transverse outflow velocity parallel to vorticity vector divided by length (w/z). $S_1 = S_2 = 0.5$, $S^* = 1,000,000$ 1/s.

temperature. Additional cases not shown here were performed with pure H_2 in-flowing from the right instead of the equimolar $\text{H}_2\text{-N}_2$ mixture of the current discussion. In this case, the location of minimum density lies upstream of the stagnation point, toward the fuel inlet boundary, and well outside the flame zone. Under this condition, the outflow is less severely altered by vorticity due to its higher density, and flammability limits are minimally extended. Cases were also tested using water to dilute the hydrogen stream in place of nitrogen. These cases showed no qualitative difference from the nitrogen case.

Examination of the four sub-figures together shows that excess oxygen enters the domain along the η -direction when vorticity is applied. This excess oxygen exits the domain along the ξ -axis as shown by the u_ξ/ξ magnitude between $-20 < \eta < 5$. The introduction of vorticity also causes undulating behavior of the u_ξ and w -velocity components in the flame zone. Without vorticity, u_ξ/ξ and w/z are equal, indicating symmetric outflow in the ξ and z directions. Furthermore, these velocity components are elevated in the flame zone showing the hot (low-density) products of combustion accelerating out of the domain. However, with strong vorticity, the low-density products of combustion are forced toward the stagnation point in the ξ direction under the centrifugal action of vorticity. This leaves only the z -direction as a path for combustion products to escape which is why the peaks of the w/z curves increase with increasing vorticity. These effects are compounded when the flamelet exists in an asymmetric strain field ($S_1 \neq S_2$), which is discussed later on.

We now consider the effects of vorticity and transverse strain rates on temperature, species, and energy profiles for the case shown in Fig. 3.6a-d. Figure 3.7a-d shows temperature, major species, total enthalpy heat release rate (HRR_T), and the integrated H_2 reaction rate profiles for the afore-discussed three cases. Inspection of the temperature profiles shows the direct relationship between peak temperature and vorticity. Next, we examine the species profiles. Unsurprisingly, reactant mass fractions decrease while major product mass fractions increase with vorticity. Essentially, the reduction in strain rate in the flame zone caused by vorticity allows for more complete combustion. Figure 3.7c and 3.7d show the decreased (HRR_T) and burning rate caused by vorticity. This is the result of decreased mass flux as the centrifugal force opposes the inflows as previously noted by Sirignano [94].

Besides vorticity, differing strain rates along ξ and z directions can also alter flamelet behavior. Figure 3.8 shows the axial velocity (u_χ) and similarity variable (f) for varying vorticity and transverse strain rates. Note that for the three cases with $\omega = 0.0$, the curves of both u_χ and f lie within a line thickness of each other and are thus visually indistinguishable; i.e., all

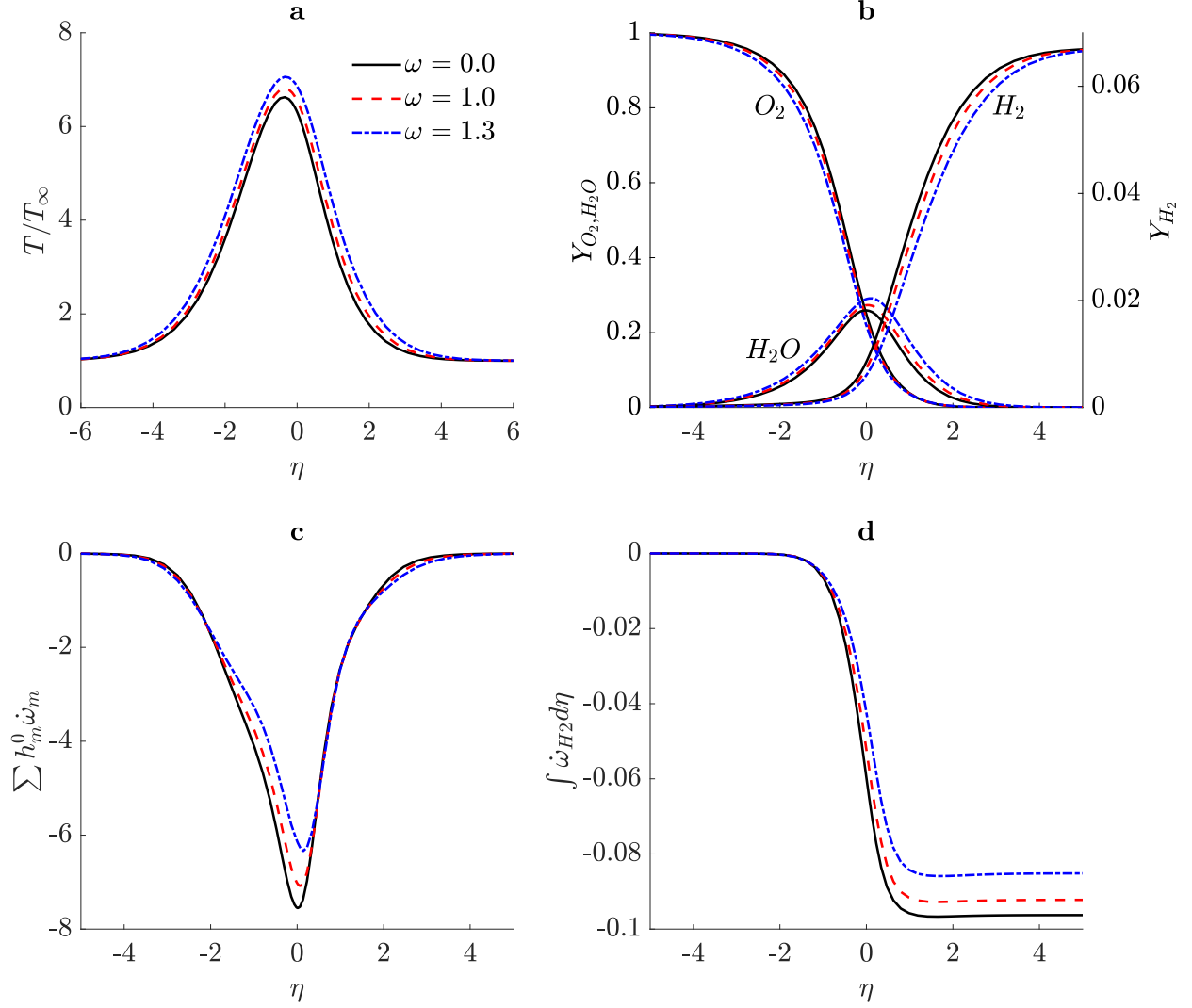


Figure 3.7: Non-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$, $S_2 = 0.5$, $S^* = 1,000,000$ 1/s.

$\omega = 0.0$ curves are coincident with the solid red line. Certain general trends are unchanged for this asymmetric case, namely the decreased strain rate in the flame zone as well as increased oxygen influx, both a result of imposing vorticity. However, the important difference is that when $S_2 > S_1$, more outflow is allowed in the z -direction which is unrestricted by vorticity. This allows more oxygen in to the domain and reduces the maximum strain rate in the flame zone. Conversely, when $S_2 < S_1$, the opposite trend is observed.

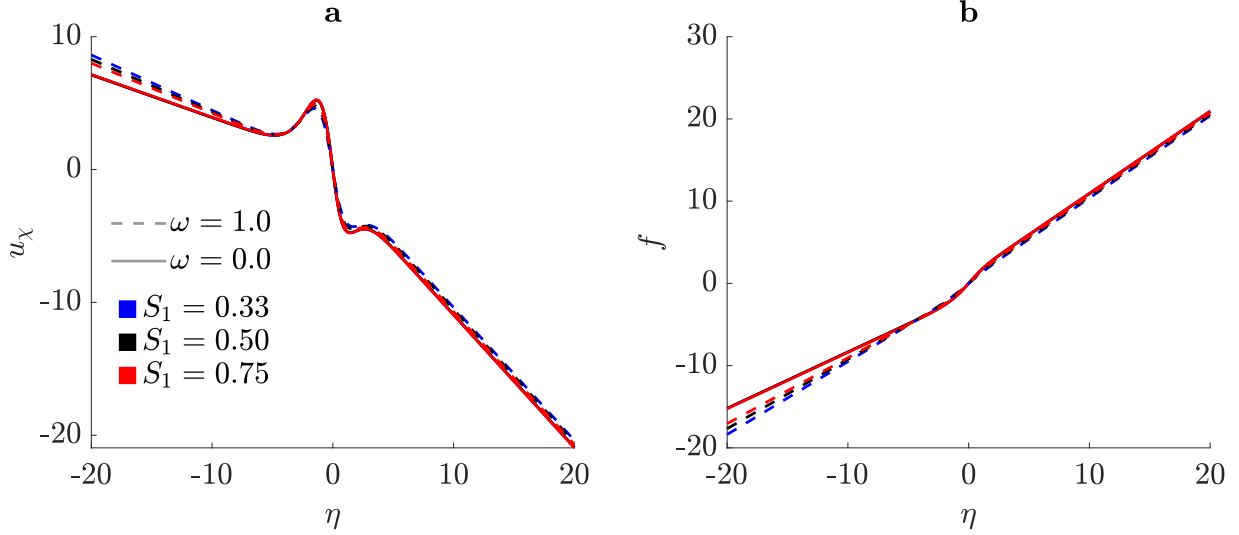


Figure 3.8: Non-premixed flame. (a) Axial (inflow) velocity u_χ ; (b) Similarity variable f . $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$, $\omega = 0.0, 1.0$, $S^* = 1,000,000$ 1/s. The three curves on each sub-figure for $\omega = 0.0$ are coincident with the solid red curve.

As is well known, it is the local strain rate in the flame zone, not a distant ambient strain rate that impacts extinction. Figure 3.9a-d compares various convective and scalar profiles of two flames on the stable branches of Fig. 3.5b having the same maximum temperature to within 0.055%. This comparison is made between the $\omega = 0.0$ and $\omega = 1.3$ curves. One may expect that all profiles between these cases would locally collapse, based on the assumption that equal maximum temperatures imply equal strain rates in the flame zone. This is not the case, although the local profiles are surely similar. The local maximum strain rates, as seen in Fig. 3.9c differ by approximately 86,000 1/s or 8% due to the variance in mass efflux caused by vorticity. It follows from the difference in convective gradients that the scalar gradients differ as well, slight though they may be. Small differences in these profiles may seem superficially unimportant; however, the ability of a flamelet model to predict similar scalar curves from vastly different S^* and ω input parameters is likely consequential when modeling turbulent reacting flows. Existing flamelet models do not represent strain rate and vorticity separately, instead characterizing them together (implicitly) with scalar dissipation rate, while mapping resolved flow quantities to sub-grid inputs.

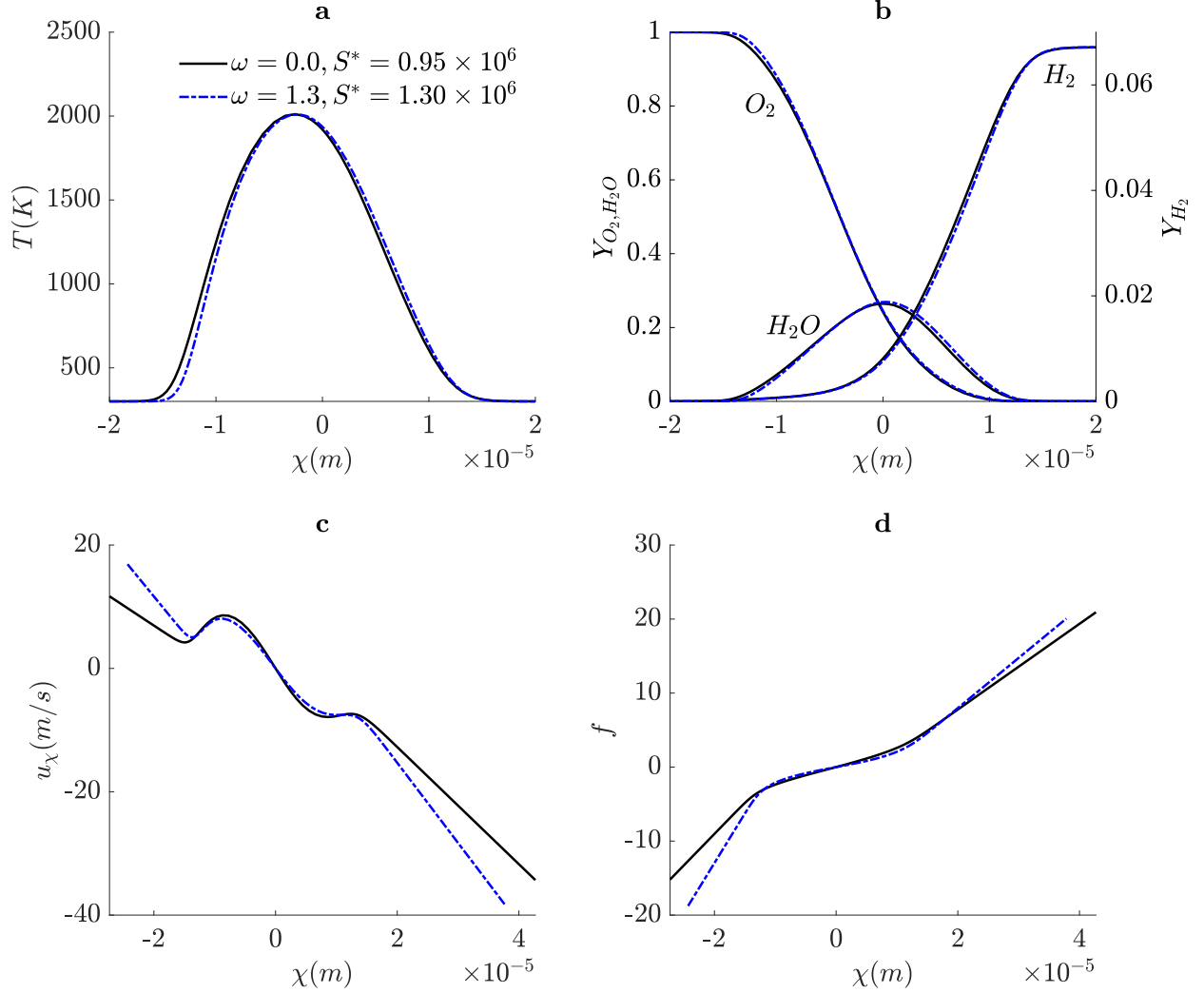


Figure 3.9: Non-premixed flame. (a) Absolute temperature; (b) Major species mass fractions; (c) Dimensional axial velocity (u_χ); Similarity variable f . $S_1 = S_2 = 0.50$, $\omega = 0.0, 1.3$, $T_{max} = 2010K$.

Figure 3.10a-d shows the velocity components in the ξ and z directions for varying vorticity and transverse strain rates. First, compare the u_ξ/ξ profiles between Fig. 3.10a and 3.10b for $S_1 = S_2 = 0.50$. In Fig. 3.10b a vorticity value of $\omega = 1.0$ (solid black) produces a straight line due to the elimination of any density effect in the ξ -momentum equation, Eq. 3.8, and the boundary condition given by Eq. 3.15. However, when $\omega \neq 1.0$ and/or $S_1 \neq 0.5$, the boundary conditions at $-\infty$ and $+\infty$ are not equal and a straight line does not occur. Further comparison of the u_ξ/ξ and w/z profiles in Fig. 3.10a-d for the case where $S_1 = 0.75, S_2 = 0.25$ (dash red) shows a conflict of influence in the flame zone between S_1 ,

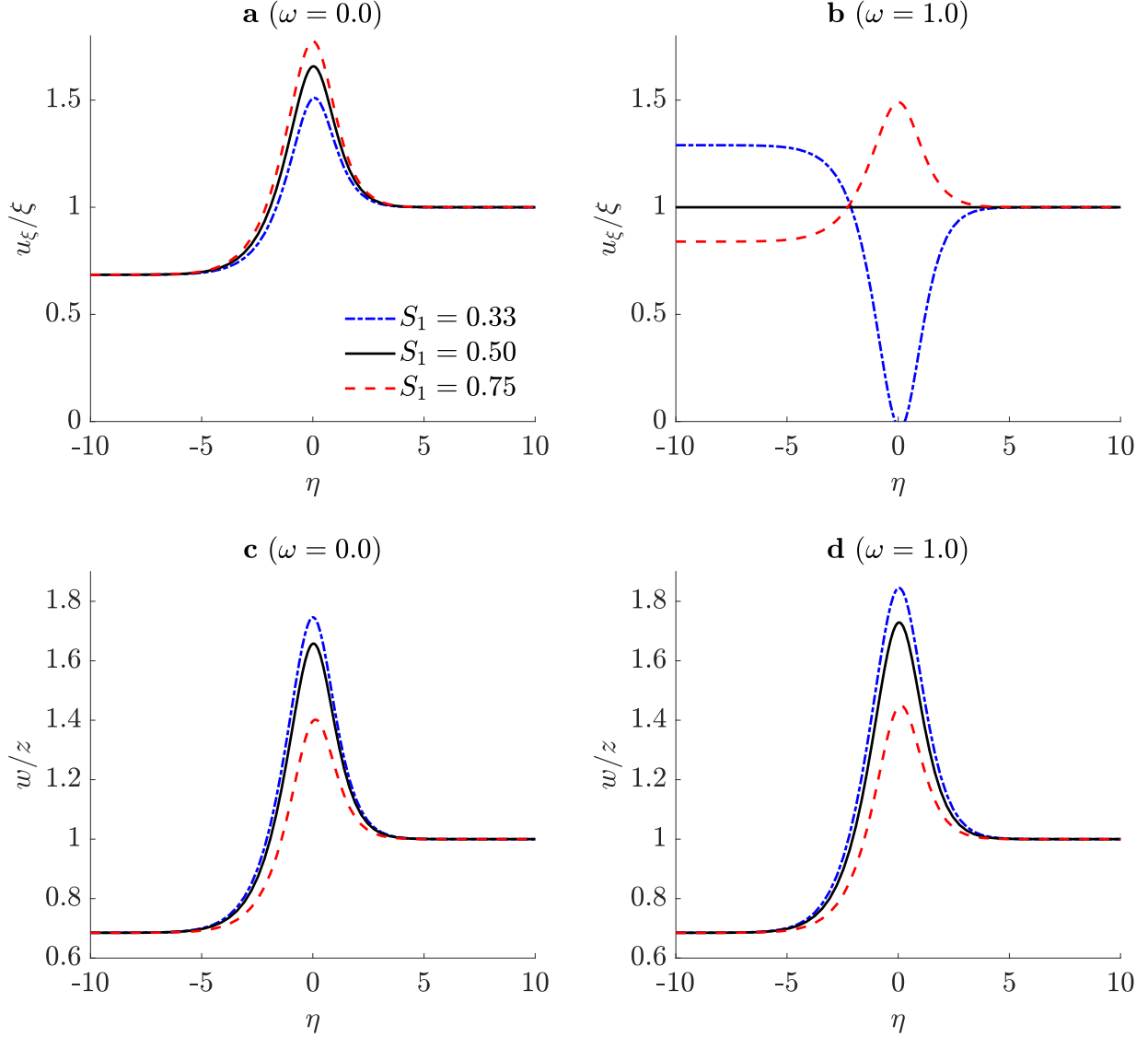


Figure 3.10: Non-premixed flame. (a) u_ξ/ξ , $\omega = 0.0$; (b) (u_ξ/ξ) , $\omega = 1.0$; (c) (w/z) , $\omega = 0.0$; (d) (w/z) , $\omega = 1.0$. $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$. $S^* = 1,000,000$ $1/s$.

S_2 , and ω . When $S_1 > S_2$, mass efflux is decreased (limited) in the z -direction (Fig. 3.10**c-d**) and increased in the ξ -direction (Fig. 3.10**a-b**). Because efflux in the ξ - η plane feels the centrifugal effect of vorticity while efflux in the z -direction does not, the centrifugal effect attempts to expel the expanding low-density products of combustion along the z -direction, but the low value of S_2 does not permit this. Instead, due to the bias toward ξ -efflux from $S_1 > S_2$, u_ξ/ξ is forced to remain positive in the flame zone. Comparing this case ($S_1 > S_2$) to the case where ($S_1 < S_2$) (dash-dot blue), we see an alignment between the preferred

efflux direction and vorticity magnitude. When vorticity is applied, efflux prefers to flow in z , and is restricted in ξ , which is why u_ξ/ξ becomes negative and the maximum of w/z is much higher for $S_1 < S_2$ than for $S_1 > S_2$. Overall, this results in a lower strain rate in the flame zone and increased residence time which explains why extinction points in Fig. 3.5c occur at a higher strain rate than the corresponding points in Fig. 3.5a and 3.5b.

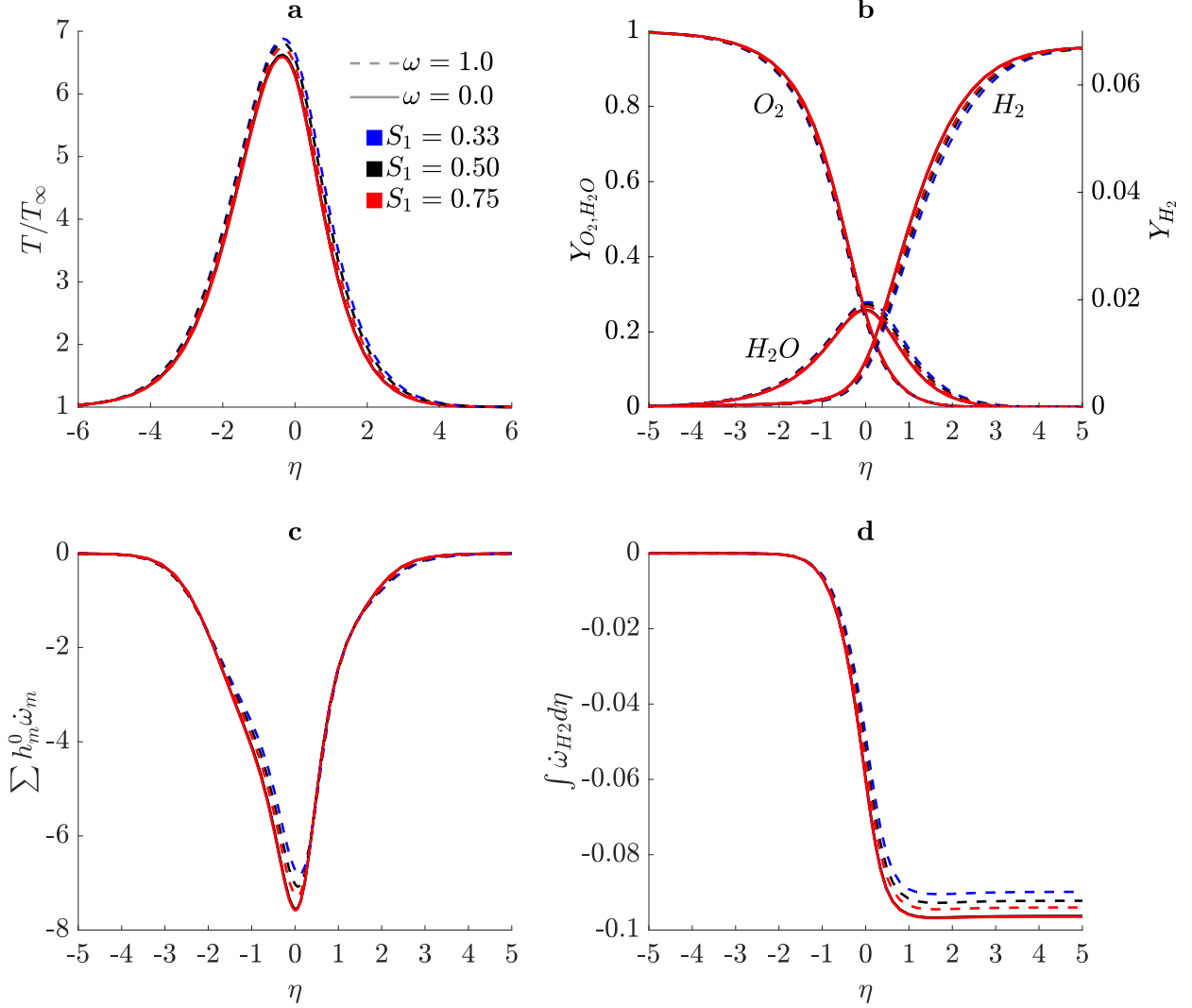


Figure 3.11: Non-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.33, 0.50, 0.75$; $S_2 = 0.67, 0.50, 0.25$. $\omega = 0.0, 1.0$, $S^* = 1,000,000$ 1/s.

Figure 3.11 shows temperature, species, and energy profiles for the symmetric and asymmetric strain rate cases at $\omega = 0.0, 1.0$. Many curves are close to one another because axial

convection differs substantially only in the negative far-field where there are no scalar gradients. Still, the deviations of strain rate and residence time arising from differing choices of S_1 , S_2 , and ω , are reflected in the scalar profiles. When $S_1 < S_2$ and $\omega = 1.0$, we see the minimum strain rate in the flame zone and the highest residence time, temperature, and product mass fraction. Interestingly, this case also produces the lowest HRR_T magnitude relative to the other rotational cases. When $S_1 > S_2$ and $\omega = 0.0$, we see the maximum strain rate in the flame zone and a reduction in residence time. This case produces the lowest temperature, product mass fraction, and HRR_T magnitude of the irrotational cases. Profiles of dependent variables on the unstable branch are qualitatively similar to those on the stable branch. While vorticity increases the maximum temperature on the stable branch, it decreases the maximum temperature on the unstable branch. Limits also exist on the maximum magnitudes of ω and S_2 that may be applied to the model. When either of these parameters exceed a critical value, centrifugal momentum overpowers the in-flow momentum and a reversal of flow occurs near the stagnation point. When this happens a pure counterflow no longer exists, instead the mass flux resembles the superposition of a counterflow and a source flow. The pressure Laplacian must be negative for the counterflow to exist, which is discussed in the coupling procedure developed in Sec. 5.1.1.

The counterflow analysis is applied only at the smallest length scales to avoid fluctuations from smaller eddies appearing in the layer. Smaller scales could not be considered small perturbations, as they would be expected to have larger strain rates, vorticity, and scalar dissipation rates. Also, they would have shorter time scales, causing problems with the quasi-steady assumption. Kinematic viscosity ν , thermal diffusivity α , and mass diffusivity D , are close in magnitude for common combusting gases. Therefore, the viscous layer near the counterflow interface and the non-premixed flame thickness are expected to have similar size. The diffusion layer centers very close to the interface for the non-premixed flamelet.

3.3.5 Premixed Flames

Here, we present the case of a stoichiometric hydrogen-air premixed twin flame. A combustible mixture of stoichiometric hydrogen and oxygen at 300 K enters the domain at $\eta = \pm\infty$. Due to the symmetry of the problem, only the positive half of the domain is calculated. The pressure is set at 10 atm. In the following figures and discussion, three combinations of ξ and z strain rates are used, $S_1 = 0.45, 0.50, 0.75$; $S_2 = 0.55, 0.50, 0.25$; and two values of vorticity are applied, $\omega = 0.0, 1.0$.

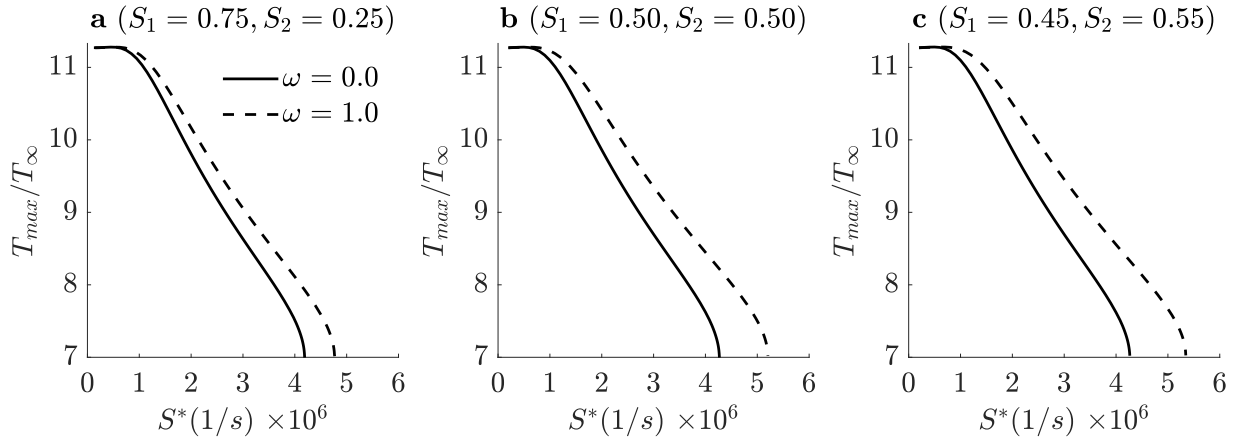


Figure 3.12: S-curves of premixed twin flames with varying strain rate and vorticity magnitudes.

Vorticity has a similar effect on the premixed twin flames as evidenced by Fig. 3.12a-c. S-curves with vorticity extinguish at a higher S^* . The preference of cases with larger S_2 values to extinguish at higher S^* is also maintained. Only the stable branches are presented here because of convergence difficulty on the unstable branch.

Figure 3.13a-d shows axial velocity u_χ , the similarity variable f , and mass effluxes in the ξ and z directions, $\rho u_\xi/\xi$ and $\rho w/z$, respectively, for the symmetric far-field strain rate case $S_1 = 0.5$, $S_2 = 0.5$ at $\omega = 0.0, 1.0$. These profiles are taken at an intermediate ambient strain rate of $S^* = 1,000,000$ 1/s. All values are non-dimensional. Efflux profiles, in the ξ and z directions, are divided by their respective spatial variables. Figure 3.13a and 3.13b show a reduction in boundary velocity and mass flux due to the centrifugal effect. Figure

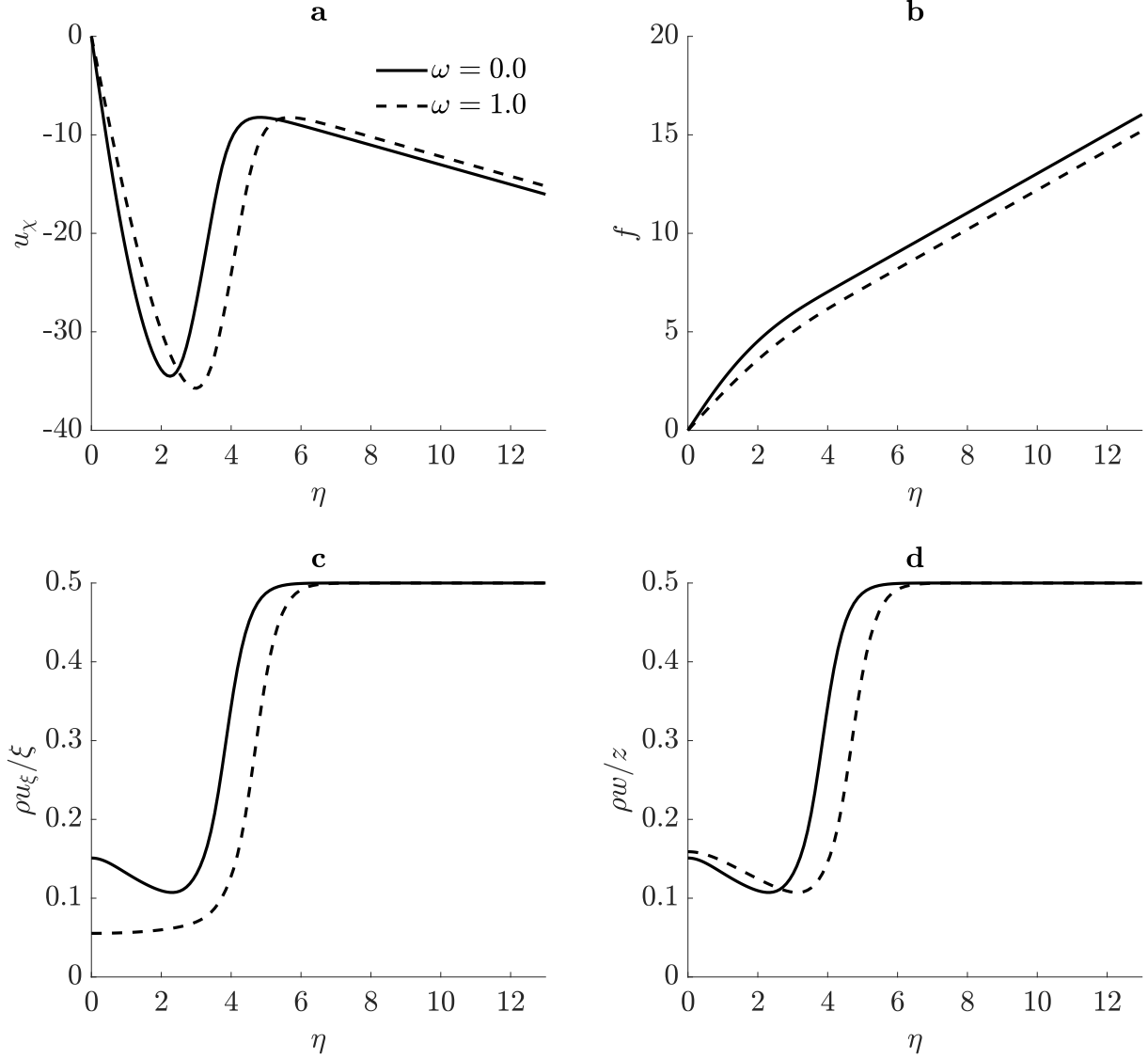


Figure 3.13: Premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse mass efflux normal to vorticity vector divided by length ($\rho u_\xi / \xi$); (d) Transverse mass efflux parallel to vorticity vector divided by length ($\rho w / z$). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 1,000,000$ 1/s.

3.13c shows a decrease in efflux component $\rho u_\xi / \xi$ when vorticity is applied. This occurs to satisfy mass conservation as a higher percentage of fluid exits in the z direction when $\omega = 1.0$ according to Fig. 3.13d. The rightward shift in all sub-figures for $\omega = 1.0$ is a consequence of the centrifugal effect reducing inflow velocity.

As the premixed flame does not have a unique peak temperature until the gradient region produced by the flame meets the stagnation point, it is beneficial to discuss the flame stand-

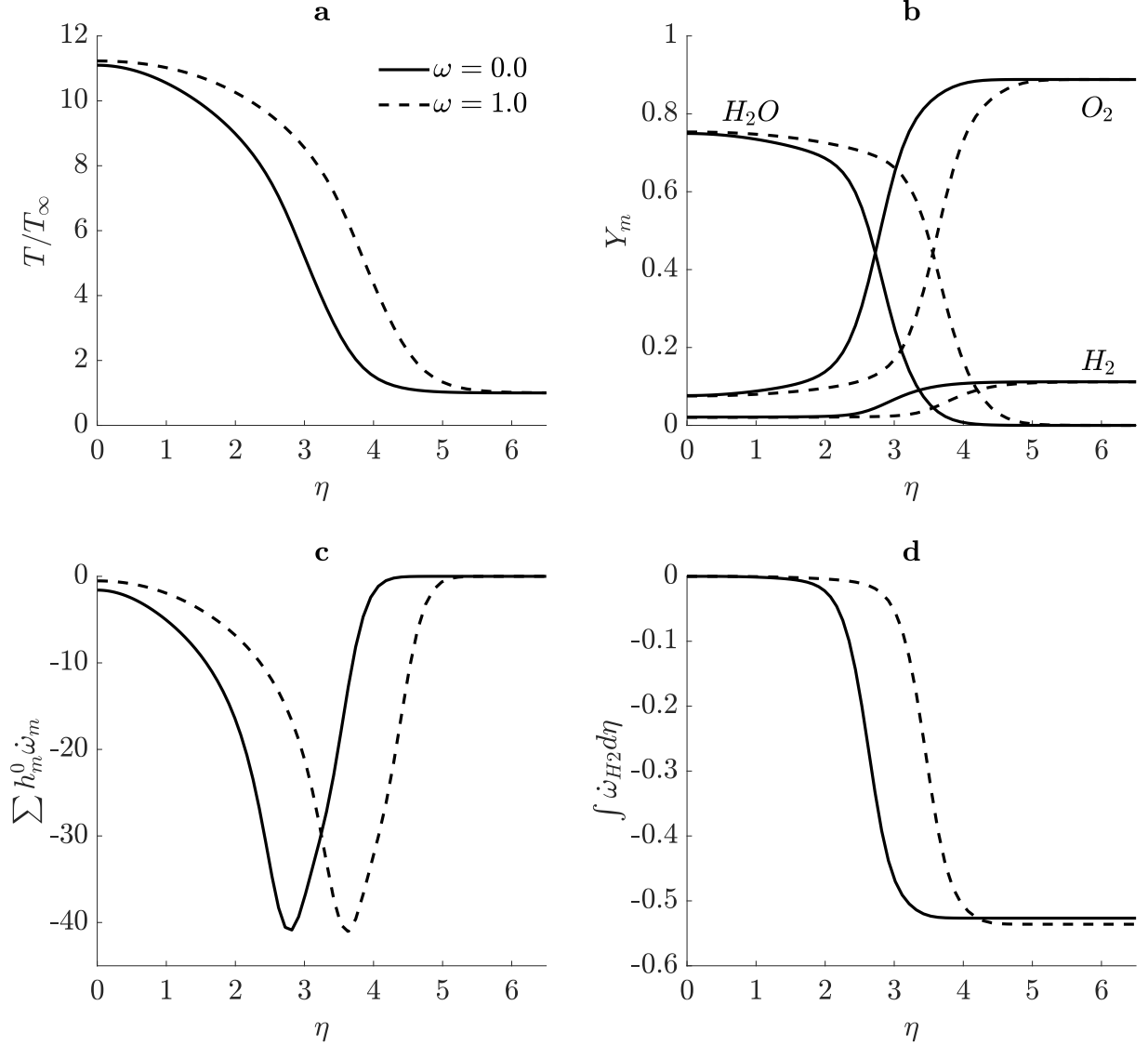


Figure 3.14: Premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 1,000,000$ 1/s.

off distance in addition to S-curves. Standoff distance is defined as the distance between the flame zone diffusion layer and the stagnation point, which decreases predictably with S^* . Figure 3.14a shows both an increased peak temperature and increased standoff distance due to the centrifugal effect. Contrary to non-premixed flames which have enhanced combustion via increased residence time, premixed flames are much less dependent on residence time because diffusion is unnecessary to create a flammable mixture. Instead, the effect of vorticity is to reduce the velocity at a given axial location which allows the flame speed, relatively

unchanged by vorticity, to move the flame to the right. This results in increased peak temperature because the scalar gradients are removed from the interface; i.e., the flame thickness increases. A comparison can be drawn here with the work of Kolla and Swaminathan [132] who examined strained premixed flames. They found that the flame brush thickness increases with the magnitude of the turbulent fluctuating velocity component normalized by unstrained laminar flame speed. Our results are in qualitative agreement as their parameterizing quantity can be likened to our non-dimensional vorticity, $\omega = \omega^*/S^*$. Our results show modifications of velocity via differing strain rates which was also reported by Knudsen et al. [133], although that work considered only normal strain rate without vorticity. The species profiles in Fig. 3.14b, heat release rate in 3.14c, and integrated H_2 reaction rate in 3.14d, reflect this shift of the diffusion layer. The temperature of the inflow is expected to affect the flame character near the extinction limit.

Figures 3.15 and 3.16 show the premixed twin flame at a higher strain rate. The flame is similarly affected by vorticity and $S_2 > S_1$ combination as non-premixed flames. Increasing vorticity increases peak temperature and flame standoff distance. When $\omega = 0.0$, the case of $S_1 = 0.5, S_2 = 0.5$ produces the highest temperature, as was the case with non-premixed flames. Figure 3.16 shows the velocity and mass flux profiles differ from non-premixed flames due to boundary-value densities. At the left boundary, non-premixed flames had increased mass flux when $\omega = 1.0$ due to the higher density there; however, the premixed flame has minimum density there because the left boundary is the stagnation point. Density differences also impose a limit on the minimum magnitude of S_1 .

The Karlovitz number Ka is often used to describe strained premixed flames and to compare flame scales to Kolmogorov scales. It can be written as the square of the ratio of premixed flame thickness to the Kolmogorov length: $Ka = (\delta_F/\delta_\kappa)^2$ where the flame thickness can be assumed to be dominated by the pre-heat layer so that $\delta_F = D/S_L$ and S_L is the premixed laminar flame speed. The mass diffusivity D is of the same order as both the kinematic

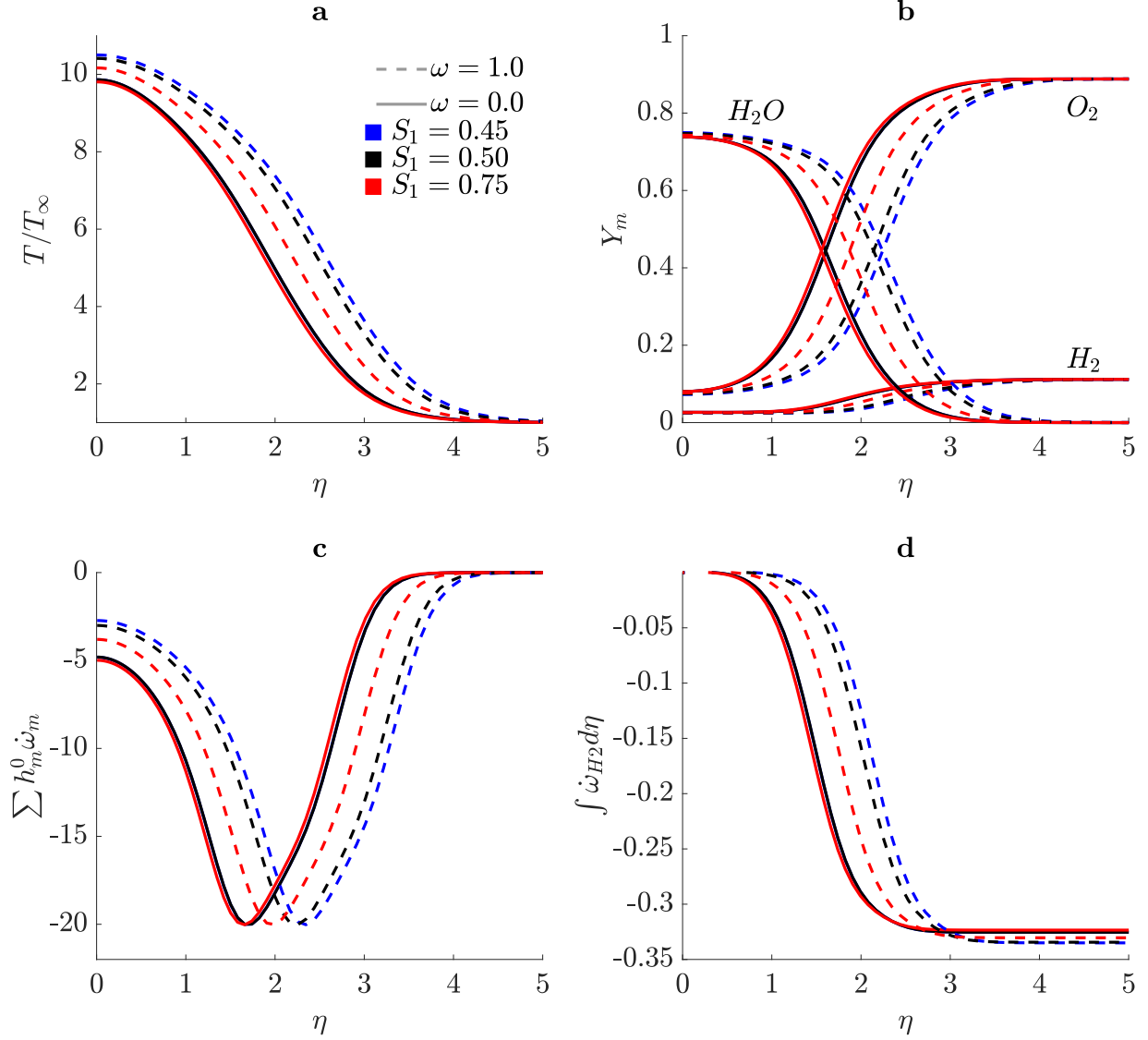


Figure 3.15: Premixed flame. (a) Temperature; (b) Major species mass fractions; (c) Heat release rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.45, 0.50, 0.75$; $S_2 = 0.55, 0.50, 0.25$; $\omega = 0.0, 1.0$; $S^* = 2,000,000 \text{ 1/s}$.

viscosity, ν , and the thermal diffusivity, α . For the counterflow at the highest strain rate (i.e., Kolmogorov value), the Kolmogorov viscous-layer thickness $\delta_\kappa = \sqrt{D/S^*}$ where S^* is the highest strain rate in the turbulent flow field; i.e., the value for the Kolmogorov scale in a shear flow is $O(Re^{1/2})$ larger than strain rates on the resolved scale in LES or RANS. A length infrequently discussed in premixed flamelet studies is the distance L of the flame from the interface in the counterflow. It follows that $LS^* = S_L$ for a quasi-steady behavior with a stationary or near-stationary distance between the flame and interface. Consequently,

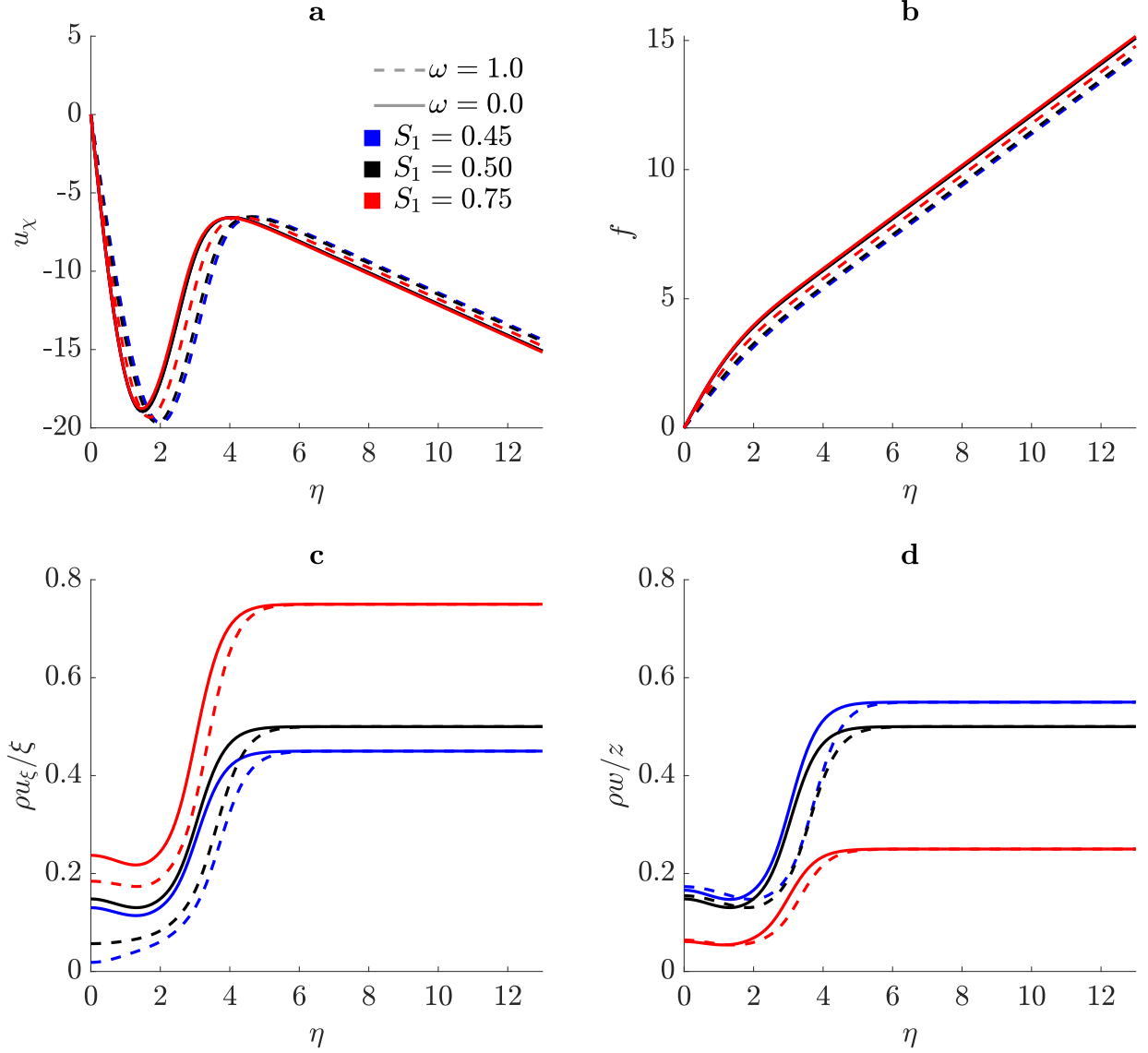


Figure 3.16: Premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse mass efflux normal to vorticity vector divided by length ($\rho u_\xi / \xi$); (d) Transverse mass efflux parallel to vorticity vector divided by length ($\rho w / z$). $S_1 = 0.45, 0.50, 0.75$; $S_2 = 0.55, 0.50, 0.25$; $\omega = 0.0, 1.0$; $S^* = 2,000,000$ 1/s.

$Ka = (\delta_\kappa / L)^2$. So, for $Ka \gg 1$, the premixed flame is thick compared to the viscous layer but its center lies close to the counterflow interface. On the other hand, if $Ka \ll 1$, the premixed flame is thin compared to the viscous layer but the distance from the interface to the viscous layer is large. This is the domain for corrugated or wrinkled laminar flamelets which occur with low to moderate levels of turbulence. This work focuses on high strain rates with a higher degree of turbulence (i.e., higher resolved-scale Reynolds number) where

the premixed flame is held in the viscous layer of the strained flow, i.e., cases with $Ka \geq 1$.

3.3.6 Partially-premixed Flames

The RFM also has the capability to compute partially-premixed flames. Below we present a flame with a slightly lean mixture inflowing from the left (1.666 H₂, 1.000 O₂, 3.760 N₂ in moles) and a rich mixture inflowing from the right (4.950 H₂, 1.000 O₂, 3.760 N₂ in moles). Both streams are at 300 Kelvin. At a low strain rate, these boundary conditions produce a counterflow with two major reaction zones (premixed) and one minor reaction zone (diffusion), see Fig. 3.18c. A lean premixed flame exists around $\eta = -4$, a non-premixed flame exists around $\eta = -1.9$, and a rich premixed flame exists around $\eta = +4$. This is an example of the established triple flame [106, 134–136] which can occur post-extinction, once the intensity of turbulent straining decreases. These mixtures were intentionally chosen to produce a triple flame. One transverse strain rate combination was used, $S_1 = S_2 = 0.5$, and evaluated for two vorticity levels, $\omega = 0.0, 1.0$.

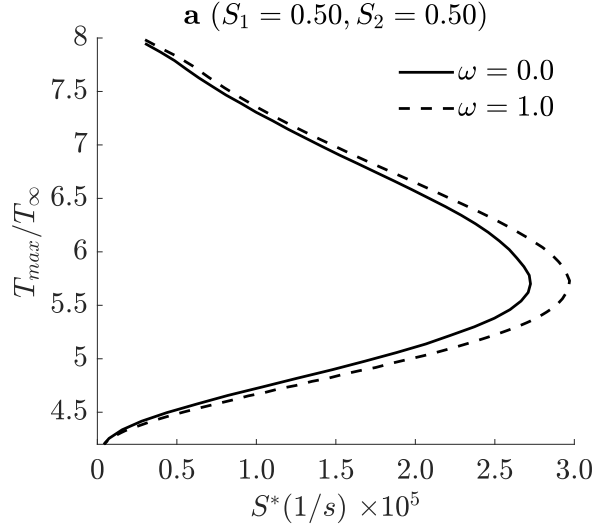


Figure 3.17: Extinction curves (S-curves) of partially-premixed flames with varying vorticity magnitudes plotted against ambient strain rate (S^*).

The S-curves of Fig. 3.17 show the vorticity effect is consistent with partially-premixed

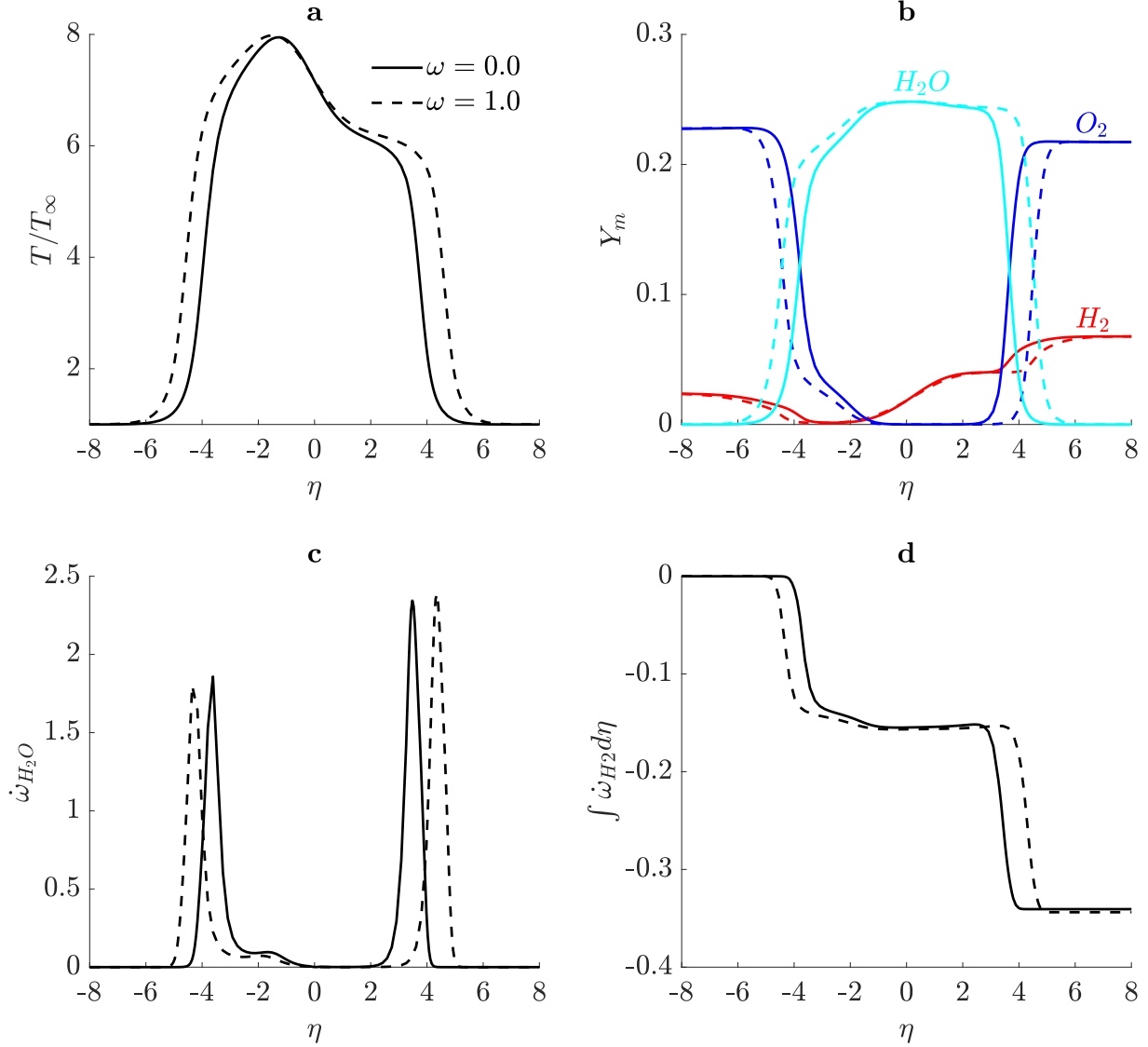


Figure 3.18: Partially-premixed flame. (a) Temperature; (b) Major species mass fractions; (c) H_2O reaction rate; (d) Integrated H_2 reaction rate (burning rate). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 30,000$ 1/s.

flames, increasing the extinction limit by 9.02 %. The extinction limit is an order of magnitude lower than the diffusion and premixed flames previously presented due to the high concentration of nitrogen in both streams. The scalar profiles in Fig. 3.18a and 3.18b show behavior reminiscent of both diffusion and premixed flames. With vorticity, the flame standoff distance increases as does the peak temperature, particularly at high strain rates. As the strain rate increases, the premixed flames on either side of the stagnation point are pushed into the non-premixed flame and it becomes difficult to distinguish three separate

flames. When the strain rate becomes very high, little to no premixed flame exists and the profiles resemble that of the non-premixed flames in Sec. 3.3.4. This is also the case across the entire unstable branch where, even at low strain rates, premixed flames do not appear on either side of the non-premixed flame. This is attributed to insufficient activation energy associated with the low peak temperatures on the unstable branch; i.e., the non-premixed flame does not produce enough energy to sustain the premixed flames.

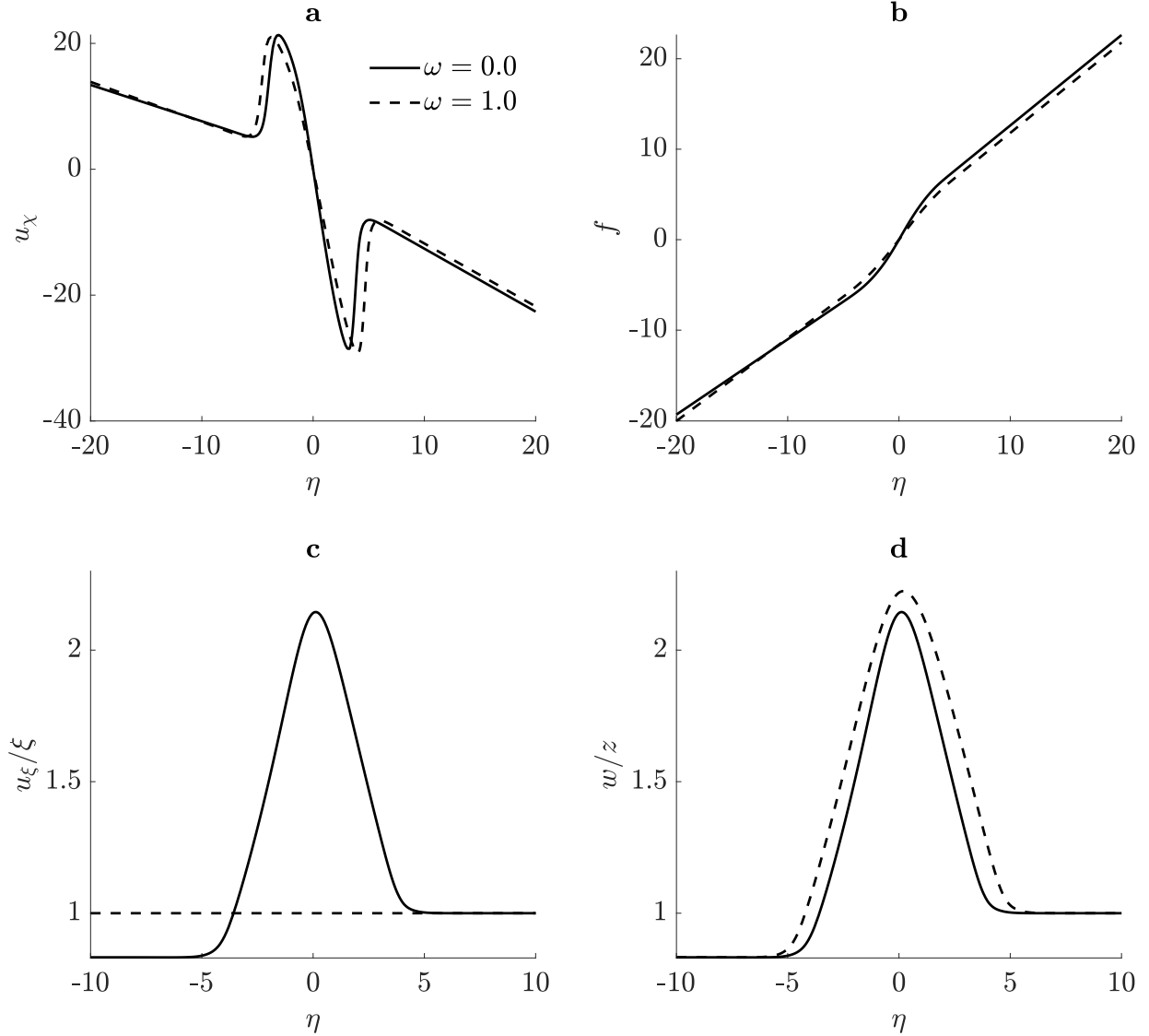


Figure 3.19: Partially-premixed flame. (a) Axial velocity u_χ ; (b) Similarity variable f ; (c) Transverse outflow velocity normal to vorticity vector divided by length (u_ξ/ξ); (d) Transverse outflow velocity parallel to vorticity vector divided by length (w/z). $S_1 = 0.5$; $S_2 = 0.5$; $\omega = 0.0, 1.0$; $S^* = 30,000$ 1/s.

Figure 3.18c shows the reaction rate of H_2O for the partially-premixed flame at a low strain rate. Two premixed flames are quite evident here while the central non-premixed flame is minimal. The centrifugal effect shifts the location of the premixed flames away from the stagnation point according to the modified axial velocity profile. The shape of integrated burning rate profiles in Fig. 3.18d differs from that of pure diffusion and pure premixed flames as individual “steps” are seen for the two premixed flames, with a slight tilting of the first step due to the central non-premixed flame. Despite the difference in shape, the overall finding that the centrifugal effect decreases burning rate is consistent with pure diffusion and pure premixed flames. Velocity and mass flux profiles of the partially-premixed flames are presented in Fig. 3.19 and have no qualitative difference from that of the non-premixed flames previously presented. Mass efflux in the z direction is increased by vorticity and there is a corresponding decrease in the ξ efflux. The axial strain rate in the flame is decreased and the boundary mass flux is increased on the oxidizer side and decreased on the fuel side.

3.3.7 Stretched Vortex Layer Hydrocarbon Non-premixed Flames

The $\text{H}_2\text{-N}_2/\text{O}_2$ flamelets presented in the prior section were primarily chosen for their chemical simplicity and relevance to upper-atmospheric and vacuum-domain engines. However, nearly all jet and in-atmospheric rocket engines burn hydrocarbons due their much greater energy density. Therefore, the RFM was investigated with hydrocarbon fuels. Jet Propellant-5 (JP-5) was selected as a representative heavy hydrocarbon fuel with significant density contrast relative to air, allowing us to assess centrifugal effects under aviation-relevant conditions. Methane-oxygen (CH_4/O_2) was selected as a well-characterized canonical system relevant to high-performance liquid rocket propulsion, enabling comparison with prior flamelet studies. The chemical kinetics models used for these hydrocarbon cases are the skeletal HyChem model for JP-5 [128, 129] and a reduced version of the FFCM-1 model for methane-oxygen combustion in rocket engines [127]. The JP-5 model has 202 reactions among 41

species and the CH₄ model has 39 reactions among 12 species. The reduced-order versions of these chemical kinetics models were chosen because it is too computationally intensive to carry hundreds or thousands of species in a coupled CFD environment. For the purposes of this work, as well as integrated RANS and LES simulations, reduced-order models are fully capable of capturing the important combustion dynamics and power or thrust output. The JP-5/Air cases have a pressure of 20 atm and the CH₄/O₂ cases have a pressure of 30 atm. Pressures were chosen as representative values for common jet engines; we did not ramp up the CH₄/O₂ pressure to modern rocket engine chamber pressures because the chemical kinetics model becomes increasingly less validated as the pressure increases.

In the RFM, scalar boundary conditions are set at $\eta = \pm\infty$ and thus the mixtures enter along the η (density-weighted y) axis. Along this axis, the far-field strain rate at $\eta = \infty$ is $-S^*$ and at $\eta = -\infty$ is $S^* \sqrt{\rho_\infty/\rho_{-\infty}}$. This axis corresponds to the mixture fraction axis in most other flamelet models. Making $S_1 > 0$ and $S_2 > 0$ then produces a counterflow with one inflow axis and two outflow axes, which, with non-zero vorticity creates a stretched vortex layer. The transverse strain rates $S_1^* = S_1 S^*$ and $S_2^* = S_2 S^*$ set the velocity gradients (relative efflux magnitudes) along the x and z axes. The two primary outputs of the RFM are curves of maximum temperature (T_{MAX}) versus ambient strain rate (S^*) and heat release rate (HRR) versus S^* . Heat release rate is defined in Eq. 3.18 where L is the computational distance along the y axis. These curves are shown in Fig. 3.20 and Fig. 3.21 for JP-5/Air and CH₄/O₂, respectively. For both of the fuel/oxidizer cases, the right ($\eta = \infty$) inlet is pure fuel at 300 K . For JP-5, the oxidizer is air (0.21% O₂, 0.79% N₂) at 300 K , and for CH₄, the oxidizer is pure O₂ at 300 K .

$$\dot{Q}_{HRR} = \frac{1}{L} \int_{-\infty}^{\infty} \sum \dot{\omega}_m h_{f,m} dy \quad \left(\frac{J}{kg \cdot s} \right) \quad (3.18)$$

The flammability limit for a given configuration of mechanical constraints and scalar bound-

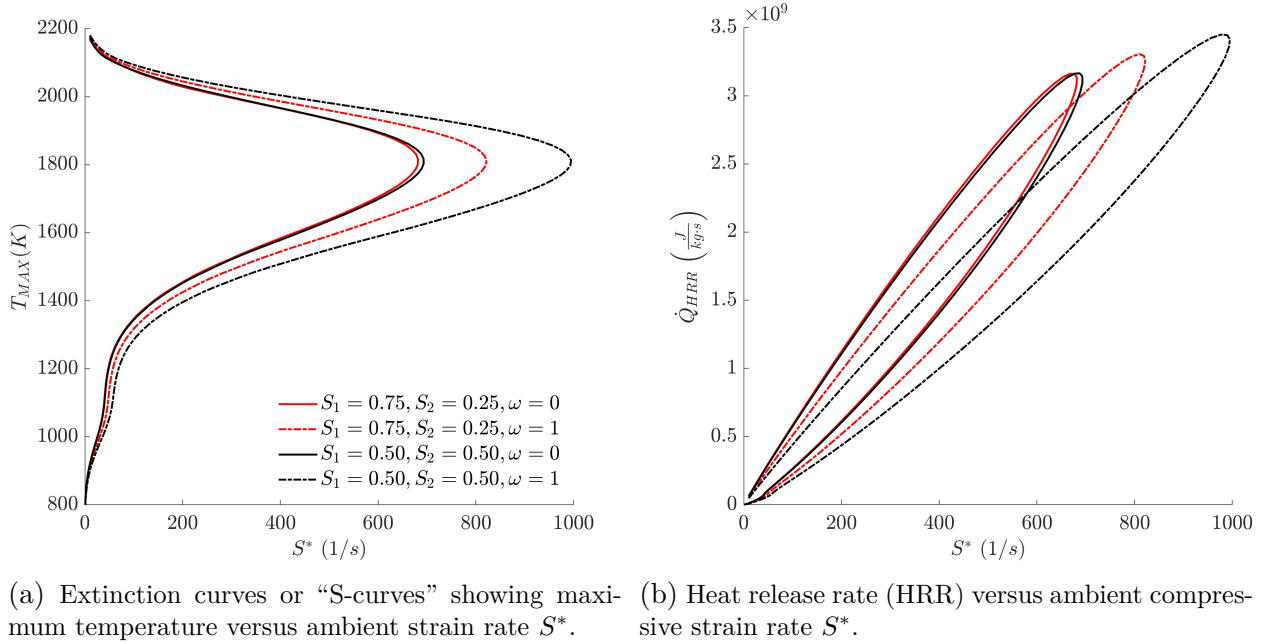


Figure 3.20: JP-5/Air non-premixed stretched vortex layer flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω .

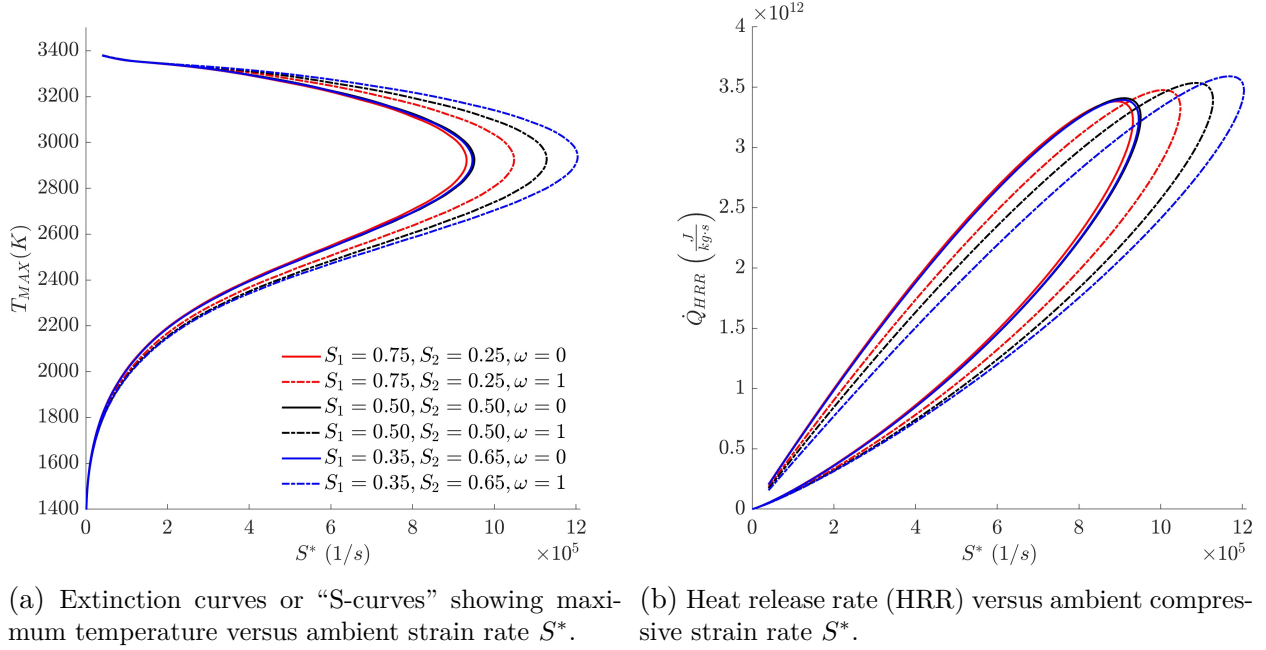


Figure 3.21: CH₄/O₂ non-premixed stretched vortex layer flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω .

any conditions is defined as the maximum ambient strain rate S^* under which a steady-state flame can burn without extinguishing; this corresponds to the locations with vertical slopes on the right sides of Fig. 3.20a and Fig. 3.21a. Inspecting the figures reveals three gen-

eral trends, consistent with the results found for $\text{H}_2\text{-N}_2/\text{O}_2$ flames in [97, 98]. First, for any combination of transverse strain rates, increasing vorticity from $\omega = 0 \rightarrow 1$ increases the flammability limit. This occurs because the centrifugal effect of vorticity counteracts the velocity gradient in the η direction, resulting in a reduction in the strain rate of the stagnation-region (flame zone) and thus an increase in residence time. Steady-state non-premixed flames extinguish when the diffusion magnitude of combustible gasses coupled with the reaction rate and heat release of exothermic reactions are insufficient to replenish the heat and radicals lost via thermal and molecular diffusion, stretching, and efflux convection in a given time. The additional residence time added by the centrifugal effect thereby allows combustion to occur at higher ambient strain rates.

The three-dimensional character of the flamelets is shown in Fig. 3.22. The streamline initializations on the oxidizer (blue) and fuel (red) sides begin from the same distance on either side of the $y = 0$ plane. Notice how the blue streamlines show a preference to exit along the z axis. This occurs because the flame zone, which is on the oxidizer side of the stagnation plane, is composed of high-temperature, low-density combustion products. Under centrifugal acceleration, low-density gas tends to flow outward along z . This is more prevalent in the JP-5/Air case because the density ratio is much larger than in the CH_4/O_2 case. On the fuel side of the stagnation plane, which is further from the flame, the density ratio, and therefore the centrifugal effect, are less pronounced, causing the streamlines to exit more evenly along the x and z directions.

The magnitude of the centrifugal force scales with density, and therefore the more dense JP-5 cases display a higher percentage increase in flammability limits than the lighter CH_4/O_2 cases. Secondly, flammability limits increase with the percentage of outflow forced in the z direction; i.e., higher values of S_2 result in higher flammability limits. Because the vorticity vector is aligned with z and S_2 , the plane experiencing centrifugal acceleration is the x - y plane. In this plane, centrifugal acceleration pushes fluid outward, thus tending to increase

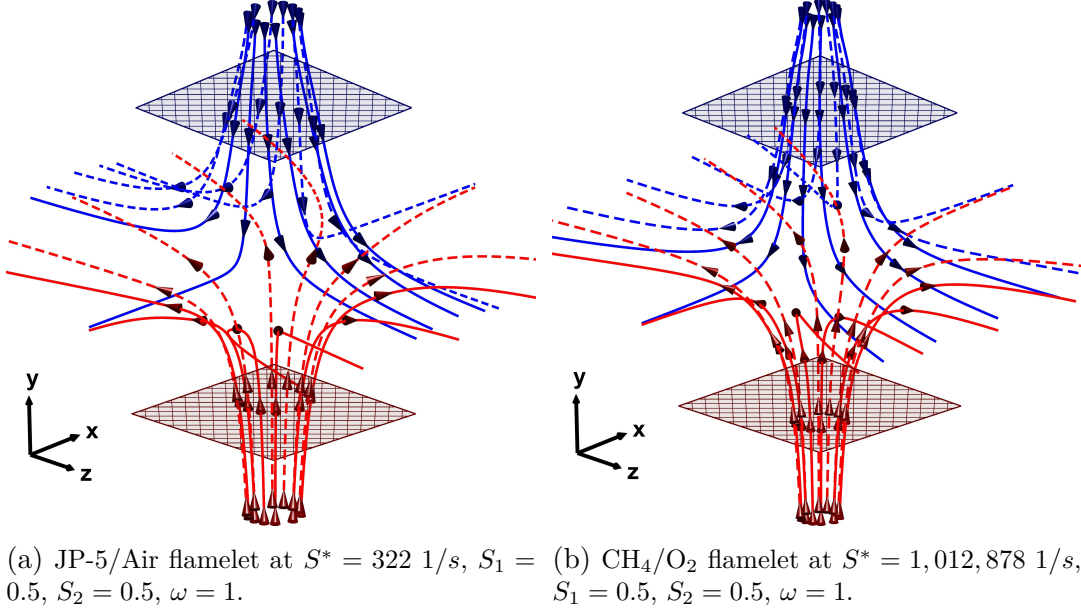


Figure 3.22: Stretched vortex layer flamelet streamlines in the non-Newtonian reference frame. Horizontal planes show surfaces of constant scalar properties. Solid and dashed lines indicate streamlines originating on the near and far sides of the inflows, respectively.

efflux in x while decreasing influx in y . When S_1 is large, this preference of increased efflux in x is permitted which yields higher flame zone strain rates and thus lower flammability limits. In contrast, when S_1 is smaller and a higher percentage of efflux is directed along the z axis (S_2 is large), the fluid is forced to turn from the x direction toward the z direction as the low S_1 strain rate prevents expulsion in x . This effectively causes a fluid bottleneck which decreases velocity and strain rate in the y direction, increasing residence time and the flammability limit. Lastly, the axisymmetric case, $S_1 = S_2 = 0.50$, produces the highest flammability limit when $\omega = 0$. The percentage increases in flammability limits, $\Delta S_{ext.}^*/S_{ext.,\omega=0}^* \times 100\%$, for the stretched vortex layer S-curves are shown in Table 3.2.

Similarly, to maximum temperature, HRR profiles are extended by the combined effects of centrifugal acceleration and increased S_2 magnitude, as shown in Fig. 3.20b and Fig. 3.21b. It is well known that turbulent combustion simulations frequently struggle to predict many experimentally-observed trends such as species concentrations (especially intermediate species and pollutants) [137, 138], extinction, re-ignition, and near-flammability limit pro-

Table 3.2: Percentage increase in flammability limits between $\omega = 0 \rightarrow 1$

Transverse Strain Rates	% increase, JP-5/Air	% increase, CH ₄ /O ₂
$S_1 = 0.75, S_2 = 0.25$	20.52%	12.48%
$S_1 = 0.50, S_2 = 0.50$	43.50%	18.62%
$S_1 = 0.35, S_2 = 0.65$	n/a	27.23%

Percentage increase in flammability limits (maximum S^* magnitude) tolerated by non-premixed flamelets when the vorticity magnitude is increased from $\omega = 0 \rightarrow 1$. Results are shown for all cases of the stretched vortex layer type. Percentages correspond to differences between solid and dashed S-curves in Fig. 3.20a and Fig. 3.21a.

cesses [139–141], onset and amplitude of combustion instabilities [142, 143], and turbulence-chemistry interaction [139, 141, 144], among others. Certainly a major component of these deviations comes from the imperfection of Reynolds stress and residual stress models, especially those developed for incompressible flows when used in an exothermically reacting flow. However, another component of the deviation comes from imperfections in the turbulent combustion model, some of which we address with the RFM, namely the combined influence of detailed chemical kinetics and transport within an asymmetric, three-dimensional, stretched vortex geometry. This is done under the quasi-steady flamelet assumption but may be treated in an unsteady framework [64].

When extrapolated to a coupled CFD + RFM framework, one can imagine a stark difference in two simulations resulting from the difference in HRR. Contrast CFD using an irrotational, symmetric flamelet model with CFD using the RFM with $\omega = 1$ (a good approximation based on DNS work). For hydrocarbon fuels, the latter framework will return larger HRRs for strain rates up to $\sim 40\%$ higher than the former framework which does not account for Kolmogorov vorticity nor asymmetric strain rates. This difference may be compounded if the former flamelet model makes a constant Lewis number assumption or otherwise restricts the transport process as seen by the differences in the FPV and RFM results in [145]. We surmise that this difference will be evident in the resolved or mean flow field and may provide a plausible explanation for part of the discrepancies often observed between CFD predictions

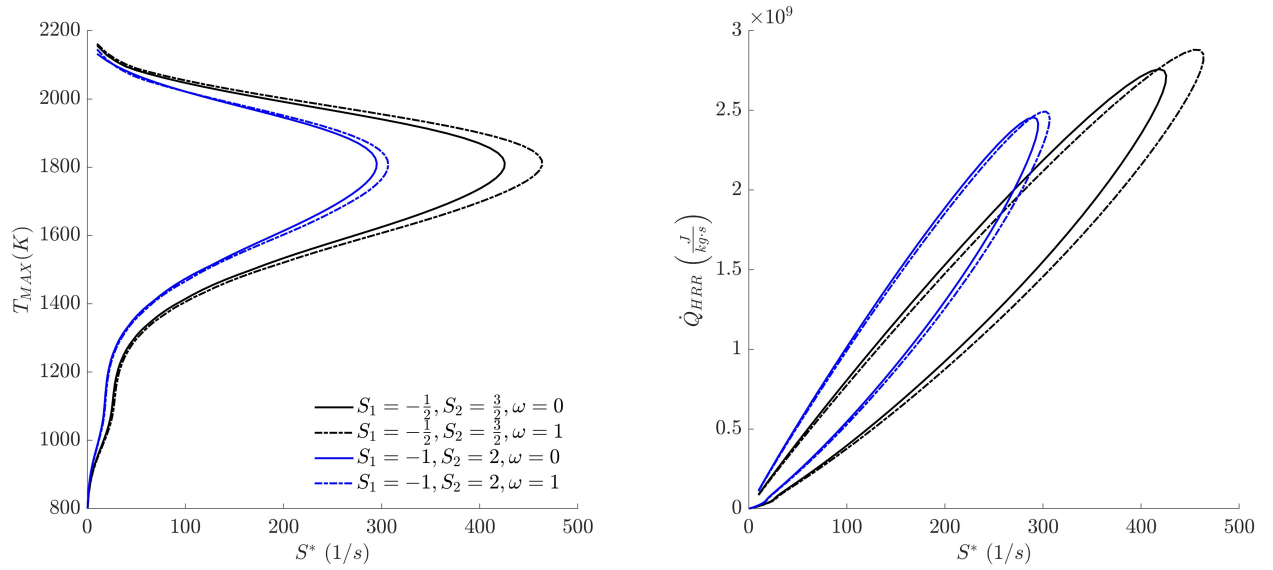
and experimental results, warranting future investigation.

Although the qualitative results of JP-5/Air flamelets are essentially the same as the CH₄/O₂ flamelets, the magnitudes of tolerable S^* values differ by five orders. This difference is due to three factors. First, CH₄/O₂ flamelets have an ambient pressure 10 *atm* higher than the JP-5 flamelets, which increases the Arrhenius rates. Secondly, the CH₄ fuel is oxidized with pure O₂ while the JP-5 fuel is oxidized with air. Lastly and most interestingly, JP-5 is a large and heavy hydrocarbon chain, while CH₄ is a foundational fuel. Therefore, JP-5 molecules must be pyrolyzed into many smaller hydrocarbons before oxidization. There are a multitude of time scales associated with the pyrolysis process, some of which are extremely long relative to CH₄, and thus require longer residence times; i.e., lower strain rates. Furthermore, due to their large size and mass, JP-5 molecules are slow to diffuse, further necessitating longer residence times to create stoichiometric conditions. As the temperature decreases, some of the reactions in the pyrolysis process are turned off, which is evident in the horizontal bump seen on the unstable branch of Fig. 3.20a around $900K < T_{MAX} < 1200K$.

The density ratio between the $\eta = -\infty$ and $\eta = +\infty$ inflows sets limits on the acceptable magnitudes of $\omega/2S_1$, and thus implicitly on S_2 , as seen by the $\eta = -\infty$ boundary condition in Eq. 3.15. The argument of the square root must be positive, which means $\rho_{\infty}^*/\rho_{-\infty}^* \leq 1$. For the same inflow temperatures and pressures, density is determined by molecular weight, which is why the JP-5 cases only show two combinations of transverse strain rates while the CH₄ cases show three. As JP-5 is much heavier than air (167.32g/mol versus 28.85g/mol, respectively), $\omega = 1$ limits $S_1 \geq 0.4551$. As there are few qualitative differences between $S_1 = 0.4551$ and $S_1 = 0.50$, we omit the results of $S_1 = 0.4551$ for JP-5. Conversely, CH₄, being lighter than O₂, produces no density ratio limitation and thus any value of S_1 other than $S_1 = 0$ is acceptable.

3.3.8 Stretched Vortex Tube Hydrocarbon Non-premixed Flames

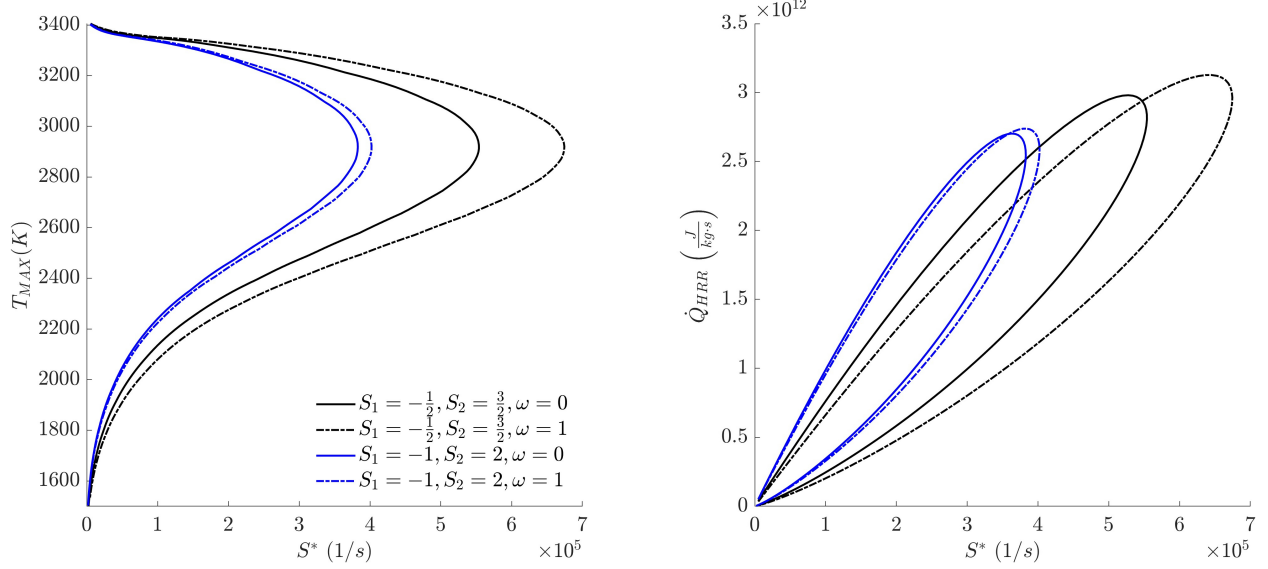
Although the DNS findings discussed previously indicate a likelihood of the stretched vortex layer geometry, it is possible for the Kolmogorov-scale flow field to have two inflows. This is achieved in the RFM by setting $S_1 < 0$, which causes influx in the x direction in addition to the y direction, creating an inward-swirling, stretched vortex tube configuration. The results of the stretched vortex tube flamelet are shown in Fig. 3.23 and Fig. 3.24 for the same set of scalar boundary conditions and ambient pressures used in the stretched vortex layer results.



(a) Extinction curves or “S-curves” showing maximum temperature versus ambient strain rate S^* . (b) Heat release rate (HRR) versus ambient compressive strain rate S^* .

Figure 3.23: JP-5/Air non-premixed stretched vortex tube flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω .

The vorticity effect, which increases the flammability limit, is qualitatively the same between the stretched vortex tube cases and the vortex layer cases. However, the trend elicited by varying the transverse strain rates, S_1 and S_2 , is reversed. For stretched vortex tube cases, more negative S_1 magnitudes and higher (positive) S_2 magnitudes result in lower flammability limits because the influxes and effluxes are stronger, resulting in higher flame zone strain rates. In contrast, when S_1 is negative but of low magnitude and S_2 is positive and also of lower magnitude, the fluid bottleneck occurs, reducing the amount by which the



(a) Extinction curves or “S-curves” showing maximum temperature versus ambient strain rate S^* . (b) Heat release rate (HRR) versus ambient compressive strain rate S^* .

Figure 3.24: CH_4/O_2 non-premixed stretched vortex tube flamelets. Both sub-figures show varying mechanical constraints: S^* , S_1 , S_2 , and ω .

flame zone is stretched and thus extending the residence time. Across all configurations, the stretched vortex tube cases show significantly lower flammability limits than the stretched vortex layer cases due to the nature of the two inflow axes, which produce increased stretching of the stagnation region and therefore higher strain rates, regardless of the magnitudes of S_1 , S_2 , or ω . The percentage increases in flammability limits, $\Delta S_{ext}^*/S_{ext, \omega=0}^* \times 100\%$, for the stretched vortex tube S-curves are shown in Table 3.3.

Table 3.3: Percentage increase in flammability limits between $\omega = 0 \rightarrow 1$

Transverse Strain Rates	% increase, JP-5/Air	% increase, CH_4/O_2
$S_1 = -0.50, S_2 = 1.50$	8.91%	21.78%
$S_1 = -1.00, S_2 = 2.00$	3.98%	5.06%

Percentage increase in flammability limits (maximum S^* magnitude) tolerated by non-premixed flamelets when the vorticity magnitude is increased from $\omega = 0 \rightarrow 1$. Results are shown for all cases of the stretched vortex tube type. Percentages correspond to differences between solid and dashed S-curves in Fig. 3.23a and Fig. 3.24a.

As in the cases of the stretched vortex layer, the stretched vortex tube flamelets show an increase in HRR for a given S^* value, as well as an increase in the maximum HRR mag-

nitude. These findings augment the HRR discussion in the vortex layer cases by providing a more complete map of the full range of possible HRRs experienced by a given fuel and oxidizer combination. Although complicated to implement, we believe that the best flamelet combustion model will account for all possible variations in S_1^* , S_2^* , S^* and vorticity ω^* . This may be prohibitively costly in terms of the look up process, and thus we identify vorticity as the primary effect and transverse strain rate variation as secondary, augmentation effects.

3.3.9 Summary of Findings for Multi-step Chemical Kinetics with Detailed Transport

The inclusion of detailed chemical kinetics, multi-component diffusion, and variable thermo-physical properties in the RFM has yielded new findings in the effects of vorticity and three-dimensional strain rate distributions. While corroborating the fundamental result that vorticity increases residence time, making a highly strained flame behave more like a moderately-strained, irrotational flame, other differences exist due to reactant composition in concert with centrifugal acceleration. Diffusion flamelets with three fuel/oxidizer pairs were investigated: $\text{H}_2\text{-N}_2/\text{O}_2$, JP-5/Air, and CH_4/O_2 . From $\omega = 0$ to $\omega = 1$, increases in flammability limits for stretched vortex layer-type flamelets ($S_1 > 0$; $S_2 > 0$) were approximately 8-17% for $\text{H}_2\text{-N}_2/\text{O}_2$, 21-44% for JP-5/Air, and 13-27% for CH_4/O_2 . The centrifugal effect is shown to be amplified when the density in the flame zone is low relative to the inflow densities. Thus, the greatest impacts of the RFM in coupled simulations are expected when the fuel is a heavy hydrocarbon such as JP-5, RP-1, or other kerosene derivatives. In preliminary testing with pure H_2/O_2 diffusion flamelets, the centrifugal effect was negligible because the pure H_2 fuel density, even at low temperature, was less dense than the high-temperature products in the flame zone. Diffusion flamelets of the stretched vortex tube type ($S_1 < 0$; $S_2 > 0$) were also computed for JP-5/Air and CH_4/O_2 cases. From $\omega = 0$ to $\omega = 1$, increases in flammability limits for these cases were approximately

4-9% for JP-5/Air and 5-22% for CH_4/O_2 . Together these findings indicate that for any distribution of three-dimensional strain rates and for any fuel combination, the centrifugal effect of vorticity increases the flammability limit; however, the extension of the limit is more substantial if the velocity gradients are of the stretched vortex layer type and/or if there is a substantial density difference between hot products and inflow streams. As stretched vortex layers are the most probable structures indicated by DNS, it is expected that the centrifugal effect will be evident in a coupled CFD framework.

Premixed and partially-premixed flamelets were also computed to showcase the ubiquity of the RFM. Both premixed and partially-premixed flames show the fundamental trend that vorticity increases the flammability limit. The primary difference between premixed or partially-premixed flames and diffusion flames is that premixed inflow mixtures stabilize wherever their laminar flame speed matches the convective inflow velocity. Thus, for low strain rates, premixed flames (including the premixed portion of partially-premixed flames) exist far from the counterflow stagnation plane; i.e., they have a large standoff distance. When strain rates increase, these premixed flames shift toward the stagnation plane, eventually merging with the diffusion layer. The tendency of premixed and partially-premixed flames to burn far away from the stagnation plane suggests that these mixtures burn outside the Kolmogorov eddy holding the central diffusion layer. Therefore, careful consideration must be taken when using non-premixed flamelet models in situations where there is substantial premixing, as it is not proper to assume that the premixed flames always burn within a few Kolmogorov radii of the stagnation plane.

3.4 Fickian Diffusion and Multi-step Chemical Kinetics: Impact on Scalar Dissipation Rate

In the prior sections, issues with scalar dissipation rate have been identified as: its creation requires Fickian diffusion, it is often used with unity Lewis numbers, and it has no scaling law grounded in turbulence cascade theory; instead the resolved scale value of SDR is often equated to the stoichiometric value, χ_{st} , in the center of the flamelet reaction zone. The other common variable used is the mixture fraction, which has its own issue: it does not allow fuel mixed into the oxidizer stream or oxidizer mixed into the fuel stream and excludes countergradient diffusion since it must vary monotonically between the oxidizer and fuel boundaries. Thus, a flamelet formulation using SDR and mixture fraction have reduced utility in terms of relaxing the classical flamelet assumptions outlined in Chap. 2.

In this study, for the limited cases where mixture fraction and SDR are meaningful variables, we make four primary points: First, the determination of both SDR and local strain rate from first principles depends on both vorticity and applied strain rate. Flammability curves (S-curves) plotted versus SDR collapse as shown in Fig. 3.25; however, there is no known first-principles approach to relate χ_{st} to resolved-scale behavior. Second, as was seen in the prior section, vorticity increases the maximum ambient strain rate above which a diffusion flame will extinguish and the ambient transverse strain rates (those normal to the inflow axis) also influence the extinction strain rate. Third, the Fickian diffusion formulation with the imposition of unity Lewis number alters the S-curves. Lastly, we argue that scaling laws for velocity gradients are both more substantiated and more representative of the physics than procedures to relate SDR to the resolved scale; however, this is our opinion and not affirmed or disputed by our results.

3.4.1 Governing Equations

This section uses the same basic set of governing equations as the prior section where vorticity is included via a transformation to a non-Newtonian reference frame after which a similarity solution is employed. The governing equations for three-dimensional steady flow in this reference frame are listed below as Eq. 3.19-3.23 where $a_i = \langle x\omega^2/4, y\omega^2/4, 0 \rangle$ is the centrifugal acceleration in the non-Newtonian reference frame. Note that because this section pertains to the classical flamelet model's use of scalar dissipation rate χ , the RFM non-Newtonian reference frame spatial directions are x, y, z in this section instead of ξ, χ, z as in the prior section so as to not confuse scalar dissipation rate with the compressive axis spatial variable. The low Mach number approximation is made to remove terms involving kinetic energy and viscous dissipation.

$$\frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (3.19)$$

$$\rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho a_i \quad (3.20)$$

$$\tau_{ij} = \mu \left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right] \quad (3.21)$$

$$\frac{\partial(\rho u_j h)}{\partial x_j} + \frac{\partial}{\partial x_j} \sum_{m=1}^{n_{sp}} \rho v_m^d Y_m h_m = \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) - \rho \sum_{m=1}^{n_{sp}} h_{f,m} \dot{\omega}_m \quad (3.22)$$

$$\frac{\partial(\rho u_j Y_m)}{\partial x_j} + \frac{\partial}{\partial x_j} (\rho Y_m v_m^d) = \rho \dot{\omega}_m ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.23)$$

In order to define the scalar dissipation rate commonly used in the literature, see Eq. 3.40, thermal and mass diffusivities for all species are taken to be equal. Unitary Lewis numbers are assumed which specifies the diffusivity at each point in the domain according to Eq. 3.24.

Diffusion velocity and diffusion flux are defined according to Eq. 3.25-3.26. Using Taylor series approximations in classical fashion for transverse velocity components in a counterflow, i.e., Eqs. 3.27-3.28, a similar solution described by ordinary differential equations, Eqs. 3.31-3.34, is obtained. The full derivation is given in [94, 95, 98].

$$D = \frac{\lambda}{\rho c_p} \quad (3.24)$$

$$v_m^d = -\frac{1}{Y_m} D \frac{dY_m}{dy} \quad (3.25)$$

$$J_m = \rho Y_m v_m^d \quad (3.26)$$

The similarity solution simplifies the solution to Eq. 3.19-3.23, reducing the scalar fields to functions of only the axial coordinate y . In doing so, we do not account for curvature effects. The velocities in the transverse directions, x and z are assumed to be functions of their respective spatial variables and of y according to Eq. 3.27-3.28.

$$u_x = S_1 x f_1' \quad (3.27)$$

$$u_z = S_2 z f_2' \quad (3.28)$$

The two constants S_1 and S_2 are the far-field strain rates at $x = +\infty$ and $z = +\infty$, respectively, non-dimensionalized by the ambient strain rate at $y = +\infty$, S^* . For the remainder of this section, * indicates a dimensional quantity. All other quantities are non-dimensional. Variables f_1' and f_2' are two of three similarity variables, all of which are functions of y only. The third similarity variable is defined according to Eq. 3.29 from which the y velocity component is found via Eq. 3.30.

$$f = S_1 f_1 + S_2 f_2 \quad (3.29)$$

$$u_y = -\frac{f}{\rho} \quad (3.30)$$

Employing a density-weighted Illingworth transformation from $y \rightarrow \eta$, i.e., $\eta \equiv \int_0^y \rho(y) dy$, allows the equations to be further simplified. After the transformation to η -space is made, we denote first derivatives with respect to η using superscript $'$. Derivatives of higher order have additional “primes”; e.g., a second derivative has superscript $''$. For a complete derivation of the similarity solution, the reader is encouraged to see Sirignano [94, pp. A21-11-16]. The similar form of the governing equations and their boundary conditions are presented below, along with the equation of state. Equations 3.31-3.32 are the momentum equations in the x and z directions. The y momentum equation is not needed to obtain the velocity field but can be used to obtain the pressure gradient.

$$\rho\mu f_1''' + f_1''(\rho\mu)' + f f_1'' + S_1 \left(\frac{1}{\rho} - (f_1')^2 \right) + \frac{\omega^2}{4S_1} \left(1 - \frac{1}{\rho} \right) = 0 \quad (3.31)$$

$$\rho\mu f_2''' + f_2''(\rho\mu)' + f f_2'' + S_2 \left(\frac{1}{\rho} - (f_2')^2 \right) = 0 \quad (3.32)$$

$$c_p f T' + (\rho \lambda T')' - T' \sum_{m=1}^{n_{sp}} J_m c_{p_m} - \sum_{m=1}^{n_{sp}} h_m^0 \dot{\omega}_m = 0 \quad (3.33)$$

$$f Y_m' - J_m' + \dot{\omega}_m = 0 \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (3.34)$$

$$P = \rho R_{sp} T \quad (3.35)$$

The boundary conditions for Eqs. 3.31-3.35 given by Eqs. 3.36-3.39.

$$f_1'(\infty) = 1 \quad ; \quad f_1'(-\infty) = \sqrt{\frac{1}{\rho_{-\infty}} + \left(\frac{\omega}{2S_1} \right)^2 \left(1 - \frac{1}{\rho_{-\infty}} \right)} \quad ; \quad f_1(0) = 0 \quad (3.36)$$

$$f_2'(\infty) = 1 \ ; \ f_2'(-\infty) = \frac{1}{\sqrt{\rho_{-\infty}}} \ ; \ f_2(0) = 0 \quad (3.37)$$

$$T(\infty) = 1 \ ; \ T(-\infty) = T_{-\infty} \quad (3.38)$$

$$Y_m(\infty) = Y_{m,\infty} \ ; \ Y_m(-\infty) = Y_{m,-\infty} \quad (3.39)$$

Realize that enstrophy, $\omega^{*2} = \omega^* \cdot \omega^*$ is actually the relevant variable. The direction of rotation in the $x - y$ plane is not relevant. Analytical and experimental studies relate enstrophy to the square and products of strain rates, concluding that they are of the same order of magnitude [123–125]. As such, we normalize vorticity by normal compressive strain rate S^* , keeping this nondimensional vorticity of $O(1)$; $0 \leq \omega = \omega^*/S^* \leq \sqrt{1.5}$.

One key difference between the RFM and former models is that the RFM geometry is three-dimensional. Specifically, three normal strain rates are allowed to differ and vorticity can be applied. Furthermore, the RFM does not use a nozzle-counterflow as many opposed-flow flame solvers do. At infinity, we take a potential counterflow which removes the imposition of zero velocity gradients at a fixed nozzle separation distance. Through the similarity solution, this three-dimensional geometry may be solved with ODEs.

3.4.2 Scalar Dissipation Rate and Mixture Fraction

Instead of strain rate, scalar dissipation rate (SDR), χ , is commonly used to classify extinction in flamelet modeling. Beginning with Eq. 3.41, conservation of mixture fraction Z , an ODE for SDR can be derived in terms of the similarity variable f and other quantities known once Eq. 3.31-3.35 have been solved. The resultant equation, Eq. 3.42, is a linear, homogeneous ODE with known boundary conditions when formulated in terms of the mixture

fraction which varies from 0 to 1.

$$\chi \equiv 2D \left(\frac{\partial Z}{\partial x_i} \right)^2 = 2D \left(\frac{dZ}{dy} \right)^2 \quad (3.40)$$

$$\rho u_y \frac{dZ}{dy} = \frac{d}{dy} \left(\rho D \frac{dZ}{dy} \right) \quad (3.41)$$

Multiplication by $2(dZ/dy)$ results in a first-order ODE for SDR.

$$\left[\frac{2f}{\rho D} + \frac{2}{\rho D} \frac{d(\rho D)}{dy} - \frac{1}{D} \frac{dD}{dy} \right] \chi + \frac{d\chi}{dy} = 0 \quad (3.42)$$

By defining C as the constant of integration in Eq. 3.42 and integrating, Eq. 3.43 is found for χ .

$$\chi = \frac{C}{\rho^2 D} \exp \left(-2 \int_0^\eta \frac{f}{\rho^2 D} d\eta' \right) \quad (3.43)$$

Replacing χ in Eq. 3.43 with $2D (dZ/dy)^2$ through the definition of SDR and integrating from $-\infty \rightarrow \infty$ in η -space such that Z varies from $0 \rightarrow 1$, allows C to be determined.

$$C = \frac{2}{\left(\int_{-\infty}^{\infty} \frac{1}{\rho^2 D} \exp \left[- \int_0^\eta \frac{f}{\rho^2 D} d\eta' \right] d\eta \right)^2} \quad (3.44)$$

3.4.3 Chemical Kinetics

As in Sec. 3.3, the skeletal version of the Foundational Fuel Chemistry Model 1.0 (FFCM-1) [127] for hydrogen-oxygen combustion was used to generate these results. This model also includes nitrogen as a non-reacting species for a total of nine species and 25 reactions. NOx formation is not considered.

3.4.4 Equal Transverse Strain Rates ($S_1 = S_2$)

The counterflow diffusion flame studied in the following sections uses oxygen (O_2) at 300 K issuing from $y = -\infty$ and an equimolar mixture of hydrogen (H_2) and nitrogen (N_2), also at 300 K, issuing from $y = +\infty$. The pressure is set at 10 atmospheres. Calculations were performed for three values of non-dimensional vorticity, $\omega = 0, 1, \sqrt{1.5}$, with $S_1 = S_2 = 1/2$ to simulate the existing flamelet models' assumption of axisymmetry. Note that our calculations are axisymmetric only when $S_1 = S_2 = 1/2$ and $\omega = 0$. When $\omega > 0$, vortex stretching implies non-symmetric behavior.

First, extinction curves, or S-curves, were calculated to determine the flammability limits at each value of ω . Figure 3.25a shows these extinction curves plotted in three ways from left to right: against the maximum SDR, χ_{max} , the ambient (i.e., inflow) axial strain rate at $y = +\infty$, S^* , and the maximum or local axial strain rate in the flame zone, S_{local}^* .

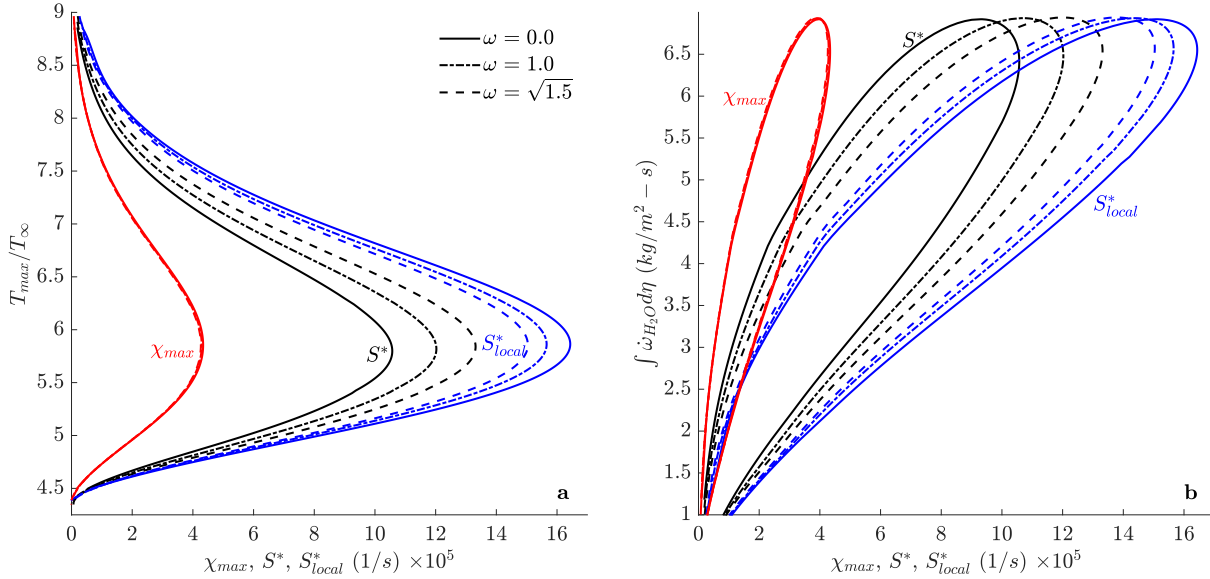


Figure 3.25: (a) Extinction curves in terms of maximum temperature; (b) Extinction curves in terms of heat release rate. Both sub-figures are plotted versus: maximum scalar dissipation rate, χ_{max} (red); ambient strain rate, S^* (black); maximum local strain rate, S_{local}^* (blue).

The black curves show a substantial impact of vorticity on the extinction ambient strain

rate of the flames with a 26% increase occurring between $\omega = 0 \rightarrow \sqrt{1.5}$. When local maximum strain rate is used on the abscissa (blue curves), those with $\omega \neq 0$ fall to the left of those with $\omega = 0$ because vorticity-induced changes to the velocity field decrease local strain rate with increasing vorticity. Since the temperature at the extinction point is nearly unchanged by vorticity, those curves with decreased local strain rate fall to the right with increasing vorticity when plotted against the inflow strain rate. When the S-curve is plotted versus maximum SDR, a near-total collapse occurs, although the order of curves follows those versus maximum local strain rate. Figure 3.25b plots the integrated burning rate of water (H_2O) along the S-curves in Fig. 3.25a. Again, the solution is highly dependent on vorticity magnitude when plotted versus S^* and S_{local}^* and significantly collapses versus χ_{max} . Actually, maximum temperature is a better predictor than SDR to capture “collapse”. From Fig. 3.25, we see that one value of ω together with one value of S^* , S_{local}^* , or χ_{max} determines two values of T_{max} and H_2O production rate. However, one value of T_{max} with one value of ω gives distinct values for S^* , S_{local}^* , χ_{max} , and H_2O production rate.

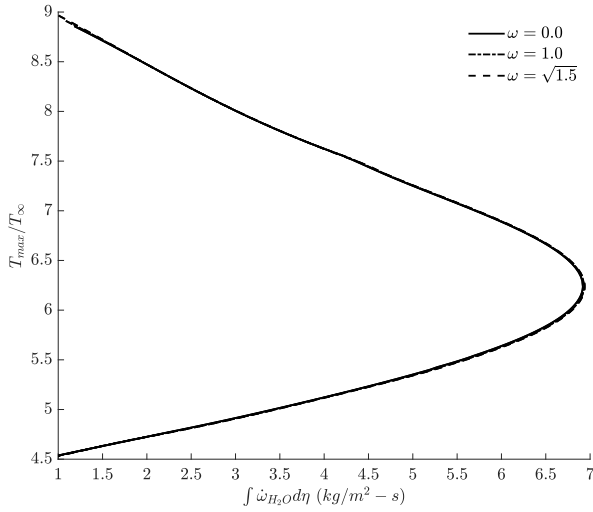


Figure 3.26: Temperature versus integrated H_2O burning rate.

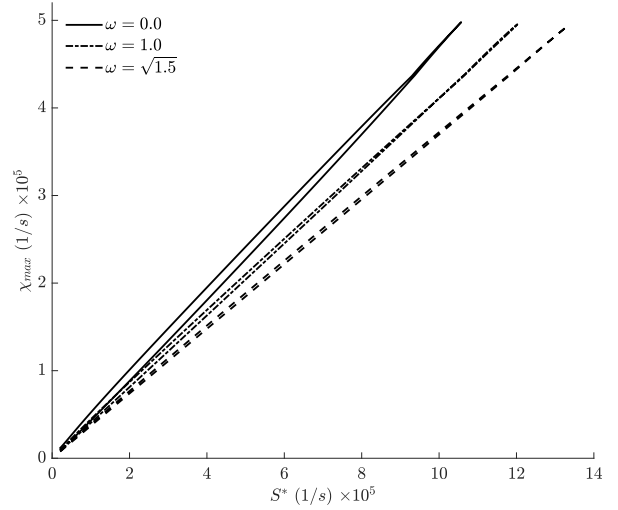


Figure 3.27: SDR versus Ambient Strain Rate.

Many flamelet approaches include only the stable branch of the S-curve. This is a viable tactic in some scenarios and simplifies computation by requiring only SDR or, in our case,

strain rate and vorticity. If one wants to use the unstable branch as well, which more accurately captures extinction, reignition, pressure oscillation, and other unsteady effects [106], an additional parameter is necessary to distinguish the branches, such as the progress variable or maximum temperature.

If output parameters are plotted versus output parameters, curves with varying vorticities collapse; see Fig. 3.25 (red) and Fig. 3.26. However, no output parameters plotted versus the two input parameters, S^* and ω , collapse; see Fig. 3.25 (black, blue) and Fig. 3.27. Obviously, integrated production rate versus maximum temperature would collapse if plotted. It is not surprising that one output plotted against another output collapses. This collapse results from the system having several input parameters, two of which (S^* and ω) similarly alter behavior. It is the reciprocal strain rate in the flame zone, i.e., residence time, that predominantly affects combustion intensity. All things being equal, an increase in S^* increases flame zone strain rate, decreasing residence time while an increase in ω does the opposite. It is just as reasonable to create a flamelet theory using maximum temperature as the primary parameter as it is to make maximum SDR (or stoichiometric SDR) the primary parameter. Temperature, in fact, was used by Knudsen and Pitsch [146] as the unique parameter is distinguishing between non-premixed flamelet solutions in the creation of a flame index for a multi-regime flamelet model. Earlier, Peters [1] used temperature to define the progress variable for premixed combustion. Maximum temperature, maximum SDR, and integrated production rate are all outputs dependent on vorticity and applied strain rate. The scaling of any of these output parameters given resolved-scale quantities is undetermined following first principles; rather, some contrivance such as a progress variable and an assumed functional form of $\chi(Z)$ is required. However, scaling rules can be found for applied strain rate and vorticity, so, we hypothesize that utilizing such rules may provide a more robust coupling procedure between sub-scale and resolved scale quantities, as done in Sec. 5.1.

The tendency of curves to collapse might at first appear convenient, allowing solutions to

be parameterized by χ_{max} instead of S^* and ω , and indeed if only stable branch solutions are considered, and one is willing to bypass direct solution of the momentum and continuity equations by assuming some $\chi(Z)$, χ_{max} is adequate; however, some issues persist. First, as discussed in Chap. 2, recent flamelet approaches utilizing a transformation to 3D mixture fraction space are exact with respect to their pre-transformed equations, however, any flaw in the pre-transformed equations or in the assumption of variables in the post-transformed equations will cause a deviation from the real physics. In the flamelet form, i.e., Eqs. 2.25-2.28, the effects of the momentum and continuity equations are contained in scalar dissipation rate, χ . That is okay provided the χ used to solve Eqs. 2.25-2.28 came from physically complete conservation equations. The vast majority of existing models, even the most current, while having a correct “flamelet equation” in terms of χ then inject some sort of assumed Gaussian variance for $\chi(Z)$ which neglects vorticity, and sometimes variable density, in the momentum equation. Secondly, at the fundamental level as a physically meaningful parameter, SDR precludes preferential (unequal Lewis numbers) and differential (non-unitary Lewis numbers) diffusion [147] since its definition stipulates a common diffusivity among all species. Incorporating detailed transport allows species and heat to locally re-distribute which notably impacts laminar flames [79, 80, 86, 88]. Corrections to models assuming constant Lewis number can be made to better capture the tendencies of differential diffusion [81–83, 85, 88], but it becomes difficult to create a useful and clearly understood conserved scalar. An alternate approach, governing a conserved scalar with a transport equation in which the diffusivity is equal to the thermal diffusivity but differs from the species diffusivity, was introduced by Pitsch and Peters [83]. Although it is named the “mixture fraction,” it differs from the classical definition and has diminished physical meaning. A complicated set of differential equations are yielded, resulting in a SDR with unclear physical interpretation and thus the problem of coupling it to the resolved scale via a “first principles” method persists. These improvements to existing flamelet models clearly show the importance of differential diffusion. Present flamelet theory, including differential and preferential diffusion,

for example Jiang et al. [88], are definite improvements on the classical theory. Therefore, differential and preferential diffusion alone, are not the major improvements pursued here. Rather it is the accrument of underlying assumptions, not all of which have been relaxed, which inspired the RFM. It is not based on existing models and is constructed from the ground up with no constraints on Lewis number, geometry, velocity derivatives, or thermo-physical relations. We hypothesize that the RFM will yield an improvement in the context of RANS and LES because it addresses previously excluded physics.

Furthermore, in application of a flamelet model to turbulent combustion, the cascades of length, velocity, and velocity derivatives (strain rate and vorticity) are much better understood than the cascades of scalar gradients [130]. Therefore, we believe it is worth investigating whether parameterizing flamelet solutions with strain rate and vorticity may improve accuracy in RANS and LES. It is noteworthy, however, that employing strain rate and vorticity adds an additional matrix parameter and is thus more computationally expensive. Also note that like SDR, strain rate and vorticity cannot distinguish the stable from the unstable branch. In lieu of an unsteady formulation, we think temperature may be the best “trigger” to differentiate between the stable reacting, and stable non-reacting branches.

The importance of solving the momentum equations with vorticity is illustrated in Fig. 3.28. Although the velocity curves have the same ambient strain rate, $S^* = 903,500$ 1/s, their slopes and magnitudes differ as a result of mass efflux changes caused by the centrifugal action of vorticity coupled with the density gradients throughout the counterflow. With vorticity, the lighter fluid (products of combustion) tends to flow outward aligned with the vorticity axis as this direction does not experience centrifugal force. The denser fluid is thrown outward in the plane normal to the vorticity axis, counteracting the incoming pressure gradient. This results in a lower strain rate at the stagnation point, and thus increased residence time, which is responsible for increased temperatures on the stable branch. Unlike temperature, SDR decreases as vorticity increases because the lower velocity gradients cause

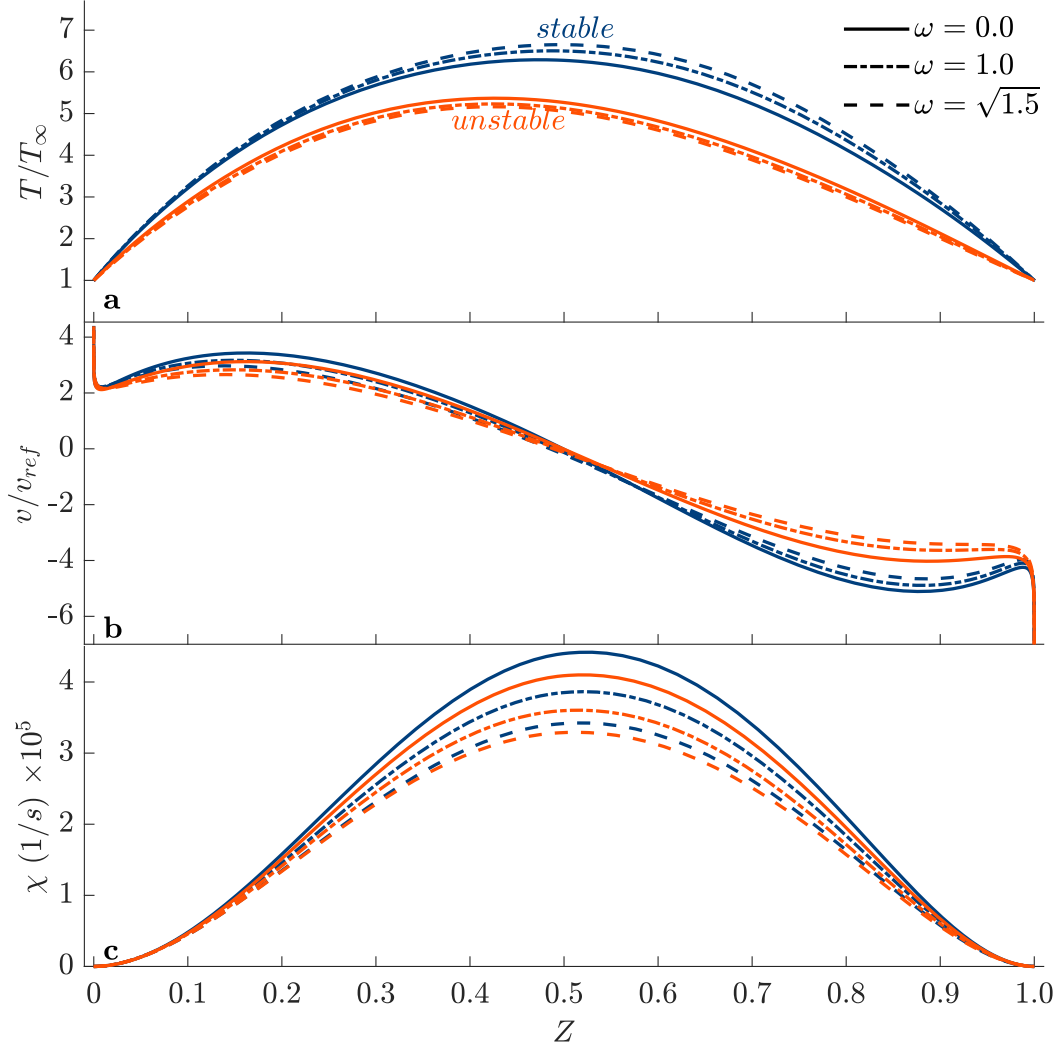


Figure 3.28: (a) Temperature versus mixture fraction; (b) Axial velocity versus mixture fraction; (c) Scalar dissipation rate versus mixture fraction. Stable branch (navy); unstable branch (orange). $S^* = 903, 500$ 1/s.

lower mixture fraction gradients. This result, shown in Fig. 3.28c, clearly indicates that vorticity must be considered to accurately determine SDR. The existing progress variable method relies on taking scalar values at the point of stoichiometric mixture fraction to define the progress variable and parameterize the S-curve [77]. These scalars are typically weighted mass fractions and SDR. It is shown here that such values depend on ω and S^* and may therefore benefit by not being characterized by one progress variable. In the case that all mass diffusivities are equal to each other but not equal to thermal diffusivity, i.e., $Le \neq 1$, another term appears in the scalar transport equations and thus an additional parameter

is needed to classify solutions. Even if the assumptions involved in deriving Eq. 2.25 were inconsequential (which they are not), the issue of coupling the flamelet solutions to the resolved flow via established scaling laws remains.

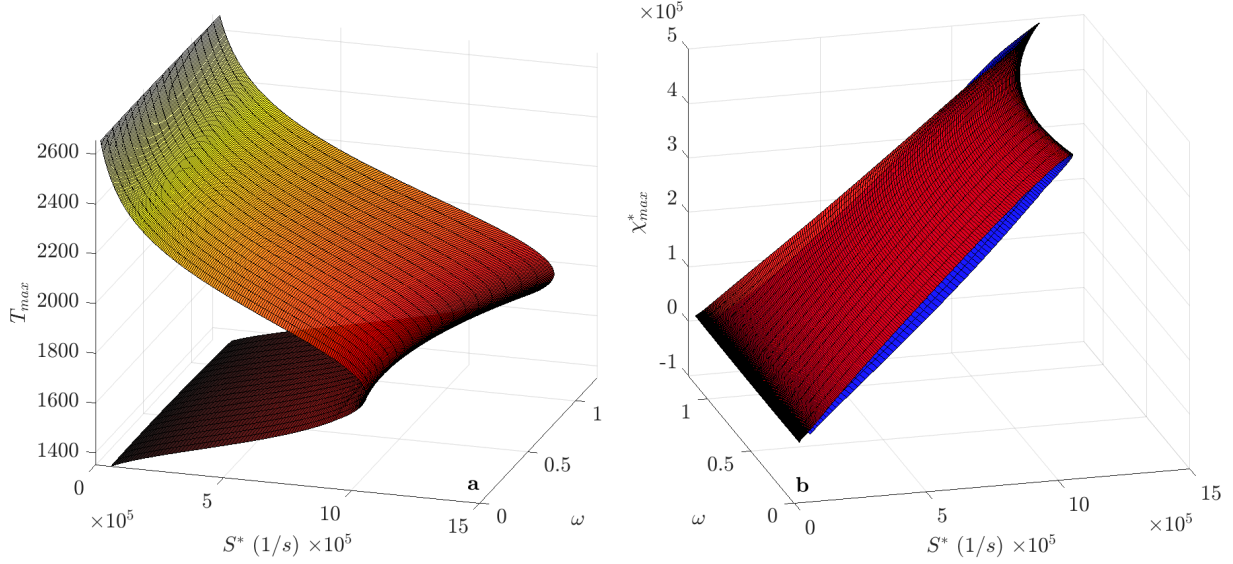


Figure 3.29: (a) Three-dimensional extinction surface; (b) Three-dimensional SDR surface. Sub-figure (a) temperature color-code from coldest to hottest (dark red $\rightarrow$ red $\rightarrow$ orange $\rightarrow$ yellow); Sub-figure (b) stable/unstable branch color code (stable: red; unstable: blue).

With a range of vorticity magnitudes, a three-dimensional surface can be created giving any output parameter as a function of the two input parameters, ω and S^* . Figure 3.29 shows two representations of these surfaces for maximum temperature and scalar dissipation rate by parabolic fitting of the three vorticity cases; $\omega = 0, 1, \sqrt{1.5}$. If viewed in the T_{max} - S^* plane, Fig. 3.29a appears as the black curves in Fig. 3.25a and Fig. 3.29b appears as Fig. 3.27. These surface plots are given to illustrate the three-dimensional character of the RFM solutions. Due to convergence difficulty near the extinction limit, the data in Fig. 3.25-3.27 and Fig. 3.29-3.31 has been post-processed to smooth transitions between the branches. The associated error with these curve fits is less than 0.5%.

3.4.5 Unequal Transverse Strain Rates ($S_1 \neq S_2$) and Non-constant Lewis Numbers

The broader theory outlined in this manuscript is not limited to the assumption of unitary Lewis number or even constant Lewis number. The Fickian diffusion formulation assumed previously can be replaced by the mixture-averaged or multicomponent diffusion formulation, as was done by Hellwig et al. [98], shown in Sec. 3.3. These are more accurate diffusion models in which the diffusivities for different species are unique and diffusion velocity depends on the gradients of multiple species. Both diffusion formulations are built on standard kinetic theory, although simplifying ad hoc assumptions are made in the mixture-averaged form. Using a multicomponent or mixture-averaged diffusion formulation allows preferential and

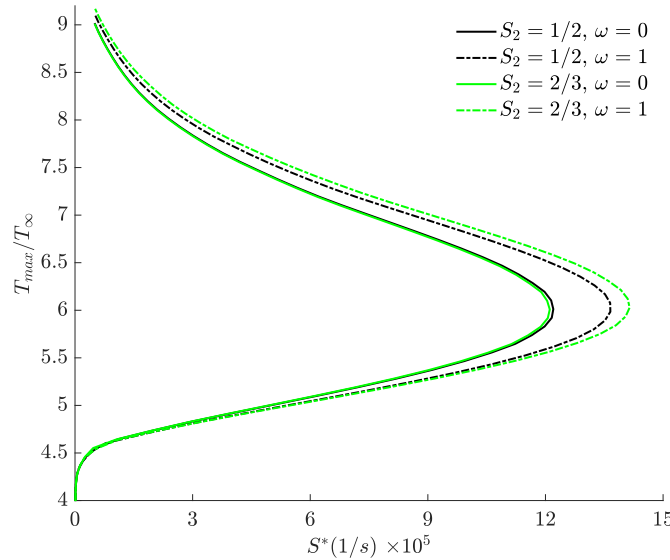


Figure 3.30: S-curves using multicomponent diffusion with transverse ambient strain rate variation.

differential diffusion which breaks two commonly used assumptions in many flamelet theories: first, scalar dissipation rate is no longer clearly defined since the mass diffusivities of each species are different; secondly, counter-gradient diffusion becomes a possibility, especially if high molecular weight fuels are considered. In this case, the mixture fraction will not vary monotonically between the oxidizer and fuel inflows which prevents the traditional method

of solving the problem in mixture fraction space with an assumed profile for $\chi(Z)$.

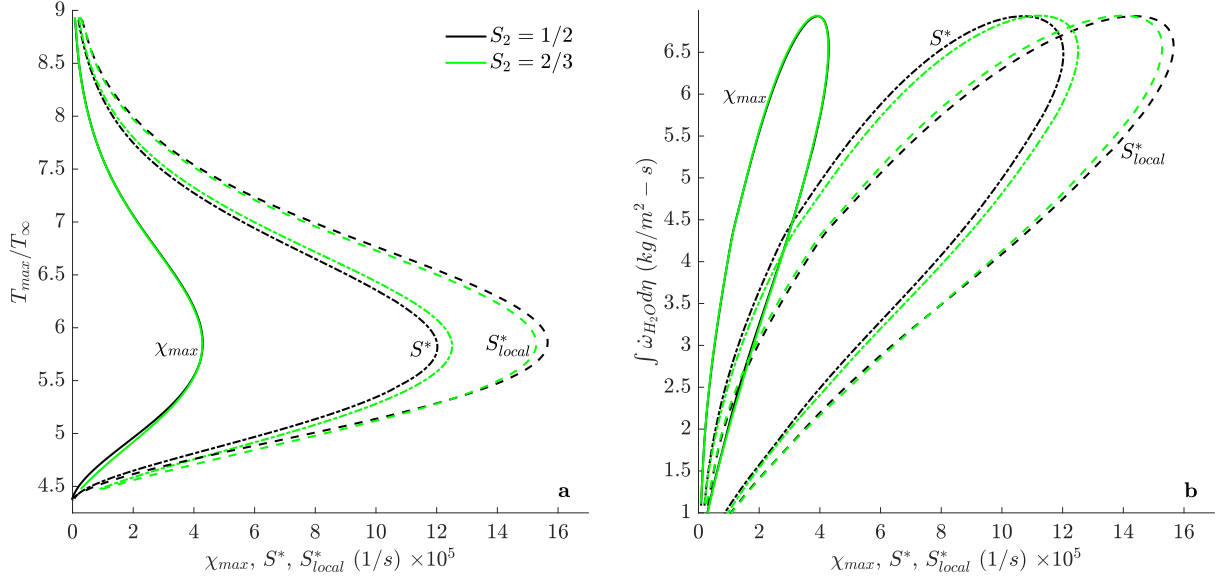


Figure 3.31: (a) Extinction curves in terms of maximum temperature; (b) Extinction curves in terms of heat release rate. Both sub-figures are plotted versus: maximum scalar dissipation rate, χ_{max} ; ambient strain rate, S^* ; maximum local strain rate, S_{local}^* . Vorticity is constant at $\omega = 1$ for all curves. $S_1 = 1/2, 1/3$, $S_2 = 1/2, 2/3$.

The data for Fig. 3.30 is taken from Hellwig [98] and shows S-curves similar to Fig. 3.25a for $S_1 = S_2 = 1/2$ and $S_1 = 1/3$, $S_2 = 2/3$ using multicomponent diffusion. Of course, SDR does not appear on the abscissa since it is now undefined. Figure 3.31 shows a repeat of certain data in Fig. 3.25 ($Le = 1$); however, vorticity is fixed at $\omega = 1$, while S_1 and S_2 vary. Here again, $S_1 = S_2 = 1/2$ and $S_1 = 1/3$, $S_2 = 2/3$. These figures illustrate three points. First, the qualitative impact of vorticity on extinction limits is common among constant and variable Lewis number formulations. Secondly, the three-dimensional character of the inflows (magnitudes of S_1 and S_2) alters the extinction limits. With vorticity, a higher transverse strain rate aligned with the vorticity vector, S_2 , yields a more stable flame for a given ambient compressive strain rate, S^* . This occurs because vorticity favors expulsion of low-density fluid outward in the direction unimpacted by centrifugal force, i.e., the direction with which S_2 and ω are aligned. Third, the diffusion formulation impacts the extinction limit. Because H_2 has a high diffusivity, imposing $Le = 1$ limits its ability to diffuse into

the oxidizer, thus the extinction limit in Fig. 3.30 (dash-dot black) is 12.5% higher than the extinction limit in Fig. 3.31a (dash-dot black).

Table 3.4: Output variables at constant transverse strain rates, S_1^*

ω	S_1, S_2	S^* (1/s)	$S_1 S^*$ (1/s)	T_{max} (K)	$\int \dot{\omega}_{H_2O} d\eta$ (kg/m ² s)	χ_{max} (1/s)
0	1/2, 1/2	660,000	330,000	2010.5	6.4088	332,350
0	1/3, 2/3	1,000,000	330,000	1817.1	6.8295	483,980
1	1/2, 1/2	800,000	400,000	1996.0	6.5094	344,740
1	1/3, 2/3	1,200,000	400,000	1813.2	6.8434	482,590

The original non-premixed flamelet formulation, using SDR as formulated by Peters [8], applies a constant transverse strain rate in the x direction. This strain rate corresponds to our S_1 only at $x = +\infty$ since our transverse strain rates vary with their respective axes and with y . Nevertheless, if two cases are compared in which the transverse strain rate in the x directions are equal at ∞ , that is $S_1 S^*$ is the same value for two cases, we find peak temperatures differ by $\sim 10\%$, burning rates differ by $\sim 5\text{-}6\%$, and maximum SDR differs by $\sim 40\text{-}45\%$ as shown in Table 3.4. Thus, it is clear that the assumptions of constant strain rates and potential flow omit certain physical behaviors that are possible to capture and should be captured.

3.4.6 Summary of Findings for Multi-step Chemical Kinetics with Fickian Diffusion

The analysis is built on two hypotheses. First, the flamelet field within the counterflow is determined by the ambient scalar and velocity fields of the two incoming flows. This hypothesis is supported by the analytical results which show that the scalar properties, normal strain rates, and vorticity are influential parameters. To be precise, enstrophy (ω^{*2}) is the parameter that appears in the analysis. Second, it is believed that these ambient properties are better suited for scaling relations with a mean or resolved flow in a turbulent

combustion analysis because they allow the sub-grid flamelet equations to determine the flame-local qualities of the reaction zone.

Depending on these inflow conditions, the analysis shows particular three-dimensional spatial variations through the counterflow for the velocity and one-dimensional variation for the scalar properties, e.g., temperature, mass fractions, and SDR. Both a stable branch and an unstable branch are described with different property variations. Thus, two different spatial profiles and values of maximum temperature and integrated burning rate can appear for the same set of ambient conditions. However, nearly the same maximum scalar dissipation rate and the same maximum local strain rate or integrated burning rate can appear on both branches. The maximum temperature is a more distinctive single parameter in distinguishing between the two branches.

For a given set of input parameters, the introduction of vorticity and varying transverse strain rates significantly changes the velocity profiles and scalar gradients within the domain. Furthermore, the ambient strain rate at which the flame extinguishes can increase by as much as 26% by vorticity for these scalar boundary conditions. Existing flamelet theories, e.g., [1, 83, 148, 149] and many others, avoid using vorticity and ambient inflow normal strain rates as input parameters. Instead, local conditions in the flame are used for input to the analysis. Specifically, the mixture fraction and SDR are used to identify all characteristics of the flame.

The identification of maximum SDR (usually assumed as a Gaussian variation) is claimed to allow identification of the important flame characteristics including production rate and maximum temperature in many existing flamelet models. While results show that the impacts of applied strain rates and vorticity are somewhat captured by maximum SDR, they also show that SDR and local strain rate depend strongly on vorticity and ambient inflow strain rate, including how strain rate distributes in a three-dimensional counterflow structure. Thus, SDR cannot be used to distinguish between all possible flamelet solutions of varying global

inputs (S^* and ω) as multiple solutions appear the same under the guise of SDR. While the local flame structures may be quite similar, the ambient velocity derivatives for the incoming flows strongly impact the coupling procedure we pursue and are significantly different from each other. For this reason, it is necessary to differentiate solutions that are locally similar but vary in the far-field. In addition, there is little literature that can guide the scaling of scalar gradients or SDR from RANS or LES to the sub-grid scale of the flamelet. SDR (as commonly constructed) is essentially impossible to scale because it asymptotes to zero outside the flamelet. The scaling of vorticity or ambient (inflow) strain rate in turbulent flows is better understood and even is discussed in textbooks [2, 125, 130, 131]. Finally, the use of SDR in flow media with preferential and differential diffusion is somewhat artificial and controversial. It is clear that a method relying on the scaling of inflow conditions for vorticity and normal strain rate is sound in its analytical foundations and in its ability to apply with models using more detailed transport; however, any realized improvements consequential of the former point remain to be seen.

Ultimately, the impacts of vorticity, transverse strain rates, and the authors decision to parameterize the flamelet solutions via scaled velocity derivatives, will be realized when the flamelet model is used in RANS and LES simulations and compared to CFD using other flamelet models and experiments. As of the time this portion of the research was conducted, implementation of the RFM in CFD simulations had not yet been done but is being pursued.

Chapter 4

Numerical Methods

This section gives an overview of the numerical methods and software used to generate the flamelet solutions presented throughout this dissertation. The original version of the RFM code used by Sirignano [94–96] was a simplified explicit pseudo-time stepping method. The small time scales of chemical reactions make the overall combustion problem very stiff, even with one-step kinetics. This means that explicit pseudo-time stepping methods require very small time steps to be stable, and thus a very large number of iterations to converge. The inclusion of detailed chemical kinetics introduces even smaller time scales, further reducing the maximum allowable Δt . This issue is an inconvenience when only one (or a few) flamelet solutions must be computed but becomes a debilitating problem for the model when hundreds or thousands of solutions must be generated to create a flamelet table. Therefore, other approaches have been incorporated and developed to drastically increase the convergence rate and improve numerical stability.

4.1 Use of Cantera

Multi-step chemical kinetics and detailed transport formulations were added to the RFM using Cantera sub-routines. This was the first core improvement to the RFM. Cantera [150], is an open-source toolbox for chemical kinetics, thermodynamics, and transport physics. Cantera allows users to load CHEMKIN-style chemical kinetics models, transport, and thermodynamics data files (“chmech”, “trans.dat”, “therm.dat”), or Cantera-style “.yaml” files (which conglomerate the three former file types) and will compute all thermodynamic properties, reaction rates, and transport coefficients given a gas state. The gas state is set using a temperature or enthalpy, pressure, and composition, all of which can be specified in various forms and using different units. An example of initializing a chemical kinetic mechanism and setting the gas state in the RFM using Cantera is shown in Fig. 4.1a. Once the gas state is set, users can call any desired property as shown in Fig. 4.1b.

```
model = 'FFCMy-CH4-12sp.yaml';
specify = 'gas';
transport = 'Multi';
gas = Solution(model,specify,transport);
set(gas,'T',T0(i),'P',P,'Y',Y0(:,i))
W = molecularWeights(gas)./1000;
R = gasconstant/1000;
```

(a) Example of initializing a chemical kinetics mechanism called “FFCMy-CH4-12sp.yaml” in Cantera and specifying that the object “gas” is a solution of this mechanism file in gas phase using multicomponent transport. Next, the thermodynamic state of “gas” is set by specifying temperature, pressure, and a vector of mass fractions. The vector of molecular weights is called from the gas object and the gas constant (a built-in Cantera property) is set to R.

```
rho(i)      = density(gas);
lam(i)      = thermalConductivity(gas);
cp_m(:,i)   = cp_R(gas)*R./W;
cp(i)       = cp_mass(gas);
mu(i)       = viscosity(gas);
om(:,i)     = ((netProdRates(gas).*W)*1000)/rho(i);
hm0(:,i)    = (enthalpies_RT(gas)./W)*R*T0(i);
Dmj(:, :, i) = multiDiffCoeffs(gas);
```

(b) Example of calling transport and chemical kinetics properties from Cantera once the gas object is set. Here the density, thermal conductivity, specific heats of each species, specific heat of the mixture, dynamic viscosity, net reaction rate of each species, total enthalpy, and multicomponent transport coefficients are called. These are the most common calls in the RFM code although Cantera is capable of many others.

Figure 4.1: Example of Cantera usage in the RFM through the MATLAB interface.

Cantera allows the user to include arbitrarily complex chemical kinetics mechanisms. However, due to the high volume of flamelet solutions which must be generated, the present work will generally employ reduced-order mechanisms to avoid exceedingly long computation times, especially for heavy hydrocarbon fuels.

Similar to CHEMKIN, Cantera includes various fluid-chemistry solvers, one of which is a nozzle-based counterflow diffusion flame called “diff flame”. The “diff flame” solver was used in Sec. 3.3 to compare with the RFM for an axisymmetric configuration without vorticity, i.e., $S_1 = S_2 = 0.5$, $\omega = 0$. However, all other results presented in this dissertation do not use the Cantera or CHEMKIN counterflow diffusion flame solvers because they are nozzle-based counterflows which force asymptotic axial strain rate to zero, negating a core tenet of the RFM. The RFM and its coupling procedure stipulate that the asymptotic axial strain rate in the counterflow is imposed by the turbulent field and is therefore of high magnitude and practically never zero.

4.2 Necessity for Fast Computations - Hybrid Scheme

On small turbulent scales within a combustor, a plethora of different conditions exist; neither temperature nor mixture are uniform within the combustor domain and velocity derivatives vary in magnitude. All of these properties impact flame extinction, heat release rate, and chemical production rates, which must be solved to close the global CFD equations. When multi-step chemical kinetic mechanisms or models are used, the number of necessary computations becomes computationally unfathomable to perform “online”, i.e., during the LES or RANS computation. Thus, creating a flamelet table, which is a large collection of flamelet solutions calculated “offline”, provides a significant saving in computational cost.

For a given set of scalar boundary conditions, many flamelet solutions exist because the ambient strain rates vary; together, they form an S-curve. Different S-curves are produced for different scalar boundary conditions, and thus the flamelet table representing all inflow mixtures is a collection of many S-curves. Two approaches are possible in terms of the flamelet scalar boundary conditions:

- The existing and simplest approach is to set the flamelet boundary conditions equal to the global-scale boundary conditions and assume *the turbulent flame samples the internal structure of a single canonical counterflow diffusion flame under various strain rates*. This method enforces the same scalar boundary conditions on all flamelets and thus requires at least an order of magnitude fewer flamelets than the following method. The coupling procedure for this approach uses the β -PDF convolution outlined in Section 2.4.2.
- The novel approach conceptualized in this dissertation is to allow the resolved-scale mixture, thermodynamic state, and TKE dissipation in a given cell to inform the boundary conditions for the flamelet in that cell. This method better respects the sub-scale physics but involves $O(10) - O(100)$ more flamelet calculations to form the table. The flamelet table dimension is also larger because the scalar boundary conditions vary. This method is further discussed in Section 5.3.

In either case, each S-curve may have $O(50) - O(100)$ flamelet solutions, and thus the flamelet table will have hundreds to tens-of-thousands of flamelet solutions depending on the scalar boundary condition method and whether or not flamelets must be calculated for varying pressure. Thus, creating the table involves solving a very large number of counterflow flames, under a variety of conditions, such that the flamelet table breadth is adequate to cover the range of possible flow conditions. However, once the table exists, it can be used for any set of global boundary conditions (provided the propellants do not change), which enables design engineers to more efficiently calculate solutions to varying combustor geometries. Note that the dimension of the flamelet table in the classical formalism is much smaller because it was assumed that the inflow mixtures to the counterflow had fixed compositions and temperatures. Allowing these to vary drastically increases the number of flamelet solutions which must be solved.

With the high number of flamelet computations necessary to form the table, the solution of

each flamelet must be efficient. The RFM governing equations, Eqs. 3.8-3.11, are stiff, non-linear, coupled ODEs, consisting of two momentum equations, an energy equation, and n_{sp} or $n_{sp} - 1$ species conservation equations (where n_{sp} is the number of species), and an equation of state. Thus, an individual flamelet solution entails solving $n_{sp} + 3$ equations, usually over a grid of a few hundred (n) nodes, for a total of $N = n \times (n_{sp} + 3)$ dependent variables. The chemical kinetics model is the primary determinant of the number of equations, and thus reduced mechanisms are opted for in the interest of computation time.

Since the governing equations are both stiff and non-linear, Newton’s method is the favored computational scheme as it works with non-linear equations (many other implicit methods do not) and it is not bottlenecked by small time steps as explicit methods are. Newton’s method is an analytical technique which obtains successively better approximations to a function or set of functions. Starting from an initial guess, the derivative of the function(s) with respect to (w.r.t.) it’s dependent variable(s) are computed, which indicates the direction the solution must move such that future derivatives are closer to zero. Iterating this process produces a numerical method which solves for the solution to the governing equation(s), i.e., the dependent variable functions, provided the initial guess is within the realm of convergence of Newton’s method and the initial derivatives are non-zero. If the initial guess is poor or the initial derivatives are near-zero or zero, Newton’s method can become stuck in infinite loops. This caveat to the ability of Newton’s method to produce a physical, converged, solution necessitates the computation of a reasonably good initial guess. In the present work, this is achieved by first explicitly marching the solution in pseudo-time before handing it over to Newton’s method to quickly converge, as shown in Fig. 4.2. The coupling of a time-marching method with Newton’s method is referred to here as a “hybrid” scheme. Generally, the first flamelet in the S-curve is the only one which must be marched in pseudo-time because once it is converged, it is a sufficient initial guess for the second flamelet at a higher strain rate. Similarly, the second converged solution is a sufficient initial guess for the third flamelet, and so on and so forth. Fortunately, this means the slower, pseudo-time marching portion

of the hybrid scheme is used much less frequently than Newton's method.

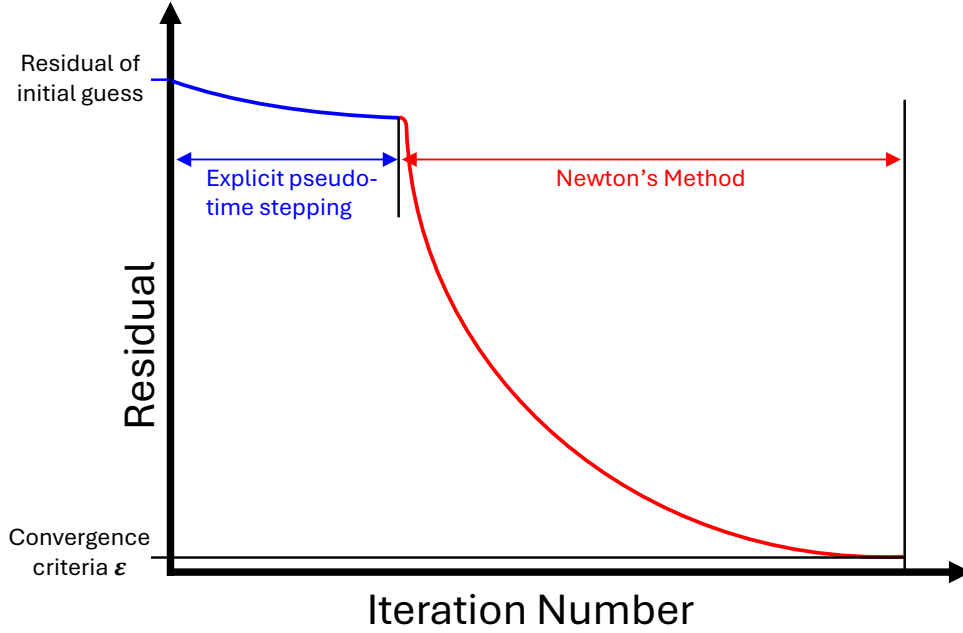


Figure 4.2: Pictorial representation of the hybrid method; explicit pseudo-time (blue) to Newton's method (red) in residual-iteration number space. Explicit marching occurs until a set pseudo-time is reached, after which Newton's method quickly iterates the solution until the convergence criteria is satisfied.

4.2.1 General Governing Equations

Over the years of development, the governing equations have gone through multiple iterations. Some have been dimensional while others were non-dimensional and different normalizations have been used. Overall, the following non-dimensional equations provided the most robust algorithm and are used in the latest version of the RFM code. These equations are shown below for Fickian and multicomponent diffusion.

The steady, three-dimensional RFM governing equations in the non-Newtonian reference frame are shown below. A Newtonian fluid is assumed invoking Stoke's hypothesis. The centrifugal acceleration vector in the momentum equation is $a_i = \langle \xi\omega^2/4, \chi\omega^2/4, 0 \rangle$.

$$\frac{\partial(\rho u_j)}{\partial x_j} = 0 \quad (4.1)$$

$$\rho u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} = \frac{\partial \tau_{ij}}{\partial x_j} + \rho a_i \quad ; \quad \tau_{ij} = -\frac{2}{3} \mu \delta_{ij} \frac{\partial u_k}{\partial x_k} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (4.2)$$

$$\frac{\partial}{\partial x_j} (\rho u_j h) + \frac{\partial}{\partial x_j} \sum_{m=1}^{n_{sp}} \rho v_{m,j} Y_m h_m = \frac{\partial}{\partial x_j} \left(\lambda \frac{\partial T}{\partial x_j} \right) - \rho \sum_{m=1}^{n_{sp}} h_{f,m} \dot{\omega}_m \quad (4.3)$$

$$\frac{\partial}{\partial x_j} (\rho Y_m u_j) + \frac{\partial}{\partial x_j} (\rho Y_m v_{m,j}) = \rho \dot{\omega}_m \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (4.4)$$

The RFM treats gas-phase mixtures obeying the ideal gas law and uses the low-Mach number approximation to simplify the energy equation. Additionally, viscous dissipation is assumed to be negligible in the energy equation. The quantities ρ , p , T , h , h_m , v_m , Y_m , λ , c_p , $c_{p,m}$, $h_{f,m}$, and $\dot{\omega}_m$ are density, pressure, temperature, mixture specific enthalpy, specific enthalpy of species m , diffusion velocity of species m , mass fraction of species m , mixture thermal conductivity, mixture specific heat, specific heat of species m , heat of formation of species m , and reaction rate of species m , respectively. The governing equations remain identical to Eqs. 4.1-4.4 when the normalizations shown in Table 4.1 are chosen. These choices are made to improve the Jacobian condition number during the numerical solution. The ambient compressive strain rate S^* is indicative of the fluid dynamic time scale and is used to non-dimensionalize the chemical reaction rate $\dot{\omega}_m$, thus, this non-dimensional ratio between the net effect of Arrhenius production/destruction rates and residence time thereby allows the input strain rate S^* to influence combustion intensity.

Using the similarity solution $u = S_1 \xi f'_1$, $v = -f/\rho$, $w = S_2 z f'_2$ with $f = S_1 f_1 + S_2 f_2$, the non-dimensional versions of Eqs. 4.1-4.4 can be reduced to the set of ordinary differential equations given by Eqs. 4.6-4.9. Here, the density-weighted Illingworth transformation from $\chi \rightarrow \eta$, i.e., $\eta \equiv \int_0^\chi \rho(\chi') d\chi'$, is made to simplify the ODEs. In the similarity variables

Table 4.1: Normalizations for dependent variables

Variable(s)	u_j, v_m	t	x_i	ρ	$h, h_m, h_{f,m}$	p
Normalization	$\sqrt{\frac{S^* \mu_\infty}{\rho_\infty}}$	S^{*-1}	$\sqrt{\frac{\mu_\infty}{\rho_\infty S^*}}$	ρ_∞	$c_{p_\infty} T_{\text{ref}}$	$S^* \mu_\infty$
Variable(s)	$\dot{\omega}_m$	μ	λ	c_p, c_{p_m}	ω	$T - T_{\text{ref}}$
Normalization	S^*	μ_∞	$\mu_\infty c_{p_\infty}$	c_{p_∞}	S^*	T_{ref}

and in Eqs. 4.6-4.9, the prime “ ’ ” indicates a derivative with respect to η . Even with non-dimensional variables, an energy equation using temperature T or sensible enthalpy h produces residuals orders of magnitude higher than the other governing equations; therefore, to aid convergence, T is replaced by θ , as defined in Eq. 4.5 with T_{ref} equal to a midpoint temperature between the maximum and minimum temperatures expected in the domain. Ideally, T_{ref} is chosen to minimize the order-of-magnitude variation for θ . For counterflow flames in which temperature varies approximately $300 \text{ K} \leq T \leq 3000 \text{ K}$, a non-dimensional temperature varies one order of magnitude while $-0.7 \leq \theta \leq 2$ remains $O(1)$. Total enthalpy is defined as $h_m^0 \equiv h_m + h_{f,m}$.

$$\theta = \frac{T - T_{\text{ref}}}{T_{\text{ref}}} \quad (4.5)$$

$$R_i^m = fY'_m - J'_m + \dot{\omega}_m \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (4.6)$$

$$R_i^{n_{sp}+1} = f\theta' + \frac{1}{c_p}(\rho\lambda\theta')' - \frac{1}{c_p}\theta' \sum_{m=1}^{n_{sp}} J_m c_{p_m} - \frac{1}{c_p} \sum_{m=1}^{n_{sp}} h_m^0 \dot{\omega}_m \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (4.7)$$

$$R_i^{n_{sp}+2} = ff_1'' + (\rho\mu f_1'')' + S_1 \left(\frac{1}{\rho} - (f_1')^2 \right) + \frac{\omega^2}{4S_1} \left(1 - \frac{1}{\rho} \right) \quad (4.8)$$

$$R_i^{n_{sp}+3} = ff_2'' + (\rho\mu f_2'')' + S_2 \left(\frac{1}{\rho} - (f_2')^2 \right) \quad (4.9)$$

Multiple forms of the mass diffusion velocity may be used. The RFM code is setup to use the multicomponent diffusion formulation or a constant Lewis number Fickian formulation. Soret effects can be included in the multicomponent formalism if desired. The two general diffusion velocity formulations are given below.

Multicomponent Diffusion	
$v_{m,j} = \frac{1}{X_m \bar{W}_{mix}} \sum_{n=1}^{n_{sp}} W_n D_{mn} \frac{dX_n}{dx_j} - \frac{D_m^T}{\rho Y_m T} \frac{dT}{dx_j} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad (4.10)$	
$v_{m,\eta} = \frac{\rho W_m}{\bar{W}_{mix}^2 Y_m} \sum_{n=1}^{n_{sp}} W_n D_{mn} \frac{dX_n}{d\eta} - \frac{D_m^T}{Y_m T} \frac{dT}{d\eta} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad (4.11)$	
$J_m \equiv \rho Y_m v_{m,\eta} = \frac{\rho^2 W_m}{\bar{W}_{mix}^2} \sum_{n=1}^{n_{sp}} W_n D_{mn} \frac{dX_n}{d\eta} - \frac{\rho D_m^T}{T} \frac{dT}{d\eta} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad (4.12)$	

Fickian Diffusion	
$V_{m,j} = -\frac{D}{Y_m} \frac{dY_m}{dx_j} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad ; \quad D \equiv \frac{1}{L_e} \frac{\lambda}{\rho c_p} \quad (4.13)$	
$V_{m,\eta} = -\frac{\rho D}{Y_m} \frac{dY_m}{d\eta} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad (4.14)$	
$J_m \equiv \rho Y_m v_{m,\eta} = -\rho^2 D \frac{dY_m}{d\eta} \quad ; \quad m = 1, 2, 3, \dots n_{sp} \quad (4.15)$	

In the above formulations, the mole and mass fractions are related according to Eq. 4.16.

$$X_m = \frac{\bar{W}_{mix}}{W_m} Y_m \quad ; \quad \bar{W}_{mix} \equiv \sum_{n=1}^{n_{sp}} X_n W_n \quad ; \quad m = 1, 2, 3, \dots, n_{sp} \quad (4.16)$$

Regardless of the diffusion velocity formulation, the boundary conditions for the governing equations, Eqs. 4.5-4.9 are given by Eqs. 4.17-4.20.

$$f'_1(-\infty) = \sqrt{\frac{1}{\rho_{-\infty}} + \left(\frac{\omega}{2S_1}\right)^2 \left(1 - \frac{1}{\rho_{-\infty}}\right)} \quad ; \quad f_1(0) = 0 \quad ; \quad f'_1(\infty) = 1 \quad (4.17)$$

$$f'_2(-\infty) = \frac{1}{\sqrt{\rho_{-\infty}}} \quad ; \quad f_2(0) = 0 \quad ; \quad f'_2(\infty) = 1 \quad (4.18)$$

$$\theta(-\infty) = \frac{T_{-\infty} - T_{ref}}{T_{ref}} \quad ; \quad \theta(\infty) = \frac{T_{\infty} - T_{ref}}{T_{ref}} \quad (4.19)$$

$$Y_m(-\infty) = Y_{m,-\infty} \quad ; \quad Y_m(\infty) = Y_{m,\infty} \quad (4.20)$$

4.2.2 Hybrid Scheme: Newton's Method + Backward Euler

To implement the hybrid scheme for a system of differential equations, we first define the vector of dependent variables over all grid points as U_j^k according to Eq. 4.21.

$$U_j^k = \left\langle \underbrace{Y_{1,1}, Y_{2,1}, \dots, Y_{n_{sp},1}, \theta_1, f'_{1,1}, f'_{2,1}, \dots}_{\text{dependent variables at grid point 1}}, \underbrace{Y_{1,n}, Y_{2,n}, \dots, Y_{n_{sp},n}, \theta_n, f'_{1,n}, f'_{2,n}}_{\text{dependent variables at grid point } n} \right\rangle^T, \quad (4.21)$$

The variables are ordered according to physical quantity and domain position as follows: mass fractions at first node, non-dimensional temperature at first node, first similarity variable at first node, second similarity variable at first node. The same order is then repeated for the second node and all nodes thereafter up to and including node n . The second index

on Y_m , f'_1 , and f'_2 , and the only index on θ , indicates the grid point (node). The subscript j on the solution vector indicates the solution number in order of increasing S^* ; i.e., $j = 1$, corresponds to the upper-most left point on the S-curve. The superscript k indicates the iteration number for a given j ; i.e., $k = 1$ is the initial guess for solution j while $k = 2$ is the solution at j after one iteration. When no superscript is written, U_j , refers to the converged j^{th} solution.

The governing equations, $R(U_j^k, S^*)$, are evaluated over all dependent variables at all grid points subject to a specified compressive strain rate S^* . Transverse strain rates S_1 and S_2 and vorticity ω are also specified. For a steady-state convergent solution, $R(U_j, S^*) = 0$; note that $R(U_j^k, S^*)$ is an $N \times 1$ ($n(n_{sp} + 3) \times 1$) vector of residuals with the same variable organization as U_j . At the beginning of the iteration loop, the dependent variable vector is guessed and the residuals will not equal zero; $R(U_j^1, S^*) = R(U_j^{guess}, S^*) \neq 0$.

Newton's method is derived by supposing $R(U_j^{k+1}, S^*) = 0$ for each iteration such that the Jacobian, as defined in Eq. 4.22 is calculable. Rearranging this equation yields an iterative method that marches $R(U_j^{k+1}, S^*) \rightarrow 0$.

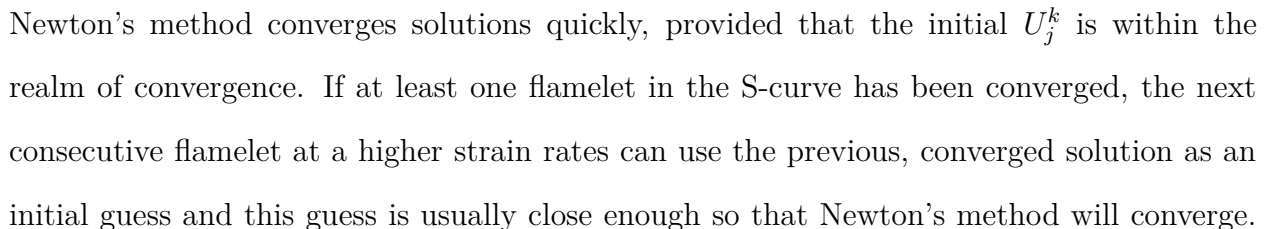
$$\frac{R(U_j^{k+1}, S^*) - R(U_j^k, S^*)}{U_j^{k+1} - U_j^k} = \frac{\partial R}{\partial U} \quad (4.22)$$

The Jacobian, is a sparse, block-tri-diagonal matrix using a three-point stencil. The upper left and bottom right corner blocks are $(n_{sp} + 3) \times (n_{sp} + 3)$ identity matrices due to Dirichlet boundary conditions on all dependent variables. Each entry in the Jacobian is the derivative of a governing equation at a specific grid point with respect to a dependent variable at a specific grid point (not necessarily the same grid point). Each block-row is indicative of the grid point of the numerator and each block-column is indicative of the grid point of the denominator. Since a three-point finite-difference stencil is used, the derivative of each governing equation is a function of variables at grid points: $i - 1$, i , and $i + 1$. Two methods

From the definition of the Jacobian in Eq. 4.22, Eq. 4.23 is obtained relating $R(U_j^k, S^*)$ to $R(U_j^{k+1}, S^*)$.

The unknown in Eq. 4.23 is the change in dependent variables, $\Delta U_j^k = (U_j^{k+1} - U_j^k)$, between consecutive iterations. Using these definitions, Eq. 4.23 is rewritten as the standard $\mathbf{A}\vec{x} = \vec{b}$ matrix equation, Eq. 4.24, which can be solved to calculate ΔU_j^k .

Starting from an unconverged solution vector, U_j^k at a fixed S^* , Eq. 4.24 is iterated via the process diagram below (Eq. 4.25) until a convergence criterion is met. Note that after one iteration, U_j^{k+1} becomes the input vector for the next iteration but S^* remains the same.



However, the initial guess for the very first flamelet in an S-curve is an extremely rough approximation to the flamelet, made out of sinusoids for the dependent variables. If Newton's method is used here, it will likely never converge. Thus, a pseudo-time marching scheme is helpful in changing a poor initial guess into one from which Newton's method can converge.

A pseudo-time marching algorithm is derived by replacing the RHS zeros of Eqs. 4.6-4.9 with pseudo-temporal derivatives of the dependent variables. This is shown in discrete form in Eq. 4.26. At steady-state, these temporal derivatives will go to zero. For the RHS of Eq. 4.26, the governing equations could be evaluated at U_j^k or U_j^{k+1} . The former will produce an explicit method that shows how the flamelet would progress in time toward a steady state. Doing so requires extremely small time steps to resolve the stiffness associated with the chemical kinetics. The latter will produce an implicit method that allows for much larger time steps and is preferred here because we are only interested in the steady state.

$$\frac{U_j^{k+1} - U_j^k}{\Delta t} = R(U_j^{k+1}, S^*) \quad (4.26)$$

Equation 4.23 is substituted into Eq. 4.26 producing Eq. 4.27.

$$\frac{U_j^{k+1} - U_j^k}{\Delta t} = R(U_j^k, S^*) + \frac{\partial R}{\partial U} (U_j^{k+1} - U_j^k) \quad (4.27)$$

Finally, Eq. 4.27 can be arranged as Eq. 4.28 where I is the identity matrix. This is essentially the same equation as Eq. 4.24; however, the main diagonal of the Jacobian is smaller by $I/\Delta t$. This is the general form of the hybrid Newton's method/backward Euler scheme for fixed S^* .

$$\left[\frac{\partial R}{\partial U} - \frac{I}{\Delta t} \right] \Delta U_j^k = -R(U_j^k, S^*) \quad (4.28)$$

4.3 Pseudo-arclength Continuation

Flamelet S-curves are characterized by three-branches: a stable branch beginning from the upper left point on the $T_{max} - S^*$ plane and extending to the flammability limit (location of infinite slope), an unstable branch beginning from the flammability limit and extending leftwards to low S^* , and finally another stable non-reacting branch beginning from the end of the unstable branch and extending rightward indefinitely. Together, these three branches form an S-shaped curve that consists of individual counterflow flamelet solutions. In practice, the non-reacting branch usually does not need to be computed because the solutions produce negligible heat and thus can be treated as zeros for the feedback to the resolved scale.

The numerical challenge is to compute the reacting stable and unstable branches efficiently and accurately. For each flamelet along the S-curve, the computation time is minimized if the initial guess is close to the final solution. Near the flammability limit, the Jacobian matrix becomes ill-conditioned and ultimately singular because the solution lies at a saddle-node bifurcation. Here $dU/dS^* \rightarrow \infty$ which causes $\partial R/\partial U$ to have a non-trivial nullspace, making $J = \partial R/\partial U$ singular. To address this, pseudo-arclength continuation is used to create accurate initial guesses and properly navigate the flammability “corners”. Pseudo-arclength continuation treats the strain rate S^* as an additional dependent variable to be solved along with the vector of field variables, U_j . As such, a constraint equation is added to the residual vector, R , that the strain rate must satisfy. The extra equation results in an additional row and column of the Jacobian matrix which allows it to be inverted even at the flammability limit.

In the pseudo-arclength formulation, the reciprocal strain rate, $\lambda = 1/S^*$, is used as the dependent variable because the solution varies more smoothly over λ than S^* . A smoother variation in the solution space aids in numerical stability. The augmented solution vector is given by Eq. 4.29. The first $N = n(n_{sp} + 3)$ elements of this vector are U_j^k from Eq. 4.21,

while the $[N + 1]^{th}$ element is λ_j^k .

$$Z_j^k = \left\langle \underbrace{Y_{1,1}, Y_{2,1}, \dots, Y_{n_{sp},1}, \theta_1, f'_{1,1}, f'_{2,1}, \dots}_{\text{dependent variables at grid point 1}}, \underbrace{Y_{1,n}, Y_{2,n}, \dots, Y_{n_{sp},n}, \theta_n, f'_{1,n}, f'_{2,n}}_{\text{dependent variables at grid point } n}, \overbrace{\lambda_j^k}^{\text{reciprocal strain rate } 1/S^*} \right\rangle^\top \quad (4.29)$$

The idea behind pseudo-arclength continuation is that once a few solutions are established, the next (unknown) solution can be expected to be roughly in-line with the tangent vector created by the existing solutions, provided the unknown solution is close to the most recent solution. The vector that points toward the location of the next solution is an $[N + 1] \times 1$ -dimensional tangent vector along the solution space, and is calculated from the two most recent solutions as shown in Eq. 4.30.

$$t_j = \frac{Z_{j-1} - Z_{j-2}}{\Delta s_{j-1}} \quad (4.30)$$

The “pseudo-arclength” between the two most recent solutions is given by Eq. 4.31 and thus the magnitude of t_j is unitary, making t_j a unit-tangent vector.

$$\Delta s_{j-1} = \sqrt{\sum_{i=1}^N (Z_{j-1} - Z_{j-2})^2} \quad (4.31)$$

Conveniently, the unit-tangent vector also happens to be the unit-normal vector of an $[N + 1] \times [N + 1]$ -dimensional hyperplane in the solution space. Any point, Z_j^k , on that hyperplane therefore satisfies the geometric constraint $t_j \cdot (Z_j^k - Z_j^0) = 0$ where Z_j^0 is the origin of the hyperplane which is a distance Δs_j away from Z_{j-1} along vector direction t_j . The constraint equation for each iteration in k is then Eq. 4.32.

$$R_s = t_j \cdot (Z_j^k - Z_j^0) \quad (4.32)$$

The initial guess of the solution is Z_j^0 and is given by Eq. 4.33 which is substituted into Eq. 4.32 to produce the final constraint equation, Eq. 4.34.

$$Z_j^0 = Z_{j-1} + t_j \Delta s_j \quad (4.33)$$

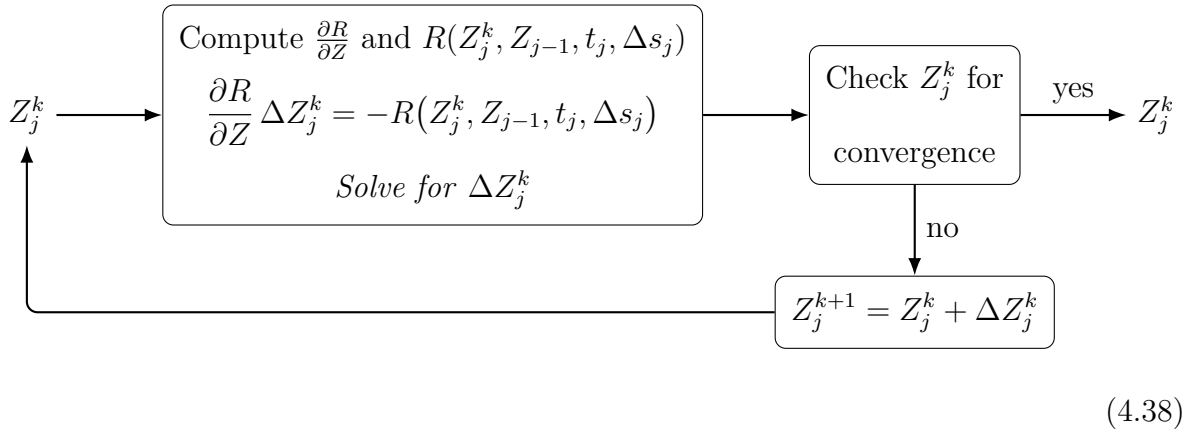
$$R_s(t_j, Z_j^k, Z_{j-1}, \Delta s_j) = t_j \cdot (Z_j^k - Z_{j-1} - t_j \Delta s_j) = t_j^\top (Z_j^k - Z_{j-1}) - \Delta s_j \quad (4.34)$$

Overall, the augmented system of equations for the pseudo-arclength continuation method is given by Eqs. 4.35-4.37. Given Z_{j-1} , t_j , and Δs_j , the process diagram is shown below in Eq. 4.38.

$$J_U = \left. \frac{\partial R}{\partial U} \right|_j^k \quad ; \quad J_\lambda = \left. \frac{\partial R}{\partial \lambda} \right|_j^k \quad (4.35)$$

$$t_U^\top = t_j^\top (1 : n(n_{sp} + 3)) \quad ; \quad t_\lambda = t_j (n(n_{sp} + 3) + 1) \quad (4.36)$$

$$\begin{bmatrix} J_U & J_\lambda \\ t_U^\top & t_\lambda^\top \end{bmatrix} \begin{bmatrix} \Delta U_j^k \\ \Delta \lambda_j^k \end{bmatrix} = - \begin{bmatrix} R(U_j^k, \lambda_j^k) \\ t_U^\top (U_j^k - U_{j-1}) + t_\lambda (\lambda_j^k - \lambda_{j-1}) - \Delta s_j \end{bmatrix} \quad (4.37)$$



Originally, a simpler version of the arc-length continuation procedure was pursued, following the work of Giovangigli and Smooke [151], Nishioka et al. [152], and Kee et al. [153,

pp. 709-711], in which the temperature at one or two specific grid points is set while the strain rate and other dependent variables adjust to satisfy the target temperature. However, this single- or dual point temperature-controlling method does not function well for the RFM because the stagnation point in the RFM is defined at a specific grid point. As S^* changes, flames, especially heavy hydrocarbon flames, shift from the oxidizer side toward the stagnation point, which results in non-monotonically decreasing temperatures, thus contradicting the arc-length constraint. Essentially, with the stagnation point fixed at $\eta = 0$, it is not possible to make an a priori choice as to which grid point will display monotonic behavior in temperature for a typical low-boundary-temperature non-premixed flame. Furthermore, with varying scalar boundary conditions, there are frequently no grid points at all which display such behavior, making single- or dual point temperature-control inadequately generalized. Therefore, following the method used by Qiao et al. [154] in determining bifurcation paths of a vortex stability problem, the high-dimensional pseudo-arclength continuation method presented above was developed for the RFM. This method forces all dependent variables at all grid points of solution Z_j to lie on an $(N + 1)$ -dimensional hyperplane which is normal to, and a distance Δs_j away from Z_{j-1} . Because this constraint considers directional changes of all variables, and is applied uniformly to the entire solution vector rather than to specific variables at specific points, the constraint holds whether or not the flames shift spatially and with or without a monotonic change in dependent variables. Regardless of the situation, the hyperplane constraint ensures that all variables are kept “in line” during the iteration process. It is therefore well-suited for any flame position with any set of scalar boundary conditions, including diffusion flames, partially-premixed flames, and triple flames, and has consistently worked well across the tested cases.

4.3.1 RFM Algorithm

So far, the governing equations and theory of the numerical method have been presented. This section details how the theory is implemented in the source code.

The decision tree for the algorithm is partially based on work by Dr. Joseph F. Grcar for the “TWOPT” boundary-value problem solver [155, 156]. Given an initial guess $U_{j=1}^{k=1}$, for the flamelet with the lowest S^* on the stable branch; e.g. the upper-most left point on the S-curve in Fig. 3.20a, the backward-Euler portion of the algorithm marches the solution in pseudo-time for a given number of time steps (PT_STEP0) to produce a reasonably good starting point for the damped Newton method. From this unconverged solution, Newton iteration attempts convergence. If Newton method fails at any step, the algorithm reverts to the pseudo-time marching scheme for a given number of steps (PT_STEP1), starting from the last solution which did not cause a failure, be it the solution Newton method began from or a subsequent successful Newton iteration. This pushes the solution into the realm in which Newton’s method can quickly converge. After the first solution $U_{j=1}$ has converged, the next solution at a higher S^* begins from an initial guess using the converged solution at $j = 1$; i.e., $U_{j=2}^{k=1} = U_{j=1}$. The $U_{j=3}$ solution is obtained in the same way from $U_{j=2}$.

Once three solutions have converged at consecutively higher S^* values, the algorithm switches to a high-dimensional pseudo-arclength continuation procedure in anticipation of the singular physical Jacobian matrix around the flammability limit. For the continuation procedure, λ_j^k becomes a dependent variable in the augmented solution vector given by Eq. 4.29.

Using the former three solutions, Z_{j-3} , Z_{j-2} , Z_{j-1} , two N -dimensional tangent vectors, t_{j-1} and t_j , are computed in addition to the curvature k_j of the solution space; here n , is the number of grid points, n_{sp} is the number of species, and $n_{sp} + 3$ is the number of dependent variables at each grid point.

$$\Delta s_{j-2} = \sqrt{\sum_{i=1}^N (Z_{j-2} - Z_{j-3})} \quad ; \quad \Delta s_{j-1} = \sqrt{\sum_{i=1}^N (Z_{j-1} - Z_{j-2})} \quad (4.39)$$

$$t_{j-1} = \frac{Z_{j-2} - Z_{j-3}}{\Delta s_{j-2}} \quad ; \quad t_j = \frac{Z_{j-1} - Z_{j-2}}{\Delta s_{j-1}} \quad (4.40)$$

From the Z_{j-1} solution, an initial guess Z_j^1 is formulated by extrapolating the current tangent vector t_j a distance Δs_j according to Eq. 4.41, where Δs_j is chosen to satisfy the maximum curvature, target ΔT_{max} , and maximum ΔS^* constraints given by Eqs. 4.42-4.45, and bounding constraints; e.g., $T_i > 0$, $-\text{Ytol_B} < Y_{m,i} < 1 + \text{Ytol_B}$, and $\lambda_j^1 > \lambda_{min} \geq 0$.

$$Z_j^1 = Z_{j-1} + t_j \Delta s_j \quad (4.41)$$

$$k = \sqrt{\frac{\sum_{i=1}^N (t_j - t_{j-1})^2}{2(\Delta s_{j-1} + \Delta s_{j-2})}} \quad ; \quad \Delta s_k = \frac{\text{KTAR}}{k} \quad (4.42)$$

$$\Delta T_{MAX,j-1} = |T_{MAX,j} - T_{MAX,j-1}| \quad ; \quad \Delta s_T = \Delta s_{j-1} \frac{\text{TTAR}}{\Delta T_{MAX,j-1}} \quad (4.43)$$

$$\Delta s_S = \text{STAR} \frac{\lambda_{j-1}^2}{\left| \frac{d\lambda}{ds} \right|} = \text{STAR} \frac{\lambda_{j-1}^2}{|t_j(\text{end})|} \quad (4.44)$$

$$\Delta s_j = \min(\Delta s_k, \Delta s_T, \Delta s_S). \quad (4.45)$$

Once the new guess is established and Newton's method begins, the residuals to all governing equations are calculated, along with the Jacobian. Using **gmres**, the code then attempts to use to solve the matrix equation, producing the update vector ΔZ_j^k as shown in the process diagram, Eq. 4.38. If **gmres** fails, the algorithm switches to pseudo-time marching for **PT_STEP1** steps, starting from the last iterate that did not fail. If **gmres** successfully produces ΔZ_j^k , convergence is checked.

The convergence criteria for the RFM is governed by two tolerance variables, **atol_P** and **rtol_P**, for absolute and relative tolerance, respectively, which check the size of the update vector, ΔZ_j^k . The convergence criteria requires that the absolute magnitude of each element of the undamped step vector, $\text{STEP} = (Z_j^k + \Delta Z_j^k) - Z_j^k$, be less than or equal to **atol_P**, or less than or equal to the respective absolute magnitude of the underlying element-wise dependent variable, multiplied by **rtol_P**. For example, suppose element *xxxx* of Z_j^k is the nondimensional temperature at some grid point and element *xxxx* of **STEP** is the discrete update to that nondimensional temperature at that grid point. For the *xxxx*th element of Z_j^k to be convergent, at least one of the following must be true: $|\text{STEP}_{xxxx}| \leq \text{atol_P}$ or $|\text{STEP}_{xxxx}| \leq \text{rtol_P} \times |Z_{j,xxxx}^k|$. For the entire solution vector Z_j^k to be convergent, every element must satisfy this condition. If one or more elements do not, iteration continues.

If the convergence criteria is not satisfied but **gmres** has successfully produced ΔZ_j^k , two damping loops begin. These loops were inspired by the work of Dr. Joseph F. Grear [155, 156]. There are two damping factors, **f_bound** and **f_damp**, both of which are initially equal to 1. The first loop chooses **f_bound** via backtracking until the updated solution vector $Z_j^{k+1} = Z_j^k + \text{f_bound} * \Delta Z_j^k$ is “in bounds”; i.e., $T_i > 0$, $-\text{Ytol_B} < Y_{m,i} < 1 + \text{Ytol_B}$, and $\lambda_j^1 > \lambda_{min} \geq 0$. This loop will run for a maximum of **max_bt** iterations, dividing **f_bound** by $\sqrt{2}$ each iteration. If elements of Z_j^{k+1} are still out of bounds after **max_bt** iterations, the update is deemed a failure and the algorithm reverts to pseudo-time marching. If all elements of Z_j^{k+1} are in bounds, the second damping loop begins.

The second damping loop chooses **f_damp**, starting from **f_damp** = 1. With the two damping factors, the updated trial solution vector is $Z_j^{k+1} = Z_j^k + \text{f_bound} * \text{f_damp} * \Delta Z_j^k$. The second damping loop requires that the infinity norm of the approximate next step vector is smaller in magnitude than the infinity norm of the current step vector; i.e., $\|\Delta Z_{j,approx}^{k+1}\|_\infty \leq \|\Delta Z_j^k\|_\infty$. The approximate step vector is calculated by computing the residuals of the governing equations at Z_j^{k+1} ; i.e, $R(Z_j^{k+1}, Z_{j-1}, t_j, \Delta s_j)$, and solving the matrix equation

$\frac{\partial R}{\partial Z}|_{curr} \Delta Z_{j,approx}^{k+1} = -R(Z_j^{k+1}, Z_{j-1}, t_j, \Delta s_j)$. Note that the Jacobian is not recalculated from Z_j^{k+1} ; i.e., the same Jacobian that produced ΔZ_j^k is used to approximate $\Delta Z_{j,approx}^{k+1}$. This is done to save computational resources as Jacobian assembly is taxing. If the current value of **f_damp** results in $\|\Delta Z_{j,approx}^{k+1}\|_\infty \leq \|\Delta Z_j^k\|_\infty$, the Newton step is accepted. If the criteria is not satisfied, **f_damp** gets divided by $\sqrt{2}$ and the new approximate step vector is checked again. If the criteria is not satisfied after **max_bt** reductions of **f_damp**, the update is deemed a failure and the algorithm reverts to pseudo-time marching.

For a given value of j , this process continues until the solution is convergent. If the solution does not converge within **max_itr** attempts of Newton’s method, the entire program is terminated. During the iteration process, the algorithm may switch between backward-Euler and damped Newton’s method if the current iterate lies outside of the realm of Newton’s method convergence or if either of the damping loops are unsatisfied. Note that the pseudo-time marching portion of the algorithm does not run through either of the damping loops because its steps are already heavily “damped” by the $I/\Delta t$ term that is subtracted from the Jacobian. Additionally, the main purpose of the pseudo-time marching sub-algorithm is to move the solution into the realm in which Newton’s method can converge, and applying more checks unnecessarily slows it down.

4.4 Jacobian Calculation

The trick to a functional Newton’s method algorithm is to properly and efficiently calculate the Jacobian matrix. The Jacobian contains the derivatives of all governing equations with respect to all dependent variables and indicates how much, and in what direction, each dependent variable must change in order to better approximate the discrete solution. There are two general methods for calculating the Jacobian: perturbation derivatives and analytical derivatives. Analytical derivatives are obviously preferable; however, they are im-

practical with detailed chemical kinetics and transport models because all of the equations are intensely coupled. In this case, perturbation derivatives are preferred for development ease. However, if one-step kinetics are used in conjunction with Shvab-Zeldovich variables, analytical derivatives may be a practical choice. Both of these methods are explained in the following sections.

4.4.1 Jacobian Matrix with Perturbation Derivatives

The simplest method of calculating the Jacobian for the detailed chemical kinetics and transport version of the RFM, i.e., Eqs. 4.6-4.9, is to artificially perturb the dependent variables at each grid point and approximate the Jacobian derivatives via first-order finite differences. To do this, the governing equations 4.6-4.9 must first be discretized.

In general, convective terms use up-winding to aid numerical stability and diffusive terms use central differences. Convective first derivatives of an arbitrary dependent variable ϕ w.r.t. an arbitrary independent variable x are approximated by Eq. 4.46.

$$\left. \frac{d\phi}{dx} \right|_i \approx \begin{cases} \frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}}, & v > 0, \\ \frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i}, & v < 0. \end{cases} \quad (4.46)$$

There are two first derivatives approximated by a second order central difference. One is the θ' in the third term on the R.H.S. of Eq. 4.7. This derivative is approximated by Eq. 4.48 which is for a non-uniform grid. Note that this expression reduces to the common central difference formula if a uniform grid is used.

$$h_1 = x_i - x_{i-1} \quad h_2 = x_{i+1} - x_i \quad (4.47)$$

$$\left. \frac{d\phi}{dx} \right|_i \approx -\frac{h_2}{h_1(h_1 + h_2)} \phi_{i-1} + \frac{h_2 - h_1}{h_1 h_2} \phi_i + \frac{h_1}{h_2(h_1 + h_2)} \phi_{i+1}. \quad (4.48)$$

The second first derivative approximated by a central difference is J'_m in Eq. 4.6. This is the trickiest of all the derivatives to approximate with a finite difference because J_m itself contains derivatives of species and, if Soret effects are included, temperature. The multicomponent diffusion flux given by Eq. 4.12 without the Soret term is calculated as follows. First, a central difference of the mole fraction of each species is calculated at the half-steps.

$$\left. \frac{dX_n}{dx} \right|_{i-1/2} \approx \frac{X_{n,i} - X_{n,i-1}}{x_i - x_{i-1}} \quad (4.49)$$

This allows J_m to be calculated with second-order-accuracy at the half-steps. Using values of $J_{m,i-1/2}$ and $J_{m,i+1/2}$ on either side of a full step, $J'_{m,i}$ can be approximated by Eq. 4.50.

$$\left. \frac{dJ_m}{dx} \right|_i \approx \frac{J_{m,i+1/2} - J_{m,i-1/2}}{x_{i+1/2} - x_{i-1/2}} \quad (4.50)$$

The other diffusive flux terms are also approximated by second order central differences as shown in Eq. 4.51 following suggestions in [157, p. 181]. Terms using this finite difference approximation are the second terms on the R.H.S. of Eqs. 4.7-4.9. Here c_ϕ is either λ in Eq. 4.7 or μ in Eqs. 4.8-4.9.

$$\left. \frac{d}{dx} \left(\rho c_\phi \frac{d\phi}{dx} \right) \right|_i \approx \frac{2}{x_{i+1} - x_{i-1}} \left[\rho_{i+1/2} c_{\phi,i+1/2} \left(\frac{\phi_{i+1} - \phi_i}{x_{i+1} - x_i} \right) - \rho_{i-1/2} c_{\phi,i-1/2} \left(\frac{\phi_i - \phi_{i-1}}{x_i - x_{i-1}} \right) \right] \quad (4.51)$$

With all the governing equations discretized, the residual vector R can be calculated for all governing equations at all grid points. By sequentially perturbing every dependent variable at every grid point, the derivatives in the Jacobian can be calculated via Eqs. 4.52-4.54. The e superscript on R_i^e is the governing equation index; i.e., $e = 1, 2, 3, \dots, n_{sp} + 3$. The v superscript on U^v indicates the dependent variable with respect to which the governing

equation is being differentiated; i.e., v indicates $Y_1, Y_2, \dots, Y_{n_{sp}}, \theta, f'_1, f'_2$.

$$\frac{\partial R_i^e}{\partial U_{i-1}^v} \approx \frac{R_i^e(U_{i-1}^{v \text{ pert}}, U_i, U_{i+1}) - R_i^e(U_{i-1}, U_i, U_{i+1})}{\epsilon} \quad (4.52)$$

$$\frac{\partial R_i^e}{\partial U_i^v} \approx \frac{R_i^e(U_{i-1}, U_i^{v \text{ pert}}, U_{i+1}) - R_i^e(U_{i-1}, U_i, U_{i+1})}{\epsilon} \quad (4.53)$$

$$\frac{\partial R_i^e}{\partial U_{i+1}^v} \approx \frac{R_i^e(U_{i-1}, U_i, U_{i+1}^{v \text{ pert}}) - R_i^e(U_{i-1}, U_i, U_{i+1})}{\epsilon} \quad (4.54)$$

Only one variable is perturbed at a time; thus the vector $U_i^{v \text{ pert}}$ is the same as U_i apart from one variable. The difference in this one variable is the perturbation ϵ ; i.e., $U_i^{v \text{ pert}} = U_i^v + \epsilon$. If $|U_i^v| > 10^{-6}$, $\epsilon = \text{sgn}(U_i^v) \max(10^{-6} * |U_i^v|, 10^{-12})$. If $|U_i^v| < 10^{-6}$, $\epsilon = 10^{-12}$.

Since a three-point stencil was used in the finite differences of the governing equations, the Jacobian is block tri-diagonal. Each block has dimension $(n_{sp} + 3) \times (n_{sp} + 3)$. The blocks below the main diagonal are a_i , the main diagonal blocks are b_i , and blocks above the main diagonal are c_i . All other blocks are null because they lie outside the stencil. The structure of blocks a_i , b_i , and c_i are shown below.

$$a_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial Y_{1,i-1}} & \cdots & \frac{\partial R_i^1}{\partial Y_{n_{sp},i-1}} & \frac{\partial R_i^1}{\partial \theta_{i-1}} & \frac{\partial R_i^1}{\partial f'_{1,i-1}} & \frac{\partial R_i^1}{\partial f'_{2,i-1}} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial R_i^{n_{sp}}}{\partial Y_{1,i-1}} & \cdots & \frac{\partial R_i^{n_{sp}}}{\partial Y_{n_{sp},i-1}} & \frac{\partial R_i^{n_{sp}}}{\partial \theta_{i-1}} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{1,i-1}} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{2,i-1}} \\ \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{1,i-1}} & \cdots & \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{n_{sp},i-1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial \theta_{i-1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{1,i-1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{2,i-1}} \\ \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{1,i-1}} & \cdots & \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{n_{sp},i-1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial \theta_{i-1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{1,i-1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{2,i-1}} \\ \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{1,i-1}} & \cdots & \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{n_{sp},i-1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial \theta_{i-1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{1,i-1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{2,i-1}} \end{bmatrix} \quad (4.55)$$

$$b_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial Y_{1,i}} & \cdots & \frac{\partial R_i^1}{\partial Y_{n_{sp},i}} & \frac{\partial R_i^1}{\partial \theta_i} & \frac{\partial R_i^1}{\partial f'_{1,i}} & \frac{\partial R_i^1}{\partial f'_{2,i}} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial R_i^{n_{sp}}}{\partial Y_{1,i}} & \cdots & \frac{\partial R_i^{n_{sp}}}{\partial Y_{n_{sp},i}} & \frac{\partial R_i^{n_{sp}}}{\partial \theta_i} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{1,i}} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{2,i}} \\ \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{1,i}} & \cdots & \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{n_{sp},i}} & \frac{\partial R_i^{n_{sp}+1}}{\partial \theta_i} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{1,i}} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{2,i}} \\ \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{1,i}} & \cdots & \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{n_{sp},i}} & \frac{\partial R_i^{n_{sp}+2}}{\partial \theta_i} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{1,i}} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{2,i}} \\ \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{1,i}} & \cdots & \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{n_{sp},i}} & \frac{\partial R_i^{n_{sp}+3}}{\partial \theta_i} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{1,i}} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{2,i}} \end{bmatrix} \quad (4.56)$$

$$c_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial Y_{1,i+1}} & \cdots & \frac{\partial R_i^1}{\partial Y_{n_{sp},i+1}} & \frac{\partial R_i^1}{\partial \theta_{i+1}} & \frac{\partial R_i^1}{\partial f'_{1,i+1}} & \frac{\partial R_i^1}{\partial f'_{2,i+1}} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial R_i^{n_{sp}}}{\partial Y_{1,i+1}} & \cdots & \frac{\partial R_i^{n_{sp}}}{\partial Y_{n_{sp},i+1}} & \frac{\partial R_i^{n_{sp}}}{\partial \theta_{i+1}} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{1,i+1}} & \frac{\partial R_i^{n_{sp}}}{\partial f'_{2,i+1}} \\ \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{1,i+1}} & \cdots & \frac{\partial R_i^{n_{sp}+1}}{\partial Y_{n_{sp},i+1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial \theta_{i+1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{1,i+1}} & \frac{\partial R_i^{n_{sp}+1}}{\partial f'_{2,i+1}} \\ \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{1,i+1}} & \cdots & \frac{\partial R_i^{n_{sp}+2}}{\partial Y_{n_{sp},i+1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial \theta_{i+1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{1,i+1}} & \frac{\partial R_i^{n_{sp}+2}}{\partial f'_{2,i+1}} \\ \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{1,i+1}} & \cdots & \frac{\partial R_i^{n_{sp}+3}}{\partial Y_{n_{sp},i+1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial \theta_{i+1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{1,i+1}} & \frac{\partial R_i^{n_{sp}+3}}{\partial f'_{2,i+1}} \end{bmatrix} \quad (4.57)$$

The blocks are assembled into the Jacobian matrix, allowing the matrix equation in Newton's method to be solved for ΔU_j^k (or ΔZ_j^k if arc-length continuation is being used). The full matrix equation is shown below in Eq. 4.58. The I matrices in the upper left and lower right corners of the Jacobian are $(n_{sp} + 3) \times (n_{sp} + 3)$ identity matrices that result from Dirichlet boundary conditions. The 0's indicate $(n_{sp} + 3) \times (n_{sp} + 3)$ null matrices.

$$\begin{bmatrix}
I & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\
a_2 & b_2 & c_2 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\
0 & a_3 & b_3 & c_3 & 0 & \dots & 0 & 0 & 0 & 0 \\
0 & 0 & a_4 & b_4 & c_4 & \dots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_5 & b_5 & \dots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \dots & b_{N-3} & c_{N-3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \dots & a_{N-2} & b_{N-2} & c_{N-2} & 0 \\
0 & 0 & 0 & 0 & 0 & \dots & 0 & a_{N-1} & b_{N-1} & c_{N-1} \\
0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & I
\end{bmatrix}
\begin{bmatrix}
\Delta U_1 \\
\Delta U_2 \\
\Delta U_3 \\
\Delta U_4 \\
\Delta U_5 \\
\vdots \\
\Delta U_{N-3} \\
\Delta U_{N-2} \\
\Delta U_{N-1} \\
\Delta U_N
\end{bmatrix}
=
\begin{bmatrix}
0 \\
-R(U_2) \\
-R(U_3) \\
-R(U_4) \\
-R(U_5) \\
\vdots \\
-R(U_{N-3}) \\
-R(U_{N-2}) \\
-R(U_{N-1}) \\
0
\end{bmatrix} \quad (4.58)$$

Although it is computationally taxing to assemble the Jacobian via perturbation methods, this is a practical way of doing so when the dependent variables, coefficients, and source/sink terms have coupled, highly nonlinear interdependency. However, perturbation techniques are known to have a variety of problems. First, rounding errors may be introduced due to numerical precision, especially when perturbations are very small, such as those for minor chemical species. This can degrade the accuracy of the solution. Second, inaccuracies, both from rounding errors and the use of first-order finite differences, contribute to numerical instability because the Jacobian is consequently less accurate, which frequently necessitates more iterations to reach convergence. In some cases, poor Jacobian accuracy prevents convergence all together. The imprecision of perturbation derivatives requires some tricky algorithmic

decision making to prevent the solution from going astray. These tricks primarily show up in the selection of ϵ , bounds checks, and damping checks. The method is computationally intensive because the coupled governing equations must be evaluated for every dependent variable, perturbed and unperturbed, at every node. Doing so involves nested loops that take longer to execute than vectorized algebraic equations. Thus, the only reason to use perturbation methods is if analytical derivatives are impractical to obtain. This is the case for the Eqs. 4.6-4.9. However, in the next section, which covers a simplified version of the RFM, analytical derivatives do exist, and the resultant Numerical method is much faster and tends to be more stable without frequent checks.

4.4.2 Jacobian Matrix with Analytical Derivatives

To illustrate the theory behind the analytical derivative method, a simpler form of the RFM governing equations is taken. This form is the same as that used by Sirignano [94] which employs a Fickian diffusion approximation, unity Prandtl, Schmidt, and Lewis numbers, constant specific heat such that non-dimensional enthalpy is equal to the reciprocal of density, and assumes $\rho\mu = 1$ in the non-dimensional form. Furthermore, a one-step reaction is used, allowing the definition of Shvab-Zeldovich variables, $\alpha = Y_F - \nu Y_O$ and $\beta = h + \nu Y_O q$. With these simplifications, the RFM governing Eqs. 3.8-3.11 reduce to Eqs. 4.59-4.63.

$$R_i^1 = f_1''' + f f_1'' + S_1 \left[\frac{1}{\rho} - (f_1')^2 \right] + \frac{\omega^2}{4S_1} \left(1 - \frac{1}{\rho} \right) = 0 \quad (4.59)$$

$$R_i^2 = f_2''' + f f_2'' + S_2 \left[\frac{1}{\rho} - (f_2')^2 \right] = 0 \quad (4.60)$$

$$R_i^3 = h'' + f h' - q \dot{\omega}_F = 0 \quad (4.61)$$

$$R_i^4 = \alpha'' + f\alpha' = 0 \quad (4.62)$$

$$R_i^5 = \beta'' + f\beta' = 0 \quad (4.63)$$

The boundary conditions become Eqs. 4.64-4.69.

$$f_1'(\infty) = 1 \ ; \ f_1'(-\infty) = \sqrt{\frac{1}{\rho_{-\infty}} + \left(\frac{\omega}{2S_1}\right)^2 \left(1 - \frac{1}{\rho_{-\infty}}\right)} \ ; \ f_1(0) = 0 \quad (4.64)$$

$$f_2'(\infty) = 1 \ ; \ f_2'(-\infty) = \frac{1}{\sqrt{\rho_{-\infty}}} \ ; \ f_2(0) = 0 \quad (4.65)$$

$$Y_m(\infty) = Y_{m,\infty} \ ; \ Y_m(-\infty) = Y_{m,-\infty} \quad (4.66)$$

$$h(\infty) = h_{\infty} \ ; \ h(-\infty) = h_{-\infty} \quad (4.67)$$

$$\alpha(\infty) = Y_{F,\infty} - \nu Y_{O,\infty} \ ; \ \alpha(-\infty) = Y_{F,-\infty} - \nu Y_{O,-\infty} \quad (4.68)$$

$$\beta(\infty) = h_{\infty} + \nu Y_{O,\infty} q \ ; \ \beta(-\infty) = h_{-\infty} + \nu Y_{O,-\infty} q \quad (4.69)$$

To calculate the derivatives of each governing equation, they must first be discretized. This is done with a finite difference approach, using second-order central differences for all derivatives except convective terms, which use first-order up-wind finite differences to increase numerical stability. As the flamelet counterflow has a convective velocity, v , that changes signs at the stagnation point, the direction of up-winding changes between the left and right halves of the domain. The discretized equations for both halves are written below.

Left side, $v > 0$

$$R_i^1 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{f'_{1,i+1} - f'_{1,i}}{x_{i+1} - x_i} - \frac{f'_{1,i} - f'_{1,i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{f'_{1,i} - f'_{1,i-1}}{x_i - x_{i-1}} \right) + S_1 h_i - S_1 f_{1,i}^{\prime 2} - h_i \frac{\omega^2}{4S_1} + \frac{\omega^2}{4S_1} \quad (4.70)$$

$$R_i^2 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{f'_{2,i+1} - f'_{2,i}}{x_{i+1} - x_i} - \frac{f'_{2,i} - f'_{2,i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{f'_{2,i} - f'_{2,i-1}}{x_i - x_{i-1}} \right) + S_2 h_i - S_2 f_{1,i}^{\prime 2} \quad (4.71)$$

$$R_i^3 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{h_{i+1} - h_i}{x_{i+1} - x_i} - \frac{h_i - h_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{h_i - h_{i-1}}{x_i - x_{i-1}} \right) - q\omega_{F,i} \quad (4.72)$$

$$R_i^4 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{\alpha_{i+1} - \alpha_i}{x_{i+1} - x_i} - \frac{\alpha_i - \alpha_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{\alpha_i - \alpha_{i-1}}{x_i - x_{i-1}} \right) \quad (4.73)$$

$$R_i^5 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{\beta_{i+1} - \beta_i}{x_{i+1} - x_i} - \frac{\beta_i - \beta_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{\beta_i - \beta_{i-1}}{x_i - x_{i-1}} \right) \quad (4.74)$$

Right side, $v < 0$

$$R_i^1 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{f'_{1,i+1} - f'_{1,i}}{x_{i+1} - x_i} - \frac{f'_{1,i} - f'_{1,i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{f'_{1,i+1} - f'_{1,i}}{x_{i+1} - x_i} \right) + S_1 h_i - S_1 f_{1,i}^{\prime 2} - h_i \frac{\omega^2}{4S_1} + \frac{\omega^2}{4S_1} \quad (4.75)$$

$$R_i^2 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{f'_{2,i+1} - f'_{2,i}}{x_{i+1} - x_i} - \frac{f'_{2,i} - f'_{2,i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{f'_{2,i+1} - f'_{2,i}}{x_{i+1} - x_i} \right) + S_2 h_i - S_2 f_{1,i}'^2 \quad (4.76)$$

$$R_i^3 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{h_{i+1} - h_i}{x_{i+1} - x_i} - \frac{h_i - h_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{h_{i+1} - h_i}{x_{i+1} - x_i} \right) - q\dot{\omega}_{F,i} \quad (4.77)$$

$$R_i^4 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{\alpha_{i+1} - \alpha_i}{x_{i+1} - x_i} - \frac{\alpha_i - \alpha_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{\alpha_{i+1} - \alpha_i}{x_{i+1} - x_i} \right) \quad (4.78)$$

$$R_i^5 = \frac{2}{x_{i+1} - x_{i-1}} \left[\frac{\beta_{i+1} - \beta_i}{x_{i+1} - x_i} - \frac{\beta_i - \beta_{i-1}}{x_i - x_{i-1}} \right] + f_i \left(\frac{\beta_{i+1} - \beta_i}{x_{i+1} - x_i} \right) \quad (4.79)$$

Equations 4.70-4.79 can now be re-written, grouping terms with common dependent variables as shown in Eqs. 4.80-4.89.

Left side, $v > 0$

$$\begin{aligned} R_i^1 &= \frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f'_{1,i+1} \\ &- \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] f'_{1,i} + S_1 f_{1,i}'^2 \\ &+ \left[\frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] f'_{1,i-1} + S_1 h_i - h_i \frac{\omega^2}{4S_1} + \frac{\omega^2}{4S_1} \quad (4.80) \end{aligned}$$

$$\begin{aligned}
R_i^2 &= \frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f'_{2,i+1} \\
&- \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] f'_{2,i} + S_2 f_{2,i}'^2 \\
&\quad + \left[\frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] f'_{2,i-1} + S_2 h_i \quad (4.81)
\end{aligned}$$

$$\begin{aligned}
R_i^3 &= \frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} h_{i+1} \\
&- \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] h_i \\
&\quad + \left[\frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] h_{i-1} - q\dot{\omega}_{F,i} \quad (4.82)
\end{aligned}$$

$$\begin{aligned}
R_i^4 &= \frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \alpha_{i+1} \\
&- \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] \alpha_i \\
&\quad + \left[\frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] \alpha_{i-1} \quad (4.83)
\end{aligned}$$

$$\begin{aligned}
R_i^5 &= \frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \beta_{i+1} \\
&- \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] \beta_i \\
&\quad + \left[\frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} - f_i \frac{1}{x_i - x_{i-1}} \right] \beta_{i-1} \quad (4.84)
\end{aligned}$$

Right side, $v < 0$

$$\begin{aligned}
R_i^1 = & \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + f_i \frac{1}{x_{i+1} - x_i} \right] f'_{1,i+1} \\
& - \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} + f_i \frac{1}{x_{i+1} - x_i} \right] f'_{1,i} + S_1 f_{1,i}'^2 \\
& + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} f'_{1,i-1} + S_1 h_i - h_i \frac{\omega^2}{4S_1} + \frac{\omega^2}{4S_1} \quad (4.85)
\end{aligned}$$

$$\begin{aligned}
R_i^2 = & \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + f_i \frac{1}{x_{i+1} - x_i} \right] f'_{2,i+1} \\
& - \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} + f_i \frac{1}{x_{i+1} - x_i} \right] f'_{2,i} + S_2 f_{2,i}'^2 \\
& + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} f'_{2,i-1} + S_2 h_i \quad (4.86)
\end{aligned}$$

$$\begin{aligned}
R_i^3 = & \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + f_i \frac{1}{x_{i+1} - x_i} \right] h_{i+1} \\
& - \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} + f_i \frac{1}{x_{i+1} - x_i} \right] h_i \\
& + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} h_{i-1} - q\dot{\omega}_{F,i} \quad (4.87)
\end{aligned}$$

$$\begin{aligned}
R_i^4 = & \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + f_i \frac{1}{x_{i+1} - x_i} \right] \alpha_{i+1} \\
& - \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} + f_i \frac{1}{x_{i+1} - x_i} \right] \alpha_i \\
& + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} \alpha_{i-1} \quad (4.88)
\end{aligned}$$

$$\begin{aligned}
R_i^5 = & \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + f_i \frac{1}{x_{i+1} - x_i} \right] \beta_{i+1} \\
& - \left[\frac{2}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} + f_i \frac{1}{x_{i+1} - x_i} \right] \beta_i \\
& + \frac{2}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})} \beta_{i-1} \quad (4.89)
\end{aligned}$$

Equations 4.80-4.89 can now be differentiated with respect to all dependent variables at indices $i - 1$, i , and $i + 1$. Fortunately, this produces many zero-valued terms. Differentiation with respect to dependent variables at $i - 1$ produces the left-most block in the Jacobian block-row, which itself is diagonal. This block is denoted a_i . Differentiation with respect to dependent variables at i produces the main diagonal block in the Jacobian block-row, which itself is not diagonal due to the presence of h_i in R_i^1 and R_i^2 and the derivatives of α_i and β_i (through the reaction rate) in R_i^3 . This block is denoted b_i . Finally, differentiation with respect to $i + 1$ produces the right-most block in the Jacobian block-row, which itself is diagonal. This block is denoted c_i . Blocks a_i , b_i , and c_i are shown by Eqs. 4.90-4.92 with only the non-zero derivatives represented.

$$a_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial f'_{1,i-1}} & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial R_i^2}{\partial f'_{2,i-1}} & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial R_i^3}{\partial h_{i-1}} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial R_i^4}{\partial \alpha_{i-1}} & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial R_i^5}{\partial \beta_{i-1}} \end{bmatrix} \quad (4.90)$$

$$b_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial f'_{1,i}} & 0 & \frac{\partial R_i^1}{\partial h_i} & 0 & 0 \\ 0 & \frac{\partial R_i^2}{\partial f'_{2,i}} & \frac{\partial R_i^2}{\partial h_i} & 0 & 0 \\ 0 & 0 & \frac{\partial R_i^3}{\partial h_i} & \frac{\partial R_i^3}{\partial \alpha_i} & \frac{\partial R_i^3}{\partial \beta_i} \\ 0 & 0 & 0 & \frac{\partial R_i^4}{\partial \alpha_i} & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial R_i^5}{\partial \beta_i} \end{bmatrix} \quad (4.91)$$

$$c_i = \begin{bmatrix} \frac{\partial R_i^1}{\partial f'_{1,i+1}} & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial R_i^2}{\partial f'_{2,i+1}} & 0 & 0 & 0 \\ 0 & 0 & \frac{\partial R_i^3}{\partial h_{i+1}} & 0 & 0 \\ 0 & 0 & 0 & \frac{\partial R_i^4}{\partial \alpha_{i+1}} & 0 \\ 0 & 0 & 0 & 0 & \frac{\partial R_i^5}{\partial \beta_{i+1}} \end{bmatrix} \quad (4.92)$$

Note, special care must be taken in the formation of block b_i due to the chemical source term in the energy equation. As the reaction rate is a function of enthalpy and mass fractions, which are recast here to enthalpy and Shvab-Zeldovich variables, $\dot{\omega}_{F,i} = \dot{\omega}_F(h_i, \alpha_i, \beta_i)$, the reaction rate derivatives can get messy depending on the powers of h_i , $Y_{F,i}$, and $Y_{O,i}$. If a one-step reaction were used having unitary powers on $Y_{F,i}$, and $Y_{O,i}$, the derivatives are simplified somewhat. The Shvab-Zeldovich variables are defined as $\alpha_i = Y_{F,i} - \nu Y_{O,i}$ and $\beta_i = h_i + \nu Y_{O,i} q$, where $\nu = 0.275$ is the stoichiometric mass ratio for propane and oxygen,

leading to the following expression for a reaction rate with unity mass fraction powers:

$$\dot{\omega}_{F,i} = -\frac{A^* \rho_{ref}^* \rho_i}{S^*} \left[\frac{1}{q} (\beta_i - h_i) + \alpha_i \right] \left[\frac{1}{\nu q} (\beta_i - h_i) \right] e^{-\frac{E_a^*}{RT_{ref}^* h_i}} \quad (4.93)$$

Equation 4.93 is differentiated w.r.t. h_i , α_i , and β_i , producing Eqs. 4.96-4.98 to be used in the calculation of $\frac{\partial R_i^3}{\partial h_i}$, $\frac{\partial R_i^3}{\partial \alpha_i}$, and $\frac{\partial R_i^3}{\partial \beta_i}$ within b_i . Note, for numerical implementation, it is beneficial to include A^* in the exponential term, as $\ln|A^*|$, to avoid rounding errors caused by multiplying very large numbers by very small numbers.

$$Y_{O,i} = \left(\frac{\beta_i - h_i}{\nu q} \right) \quad (4.94)$$

$$Y_{F,i} = \left(\frac{\beta_i - h_i}{q} - \alpha_i \right) \quad (4.95)$$

$$\begin{aligned} \frac{d\dot{\omega}_{F,i}}{dh_i} = & -\frac{\rho_{ref}^* \rho_i}{S^*} \left[-\frac{1}{q} \left(\frac{\beta_i - h_i}{\nu q} \right) - \frac{1}{\nu q} \left(\frac{\beta_i - h_i}{q} - \alpha_i \right) \right. \\ & \left. + \frac{E_a^*}{RT_{ref}^* h_i^2} \left(\frac{\beta_i - h_i}{q} - \alpha_i \right) \left(\frac{\beta_i - h_i}{\nu q} \right) \right] e^{\ln|A^*| - \frac{E_a^*}{RT_{ref}^* h_i}} \end{aligned} \quad (4.96)$$

$$\frac{d\dot{\omega}_{F,i}}{d\alpha_i} = -\frac{\rho_{ref}^* \rho_i}{S^*} \left(\frac{\beta_i - h_i}{\nu q} \right) e^{\ln|A^*| - \frac{E_a^*}{RT_{ref}^* h_i}} \quad (4.97)$$

$$\frac{d\dot{\omega}_{F,i}}{d\beta_i} = -\frac{\rho_{ref}^* \rho_i}{S^*} \left[\frac{1}{q} \left(\frac{\beta_i - h_i}{\nu q} \right) + \frac{1}{\nu q} \left(\frac{\beta_i - h_i}{q} - \alpha_i \right) \right] e^{\ln|A^*| - \frac{E_a^*}{RT_{ref}^* h_i}} \quad (4.98)$$

With all derivatives and blocks calculated, Newton's method, as applied to the present problem with Dirichlet boundary conditions, i.e., Eq. 4.24, can be written with a_i , b_i , and c_i as Eq. 4.99 where I represents a 5×5 identity matrix and 0 represents a 5×5 null matrix.

$$\begin{bmatrix}
I & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\
a_2 & b_2 & c_2 & 0 & 0 & \dots & 0 & 0 & 0 & 0 \\
0 & a_3 & b_3 & c_3 & 0 & \dots & 0 & 0 & 0 & 0 \\
0 & 0 & a_4 & b_4 & c_4 & \dots & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & a_5 & b_5 & \dots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \dots & b_{N-3} & c_{N-3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \dots & a_{N-2} & b_{N-2} & c_{N-2} & 0 \\
0 & 0 & 0 & 0 & 0 & \dots & 0 & a_{N-1} & b_{N-1} & c_{N-1} \\
0 & 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & I
\end{bmatrix}
\begin{bmatrix}
\Delta U_1 \\
\Delta U_2 \\
\Delta U_3 \\
\Delta U_4 \\
\Delta U_5 \\
\vdots \\
\Delta U_{N-3} \\
\Delta U_{N-2} \\
\Delta U_{N-1} \\
\Delta U_N
\end{bmatrix}
=
\begin{bmatrix}
0 \\
-R(U_2) \\
-R(U_3) \\
-R(U_4) \\
-R(U_5) \\
\vdots \\
-R(U_{N-3}) \\
-R(U_{N-2}) \\
-R(U_{N-1}) \\
0
\end{bmatrix} \quad (4.99)$$

This matrix equation could be solved via inversion, block-Thomas algorithm, generalized minimum residuals, and many other common algorithms; however, a shortcut exists here due to the sparse structure. Consider the variable β . If all elements of a_i , b_i , and c_i pertaining to β are assembled into an $\mathbf{A}\vec{x} = \vec{b}$ equation, a purely tridiagonal matrix results which can be solved with the Thomas algorithm, yielding $\Delta\beta$. The same may be done for α . However, for h , the assembled matrix is not tridiagonal but can be made tridiagonal by moving the non-tridiagonal elements into the $\vec{b}$ vector. Furthermore, since $\Delta\beta$ and $\Delta\alpha$ are known, the derivatives $\frac{\partial R_i^3}{\partial \alpha_i}$ and $\frac{\partial R_i^3}{\partial \beta_i}$ can be calculated with the updated values of α and β . After Δh is known, the same process of moving off-tridiagonal elements into the $\vec{b}$ vector can be done to solve for $\Delta f'_1$ and $\Delta f'_2$. This solving process is iterated to solve for the updated dependent variables until the grid-average 2-norm residual, given by Eq. 4.100, of each governing

equation has decreased by a given order of magnitude relative to the first iteration. Note that a 2-norm residual is calculated for each dependent variable; i.e., $\|R\|_2$ is a 5×1 vector. The solution is said to be converged when each residual has decreased by around three orders of magnitude; however, this could be reduced if more accuracy is desired. In testing, even a two-order-of-magnitude reduction was adequate to converge the solution within a plot line thickness of a solution obtained with a more stringent convergence criterion.

$$\|R\|_2 = \sqrt{\frac{1}{N} \left(\sum_{i=2}^{N-1} |R(V_i)| \right)^2} \quad (4.100)$$

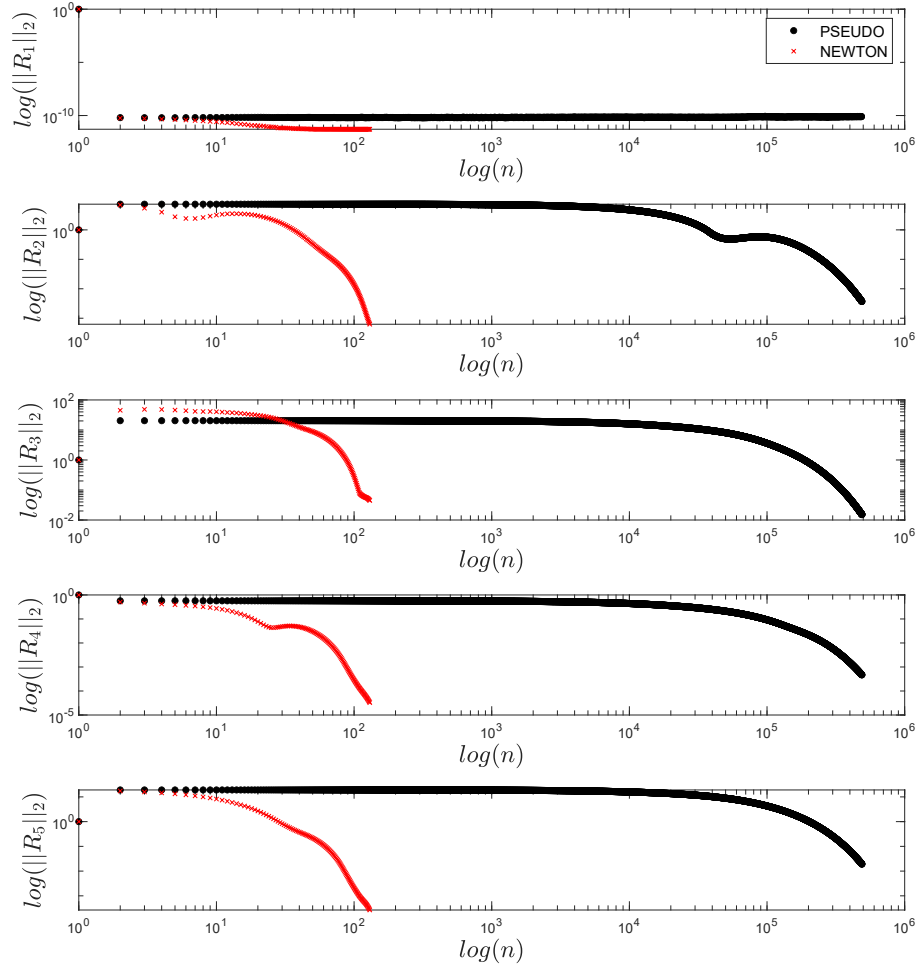


Figure 4.3: Log of residual magnitudes, $\|R\|_2$, versus log of iteration number, n , (base 10) for a lightly-strained diffusion flamelet. Residuals 1-5 pertain to f'_1 , f'_2 , h , α , and β , respectively.

This algorithm was used to solve Eqs. 4.59-4.63 and was compared against the explicit method. Newton's method showed a 99.6273% reduction in computation time. Figure 4.3 plots the residuals of the five dependent variables versus iteration number on a log-log scale. The explicit algorithm converged in 489,611 iterations, while the Newton's method converged in 130 iterations. Note that this difference is subdued by the log scale on the abscissa.

Chapter 5

Coupling the Flamelet Model to RANS/LES

The Rotational Flamelet Model presented in Chap. 3 is only half of the turbulent combustion modeling theory presented in this dissertation. The remaining improvements stem from the coupling procedure which relates the resolved or mean flow quantities in LES or RANS to boundary conditions for the RFM. These aspects are critical in determining which flamelet solution best represents the qualities of combustion occurring at a given location and time in the global flow.

As discussed in Chap. 2, the classical theory on which modern non-premixed flamelet modeling is built makes two assumptions regarding the scales and boundary conditions. First, it is assumed that in any location and at any time in the global domain, *the turbulent flame samples the internal structure of a single canonical counterflow diffusion flame under various strain rates*; that is, the inflow mixtures and temperatures to the flamelet are fixed regardless of the local scalar conditions computed by LES or RANS. The second assumption is that the only mechanical constraint relating the scales is the scalar dissipation rate, χ , or

the progress variable, C , which both map from the global scale to non-ambient (flame-local) conditions on the flamelet scale. Chapters 2 and 3 have discussed the issues seen with χ and C but they are summarized as follows.

- The scalar dissipation rate χ or flamelet progress variable (FPV) C are mapped from their mean or filtered values ($\tilde{\chi} = 2D|\widetilde{\nabla Z}|^2$) to the reaction zone of the flamelet. A delta function is often assumed for the marginal PDF of χ (or C) in the presumed PDF coupling procedure which essentially equates the value of χ in the center of the flamelet, χ_{st} , to the Favre-averaged value, $\tilde{\chi}$, produced by the LES or RANS code. Doing so ignores the concept of scale separation established in turbulence literature which says that the magnitudes of the gradients increase as the length scale decreases; thus, $\chi_{st} \gg \tilde{\chi}$ in principle, yet the models assume $\chi_{st} \approx \tilde{\chi}$ for convenience. This does not account for the trend in gradient magnitude or for intermittency. Some methodologies use a log-normal PDF which respects scale separation much better; however, this is infrequent. The delta function is also used for the FPV. Because scalar dissipation rate and the progress variable are taken at or near the stoichiometric point on the flamelet scale, scaling laws derived from cascade theory have difficulty relating the flame-local value to the mean or resolved flow.
- If the FPV is used, the S-curves are mapped to C monotonically, which has the benefit of including the unstable branch; however, doing so causes the equilibrium reacting solution to correspond to a maximization of C . In a simple turbulent shear layer in which fuel and oxidizer originate from different sides of a splitter plate and a central flame develops at the fuel-oxidizer interface, the progress variable will maximize at the center of the layer, roughly in line with, and downstream of, the splitter plate. A location in line with the splitter plate will have high turbulence intensity and thus should not correspond to a low strain rate, near-equilibrium solution. The progress variable should generally increase with downstream distance, which is why Pierce and

Moin [77] were able to predict flame lift-off; however, there is an arbitrariness to its usage that can be avoided with a different coupling procedure.

The coupling procedure pursued for the RFM is based on scale separation between the global flow and the flamelet and will use cascade theory to deduce mechanical flamelet boundary conditions given global quantities. The word “global” here is used as a placeholder for “LES resolved scale and RANS mean quantities.” Specifically, the flamelet is viewed as a laminar Kolmogorov-scale model, and thus fixed to the flamelet counterflow origin, one would “see” far-field strain rates, vorticity, and scalar values imposed by the turbulent field. The strain rates and vorticity are mechanical constraints on the flamelet model while mixture and temperature (or enthalpy) are scalar constraints. Note, the scalar constraints are included here because a true Kolmogorov-scale model would see various inflow mixtures depending on the mixture and temperature of the RANS or LES cell. The following sections cover the theory used to obtain these far-field conditions from quantities in LES and RANS codes.

5.1 Mechanical Forward Coupling

Velocity gradients are scaled following the work of Sirignano, Hellwig, and Walsh [109, 145]. Here, the turbulence kinetic energy dissipation rate, ϵ , is used to connect the global scale to the flamelet scale. ϵ is a well-established parameter in turbulence theory [2, 158] and will be used to determine the approximate vorticity and strain rate magnitudes at the Kolmogorov scale which are the mechanical constraints for the RFM. Before the in-depth analysis, consider this simple argument. Kolmogorov’s 1941 hypothesis [7] says that ϵ , the transfer rate of turbulence kinetic energy from larger scales to smaller scales is constant through the inertial range of the cascade process (on average). ϵ is then equal in magnitude to the actual energy dissipation rate in the viscous sub-range where the flamelet lives. The small amount of viscous dissipation on larger length scales is neglected in this approximation.

In other words, the energy injection rate on the large scales equals the energy transfer rate through the intermediate scales, which equals the viscous dissipation rate on the small scales. The Kolmogorov time scale is $\tau_\kappa = (\nu/\epsilon)^{1/2}$ which means the Kolmogorov strain rate is approximately $S_\kappa \approx (\epsilon/\nu)^{1/2}$. The RFM is constructed from the viewpoint that a diffusion flamelet sees this Kolmogorov strain rate in the far-field. Since turbulence kinetic energy is dissipated over a range of the smaller scales, a modeling constant, informed by DNS, is needed. Thus, the far-field strain rate seen by the flamelet should go as $S^* \approx CS_\kappa \approx C\sqrt{\epsilon/\nu}$.

Since the RFM is governed by ω , S_1 , and S_2 in addition to S^* , a more detailed mechanical coupling procedure is necessary than $S^* \approx C\sqrt{\epsilon/\nu}$; however, the end result should reflect this behavior. Figure 5.1 shows the transformation from the non-rotating coordinate system with spatial coordinates x, y, z and velocity components u, v, w to the coordinate system rotating about the z -axis with coordinates ξ, χ, z and velocity components u_ξ, u_χ, w [94]. Scalar gradients and the major principal compressive strain rate are aligned with χ , while the other principal strain rates are aligned with ξ and z . In the stretched vortex layer situation, the major tensile strain rate is aligned with the ξ axis and the intermediate tensile strain rate is aligned with the z axis. In the stretched vortex tube situation, there are two compressive principal strain rates and one tensile principal strain rate. In this case, the intermediate compressive strain rate is aligned with the ξ axis and the only tensile strain rate is aligned with the z axis. Also note that the x, y, z directions are not correlated with coordinates on the resolved scale. The transformation removes material rotation from the $\xi - \chi$ plane by having it rotate at angular velocity $d\theta/dt = \omega/2$ relative to x and y . The sub-grid domain is assumed to be sufficiently small to consider a uniform vorticity magnitude across it. The geometry and transformation presented here is the same as that in Sec. 3.2 and is informed by trends observed in non-premixed DNS studies. The dependent and independent variables are presented in dimensional form unless otherwise stated. The relations between the velocity components and spatial coordinates in both reference frames are given by Eqs. 5.1-5.4.

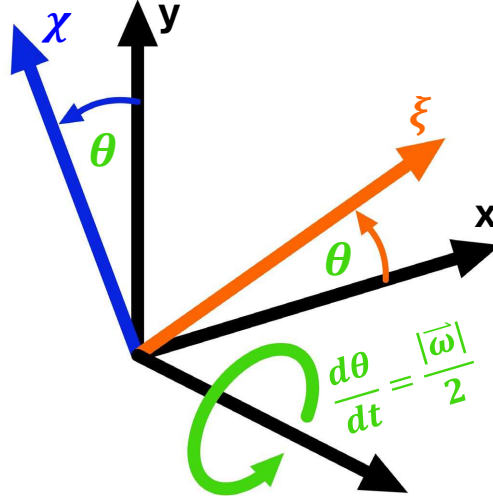


Figure 5.1: Transformation from the Newtonian reference frame (x, y, z) to the rotating non-Newtonian reference frame (ξ, χ, z) .

$$\xi = x \cos \theta + y \sin \theta ; \chi = y \cos \theta - x \sin \theta \quad (5.1)$$

$$u_\xi = u \cos \theta + v \sin \theta + \chi \frac{\omega}{2} ; u_\chi = v \cos \theta - u \sin \theta - \xi \frac{\omega}{2} \quad (5.2)$$

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial \xi} \cos \theta - \frac{\partial u}{\partial \chi} \sin \theta ; \frac{\partial u}{\partial y} = \frac{\partial u}{\partial \xi} \sin \theta + \frac{\partial u}{\partial \chi} \cos \theta \quad (5.3)$$

$$\frac{\partial v}{\partial x} = \frac{\partial v}{\partial \xi} \cos \theta - \frac{\partial v}{\partial \chi} \sin \theta ; \frac{\partial v}{\partial y} = \frac{\partial v}{\partial \xi} \sin \theta + \frac{\partial v}{\partial \chi} \cos \theta \quad (5.4)$$

From Eq. 5.1, it follows that $\sqrt{x^2 + y^2} = \sqrt{\xi^2 + \chi^2}$. Thus, the units of length are equal in both reference frames. Differentiation of Eq. 5.2, together with constraints that u_ξ is independent of χ and u_χ is independent of ξ , yields Eqs. 5.5-5.6.

$$\frac{\partial u_\xi}{\partial \xi} = \frac{\partial u}{\partial \xi} \cos \theta + \frac{\partial v}{\partial \xi} \sin \theta ; \frac{\partial u_\xi}{\partial \chi} = 0 = \frac{\partial u}{\partial \chi} \cos \theta + \frac{\partial v}{\partial \chi} \sin \theta + \frac{\omega}{2} \quad (5.5)$$

$$\frac{\partial u_\chi}{\partial \chi} = \frac{\partial v}{\partial \chi} \cos \theta - \frac{\partial u}{\partial \chi} \sin \theta ; \frac{\partial u_\chi}{\partial \xi} = 0 = \frac{\partial v}{\partial \xi} \cos \theta - \frac{\partial u}{\partial \xi} \sin \theta - \frac{\omega}{2} \quad (5.6)$$

Equations 5.5-5.6 then yield 5.7-5.8.

$$\frac{\partial u_\xi}{\partial \xi} = \frac{\partial u}{\partial x} + \left(\frac{\partial u}{\partial y} + \frac{\omega}{2} \right) \tan \theta \quad (5.7)$$

$$\frac{\partial u_\chi}{\partial \chi} = \frac{\partial v}{\partial y} - \left(\frac{\partial v}{\partial x} - \frac{\omega}{2} \right) \tan \theta \quad (5.8)$$

We focus on the inflow on either side of the counterflow induced by a compressive normal strain rate imposed on the rotating mass of fluid. Asymptotically, i.e., removed from the center of rotation, the inflow has uniform density, although exothermic reaction in the center of the rotating fluid will cause variable density locally. The divergence of velocity in either coordinate system will be zero for the incoming flow. The inflow should be independent of θ position. That occurs if $\partial v / \partial x = -\partial u / \partial y = \omega / 2$. This implies that the shear strain rate $S_{xy} = [\partial u / \partial y + \partial v / \partial x] / 2 = 0$. Since w depends only on z and u and v are independent of z for the inflow, $S_{xz} = 0$, $S_{yz} = 0$ as well. Thereby, only normal strain rate occurs in the inflow for either coordinate system. With the aim towards establishing scaling relations to the flamelet far-field, the incoming counterflow streams are sufficiently removed from the reaction zone such that density, other scalar properties, and strain rates are constant. The scaling from resolved-scale values for RANS or LES will impose boundary conditions on the flamelet but will not directly prescribe the values in or near the reaction zone; in this critical manner, the approach differs from the SDR and FPV methods discussed previously.

Equation 5.9 is obtained given the relations for vorticity in the original and transformed reference frames. The dilation remains identical in both frames; thus, the divergence of velocity is unchanged as in Eq. 5.10.

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = \omega \quad ; \quad \frac{\partial u_\chi}{\partial \xi} - \frac{\partial u_\xi}{\partial \chi} = 0 \quad (5.9)$$

$$\frac{\partial u_\chi}{\partial \chi} + \frac{\partial u_\xi}{\partial \xi} + \frac{\partial w}{\partial z} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \quad (5.10)$$

Furthermore, the divergence of velocity will be zero for the incoming flow; although density variation will occur in the flamelet interior due to exothermic reaction. For flow into the flamelet counterflow at a distance far removed from the stagnation interface, u_ξ is only a function of ξ and u_χ is only dependent on χ , and thus the velocity derivatives $\partial u_\xi/\partial \chi$ and $\partial u_\chi/\partial \xi$ are each zero. That is, the vorticity does not appear explicitly for the inflow in the description within the rotating frame; however, it can have the important implicit effect through the centrifugal acceleration in the flamelet momentum equation and boundary condition, Eq. 4.8 and Eq. 4.17.

5.1.1 Vorticity, Enstrophy, and Viscous Dissipation

The vorticity is $\omega = \epsilon_{ijk} \partial u_j / \partial x_i$ where ϵ_{ijk} is the Levi-Civita tensor. The enstrophy is defined as the dot product of the vorticity vector with itself: $\vec{\omega} \cdot \vec{\omega} = \omega^2$. Thus, in the original coordinates, vorticity and enstrophy are given by Eqs. 5.11-5.12.

$$\vec{\omega} = \left\langle \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z}, \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x}, \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right\rangle ; \quad \vec{\omega} \cdot \vec{\omega} = \omega^2 \quad (5.11)$$

$$\begin{aligned} \omega^2 = & \left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 \\ & - 2 \left(\frac{\partial v}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial u}{\partial z} \frac{\partial w}{\partial x} + \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} \right) \end{aligned} \quad (5.12)$$

Assuming a Newtonian fluid with Stokes' hypothesis, the viscous stress τ_{ij} and the viscous dissipation rate Φ are given by Eqs. 5.13-5.15.

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \quad (5.13)$$

$$\Phi = \tau_{ij} \frac{\partial u_i}{\partial x_j} = \mu \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} - \frac{2}{3} \left[\frac{\partial u_k}{\partial x_k} \right]^2 \right) \quad (5.14)$$

$$\begin{aligned}
\frac{\Phi}{\mu} = & \frac{4}{3} \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] + \left(\frac{\partial u}{\partial y} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 + 2 \frac{\partial u}{\partial y} \frac{\partial v}{\partial x} \\
& - \frac{4}{3} \left[\frac{\partial u}{\partial x} \frac{\partial v}{\partial y} + \frac{\partial u}{\partial x} \frac{\partial w}{\partial z} + \frac{\partial v}{\partial y} \frac{\partial w}{\partial z} \right] \\
& + \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 + \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial w}{\partial y} \right)^2 + 2 \frac{\partial u}{\partial z} \frac{\partial w}{\partial x} + 2 \frac{\partial v}{\partial z} \frac{\partial w}{\partial y} \right] \quad (5.15)
\end{aligned}$$

Because we treat only the far-field inflows to the flamelet counterflow and not a region in the vicinity of the reaction zone, the following conditions hold:

- $u_\xi = f(\xi); u_\chi = f(\chi); w = f(z)$
- $\rho = \text{const}$ and $\mu = \text{const}$ as the far-field is sufficiently removed from the reaction zone
- the velocity field is divergence free, i.e., $\nabla \cdot \vec{u} = 0$

Since u and v are independent of z , four terms on the last line of Eq. 5.15 are zero-valued. The other two terms on that line are also zero-valued because w depends only on z . With $\omega/2 = \partial v/\partial x = -\partial u/\partial y$, as shown above, Eqs. 5.7-5.8 yield $\partial u/\partial x = \partial u_\xi/\partial \xi$ and $\partial v/\partial y = \partial u_\chi/\partial \chi$. Also, the last three terms on the first line of Eq. 5.15 become $\omega^2/4 + \omega^2/4 - 2\omega^2/4 = 0$. Equation 5.15 then reduces to Eq. 5.16.

$$\begin{aligned}
\frac{\Phi}{\mu} = & \frac{4}{3} \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 - \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} - \frac{\partial u}{\partial x} \frac{\partial w}{\partial z} - \frac{\partial v}{\partial y} \frac{\partial w}{\partial z} \right] \\
= & \frac{4}{3} \left[\left(\frac{\partial u_\xi}{\partial \xi} \right)^2 + \left(\frac{\partial u_\chi}{\partial \chi} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 - \frac{\partial u_\xi}{\partial \xi} \frac{\partial u_\chi}{\partial \chi} - \frac{\partial u_\xi}{\partial \xi} \frac{\partial w}{\partial z} - \frac{\partial u_\chi}{\partial \chi} \frac{\partial w}{\partial z} \right] \quad (5.16)
\end{aligned}$$

Because the inflows are divergence free, Eqs. 5.13-5.14 and Eq. 5.16 reduce to Eqs. 5.17-5.19.

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (5.17)$$

$$\Phi = \tau_{ij} \frac{\partial u_i}{\partial x_j} = \mu \left(\frac{\partial u_i}{\partial x_j} \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} \right) \quad (5.18)$$

$$\frac{\Phi}{\mu} = 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] = 2 \left[\left(\frac{\partial u_\xi}{\partial \xi} \right)^2 + \left(\frac{\partial u_\chi}{\partial \chi} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] \quad (5.19)$$

Using relations for Φ and ω^2 , the divergence of the momentum equation reduces to Eq. 5.20.

$$\frac{1}{\rho} \frac{\partial^2 p}{\partial x_i^2} = \frac{\omega^2}{2} - \frac{\Phi}{2\mu} \quad (5.20)$$

In the rotating frame, the centrifugal acceleration is given as $\vec{a} = \langle \xi \omega^2/4, \chi \omega^2/4 \rangle$. Therefore, $\nabla \cdot \vec{a} = \omega^2/2$. Since viscous dissipation maintains the same value in both reference frames, the implication is that the Laplacian of the pressure is identical in both reference frames. In order to maintain a pressure maximum at the stagnation point, the centrifugal effect must be overcome by the effect of the strain rate, i.e., $\omega^2 < A_{ij}A_{ij}$ where $A_{ij} \equiv \partial u_i / \partial x_j$. Here, we have a strong argument for the importance of balance between the vorticity and strain-rate magnitudes, or more precisely, between dissipation rate and enstrophy. There are many studies on these quantities, especially for incompressible flows [159–161]. If enstrophy, ω^2 , becomes too large compared to the dissipation rate divided by dynamic viscosity, Φ/μ , the pressure Laplacian becomes positive, destroying the counterflow since the required stagnation point located at a pressure maxima cannot occur. This vital issue of balance cannot be addressed in a formulation that considers strain rate but neglects vorticity. For incompressible turbulent flows, this balance has been addressed by Yeung et al. [161] who found that the temporal statistics of both quantities have similar magnitudes and that large values of both parameters tend to occur together with $\Phi/\mu > \omega^2$ for 60-65% of the data. Although the study does not include dilatation, it shows support for the concept of mixing

and reaction occurring in rotating counterflows provided by the turbulent eddies. When combustion is rate-limited by mixing, the higher-strain rate (smaller) eddies would provide the highest burning rates (provided the mixing rate does not exceed the reaction rate).

The turbulence kinetic energy dissipation rate, $\epsilon = \Phi/\rho$, when combined with Eq. 5.19, relates ϵ to the three strain rates in the rotating reference frame, S_1^* , S^* , and S_2^* . Recall from Chap. 3 that the non-dimensional strain rates S_1 and S_2 in the ξ and z directions are the dimensional strain rates S_1^* and S_2^* normalized by the dimensional compressive strain rate S^* in the χ direction. In non-dimensional form, $S_1 + S_2 = 1$.

$$\begin{aligned}\epsilon &= 2\nu \left[\left(\frac{\partial u_\xi}{\partial \xi} \right)^2 + \left(\frac{\partial u_\chi}{\partial \chi} \right)^2 + \left(\frac{\partial w}{\partial z} \right)^2 \right] = 2\nu [(S^* S_1)^2 + S^{*2} + (S^* S_2)^2] \\ &= 2\nu S^{*2} [S_1^2 + 1 + S_2^2] = 4\nu S^{*2} [S_1^2 + 1 - S_1] \quad (5.21)\end{aligned}$$

The implication of Eq. 5.21 is that if ϵ were known from the mean or resolved flow, a relation between S^* and S_1 is established for the RFM. This relation could be useful for SDR and FPV -based models as well. For example, with $S_1 = 1/2$, we find $S^* = \sqrt{\epsilon/(3\nu)}$, its peak value. As S_1 varies in the range $0 \leq S_1 \leq 1$, S^* varies narrowly between $\sqrt{\epsilon/(4\nu)}$ and $\sqrt{\epsilon/(3\nu)}$. In the range $-1 \leq S_1 \leq 0$ (stretched vortex tube), S^* varies more strongly between $\sqrt{\epsilon/(12\nu)}$ and $\sqrt{\epsilon/(3\nu)}$. Viscous dissipation actually occurs over a range of the smallest scales, not entirely at the Kolmogorov scale. Therefore, there is reason to multiply ϵ in Eq. 5.21 by the coefficient C_{vd} (with $0 < C_{vd} < 1$), which produces the first coupling relation for the mechanical constraints on the flamelet counterflow.

$$C_{vd}\epsilon = 4\nu S^{*2} [S_1^2 + 1 - S_1] \quad (5.22)$$

5.1.2 Kinetic Energy

Turbulence cascade theory suggests that the transfer rate of turbulence kinetic energy is the same from any scale to a lower scale within the inertial range; $\epsilon \approx (u')^2/\tau' \approx (u')^3/l'$, where u' , τ' and l' are the associated velocity, time, and length scales for a given portion of the turbulence spectrum. At the Kolmogorov scale, those scales are u_κ , τ_κ , and δ_κ , respectively, the Reynolds number $Re = u_\kappa \delta_\kappa / \nu \approx 1$, and the strain rate $u_\kappa / \delta_\kappa \approx \epsilon / u_\kappa^2$ is the largest value across all scales. The Kolmogorov velocity scale is $u_\kappa \approx (\epsilon \nu)^{1/4}$ and the Kolmogorov length scale is $\delta_\kappa \approx (\nu^3 / \epsilon)^{1/4}$ [2]. In the incompressible far-field, the counterflow is described by the velocity components in Eq. 5.23.

$$u_\xi = \frac{\partial u_\xi}{\partial \xi} \xi \quad ; \quad u_\chi = \frac{\partial u_\chi}{\partial \chi} \chi \quad ; \quad w = \frac{\partial w}{\partial z} z \quad (5.23)$$

Therefore, for the inflows, the kinetic energy is Eq. 5.24.

$$\begin{aligned} \frac{u^2 + v^2 + w^2}{2} &= \frac{1}{2} \left(\frac{\partial u_\xi}{\partial \xi} \right)^2 \xi^2 + \frac{1}{2} \left(\frac{\partial u_\chi}{\partial \chi} \right)^2 \chi^2 + \frac{1}{2} \left(\frac{\partial w}{\partial z} \right)^2 z^2 \\ &\quad + \frac{1}{8} \omega^2 (\xi^2 + \chi^2) + \left(\frac{\partial u_\chi}{\partial \chi} - \frac{\partial u_\xi}{\partial \xi} \right) \frac{\omega \xi \chi}{2} \end{aligned} \quad (5.24)$$

The right-hand side of Eq. 5.24 requires knowledge of three quantities: S^* , S_1 , and ω and the left-hand side can be related to the kinetic energy per unit mass, based on Kolmogorov scale velocity fluctuations. Note, this kinetic energy will be less than the statistical value for turbulence kinetic energy k since some has been dissipated at larger scales. The left-hand side can be related to ϵ through $u_\kappa \approx (\epsilon \nu)^{1/4}$ while the right hand side can be averaged over a volume of δ_κ^3 . This reduces Eq. 5.25.

$$C_{ke} \frac{\epsilon}{\nu} = 2S^{*2} \left[S_1^2 + 1 - S_1 + \left(\frac{\omega}{2S^*} \right)^2 \right] \quad (5.25)$$

$C_{ke} \leq 1$ is a nondimensional coefficient that appears in the averaging process for the kinetic energy term on the left side of Eq. 5.24. It accounts for both approximations made in the averaging process and the adjusted decrease in kinetic energy at the Kolmogorov scale because dissipation has occurred over a range of the smallest scales. Thus, a second coupling relation is obtained relating ϵ to the mechanical constraints on the RFM. Equations 5.22 and 5.25 can be combined to form Eq. 5.26.

$$\frac{\omega^2}{2} = \left(C_{ke} - \frac{1}{2}C_{vd} \right) \frac{\epsilon}{\nu} \quad (5.26)$$

This quadratic equation yields two solutions for ω of equal magnitude and opposite rotational direction; the direction is irrelevant. S_1 and S_2 magnitudes are also irrelevant to the magnitude of ω . Vorticity is of the same order of magnitude as the applied compressive strain rate. The enstrophy value determines whether the pressure Laplacian, from Eq. 5.20, is negative, which is needed for the counterflow flamelet to exist.

$$\frac{1}{\rho} \frac{\partial^2 p}{\partial x_i^2} = \frac{\omega^2}{2} - \frac{\Phi}{2\mu} = \left(C_{ke} - \frac{1}{2}C_{vd} \right) \frac{\epsilon}{\nu} - C_{vd} \frac{\epsilon}{2\nu} = (C_{ke} - C_{vd}) \frac{\epsilon}{\nu} \quad (5.27)$$

Specifically, the positive coefficient requires $C_{ke} < C_{vd}$ for the counterflow to exist. Each ϵ value produces one acceptable ω value and one acceptable S^* value. In this way, the dimension of the flamelet table actually remains the same (in terms of mechanical constraints) as the existing models using SDR or FPV since S^* and ω are given by ϵ , provided the various constants are prescribed.

When put together, we obtain relations whereby knowledge of ϵ from the mean or resolved flow determines the strain rate and vorticity applied to the flamelet model (mechanical constraints), and the pressure Laplacian and viscous dissipation. Velocity gradients will therefore differ from (be larger than) values of the mean or resolved flow, which is the goal. The scaling from mean or resolved scales for RANS or LES will impose boundary conditions

on the flamelet but will not prescribe directly the values in or near the reaction zone; in this critical manner, the approach differs from Peters' work [1, 8], models stemming from Peters' work, and the Flamelet Progress Variable method [77]. The variable ϵ is best described here as a "tracking variable" not a "progress variable" since it can increase or decrease in any spatial direction at any time.

The final-forms of the equations relating ϵ to the mechanical constraints of the RFM are given by Eqs. 5.28-5.29. Fortunately, the derivation recovers the behavior expected from the simple example given at the beginning of this section; i.e., that $S^* \approx C \sqrt{\epsilon/\nu}$.

$$S^* = \frac{1}{2} \sqrt{\frac{C_{vd} \epsilon}{\nu[S_1^2 + 1 - S_1]}} ; \quad \omega^* = \sqrt{\frac{2[C_{ke} - C_{vd}/2] \epsilon}{\nu}} \quad (5.28)$$

$$\frac{1}{\rho} \frac{\partial^2 p}{\partial x_i^2} = (C_{ke} - C_{vd}) \frac{\epsilon}{\nu} ; \quad \frac{\Phi}{\mu} = C_{vd} \frac{\epsilon}{\nu} \quad (5.29)$$

With application of the flamelet model to Kolmogorov scales, $C_{vd} < C_{ke} < C_{vd}$ must be supportable at least in a statistical sense because a counterflow-based flamelet model cannot be justified with a positive pressure Laplacian (see Eq. 5.29). The relation obtained between S^* , S_1 , and ϵ is similar in principle to Eq. 19 of Sanders and Lamers [162], relating small-scale strain rate to ϵ . Although Sanders and Lamers do not consider transverse strain rate magnitudes or vorticity in their derivation, they too adopt a coefficient called $C_{s,1}$ (similar to C_{vd}) which is empirically tuned to match flame liftoff height. They obtain $C_{s,1} \approx 0.1$ which corresponds to $C_{vd} = 0.015$ for $S_1 = 0.5$. Bradley et al. [163] state that the flamelet strain rate should be "appreciably less than $\epsilon/6\pi\nu$ " which corresponds to $C_{vd} < 0.159$. Thus, while the coefficients are somewhat case-dependent, one can expect $C_{vd} \ll 1$ and $C_{ke} \ll 1$. As of the writing of this dissertation, the Sirignano-Liu research group at UC Irvine is conducting DNS studies to hone in on values for C_{vd} and C_{ke} , among other goals.

The ϵ -based coupling procedure has been used in conjunction with the traditional flamelet ap-

proach in two works. The first is a comparison of ϵ -based mechanical coupling with FPV coupling in an accelerated mixing layer produced by a convergent-divergent nozzle. In this work, Walsh et al. [164] generated flamelet solutions following Eq. 2.25, and coupled the flamelet model to 2-dimensional RANS via ϵ as in Eq. 5.28 and via the Flamelet Progress Variable (FPV) approach [77]. The FPV method was found to place near-equilibrium flamelet solutions ($S^* \approx 0$) in regions of high strain rate. This is because there is no physical mechanical coupling in the FPV approach; rather, the flamelet representing a given mean-flow cell is chosen by matching the amount of products present in the mean flow to the amount of products present at a particular Z value in the flamelet. Regardless of the strain rate, if the mean flow cell has substantial products, the FPV will choose a flamelet with a similarly large amount of products, which generally occurs when the flamelet strain rate is low. It may be possible to avoid this to some degree by trial and error testing of the weights of products defining the progress variable, but correct results are not ensured and significant ambiguity remains. Using the ϵ -based approach resulted in the flamelet strain rate S^* having substantial spatial correlation with the resolved scale strain rate (as it should), and thus equilibrium solutions were only present in regions of near-zero strain. Regions of high strain rate showed flamelet solutions closer to, at, and beyond, flammability limits, thus giving more believable results for flame extinction and standoff. Furthermore, by allowing for mean-flow species transport equations in which the flamelet model quantifies only the source terms, convective and diffusive redistribution of products to quenched zones promotes re-ignition. This aspect is critical to the simulation of combustors that achieve flame stability via recirculating hot products. The second utilization of the ϵ -based coupling procedure with traditional flamelets (Walsh et al. [165]) investigated JP-5 combustion in a turbine passage for the established turbine-burner concept [166–169]. The ϵ coupling procedure enabled this investigation because it does not suffer from the FPV equilibrium solution issue and because it removes the need to choose ambiguous FPV weights among the 119-species in the mechanism.

5.2 RFM Backward Coupling to RANS or LES

As was discussed throughout this manuscript, the RFM is a fundamentally different type of flamelet model than scalar dissipation rate or FPV-based models. Within a RANS or LES cell, there are many Kolmogorov volumes. Theoretically, each of those Kolmogorov volumes is represented by a three-dimensional counterflow subjected to the local Kolmogorov-scale velocity gradients and scalars that exist there. Since there is no way of separately specifying the conditions for each Kolmogorov volume within the larger CFD cell, the RFM approximates the heat release rate (HRR) and species production rates of the CFD cell via one representative three-dimensional counterflow, subjected to the approximate or averaged Kolmogorov velocity gradients and scalars that best represent the cell. Therefore, the output fed back to the RANS or LES equations is an integrated value over flamelet domain, which is then scaled by the size of the volume it represents. Once the raw flamelets have been computed, the thermochemical state is a function of physical position along the counterflow axis. Using these vectors, the raw heat release rate (HRR, or $\dot{Q}''_{\kappa}$) is calculated according to Eq. 5.30 and the raw species production rates (SPR or $\dot{\omega}''_{m,\kappa}$) are calculated via Eq. 5.31. The number of “primes” (') indicates the exponent of the length unit in the denominator.

$$\dot{Q}''_{\kappa} = \int_{-\infty}^{\infty} \sum_{m=1}^{n_{sp}} \dot{\omega}_m(\chi) h_{f,m} d\chi \quad \left(\frac{J}{m^2 \cdot s} \right) \quad (5.30)$$

$$\dot{\omega}''_{m,\kappa} = \int_{-\infty}^{\infty} \dot{\omega}_m(\chi) d\chi \quad \left(\frac{kg}{m^2 \cdot s} \right) ; \quad m = 1, 2, 3, \dots n_{sp} \quad (5.31)$$

Since the flamelet represents a volume rather than an area and because RANS and LES equations typically use per $m^3 \cdot s$ basis units, another length must be divided into the HRR and SPR. The raw flamelet properties cannot use their own domain size as a reference length because the domain size varies from flamelet to flamelet. Thus, the flamelet outputs are computed per $m^2 \cdot s$ instead of $m^3 \cdot s$ due to the arbitrariness of the additional length

parameter. In other words, the integrated $\dot{Q}''_{\kappa}$ and $\dot{\omega}''_{m,\kappa}$ directly from the flamelets are not divided by the flamelet domain length in order to achieve a per $m^3 \cdot s$ basis. Instead, the flamelet outputs $\dot{Q}''_{\kappa}$ and $\dot{\omega}''_{m,\kappa}$ are divided by the Kolmogorov-scale reference length as computed from ϵ , $\delta_{\kappa} = (\nu^3/\epsilon)^{1/4}$, to achieve the proper units. These are the values fed back to the RANS or LES code and are shown in Eqs. 5.32-5.33.

$$\dot{Q}'''_{CFD} = \frac{1}{\delta_{\kappa}} \dot{Q}''_{\kappa} = \frac{1}{(\nu^3/\epsilon)^{1/4}} \dot{Q}''_{\kappa} \quad \left(\frac{J}{m^3 \cdot s} \right) \quad (5.32)$$

$$\dot{\omega}'''_{m,CFD} = \frac{1}{\delta_{\kappa}} \dot{\omega}''_{m,\kappa} = \frac{1}{(\nu^3/\epsilon)^{1/4}} \dot{\omega}''_{m,\kappa} \quad \left(\frac{kg}{m^3 \cdot s} \right) \quad (5.33)$$

5.3 Scalar Coupling

The second aspect of flamelet forward coupling pertains to the actual mixture that is combusting. Classical flamelet theories assume that every flamelet has the same mixture and temperature (or enthalpy) boundary conditions, which means that the flamelet counterflow itself has no relation to the specific mixture or temperature in a given CFD cell. The inflows in the classical theories simply use the global inflow conditions; e.g. pure oxygen and pure fuel at low temperature as would emanate from a rocket engine injector plate. Since these flamelets do not respect the local scalar values in a RANS or LES cell, the β -PDF is necessary to “slice out” a portion of the flamelet counterflow domain over which the flamelet mixture fraction varies in the same statistical range as that suggested by the specific RANS or LES cell. While this coupling method is certainly numerically feasible for the RFM, and may be sufficient in certain applications, it presents a physicality problem because the RFM is a true sub-grid model. As the β -PDF method is covered in the literature, it will not be discussed here. The foundational basis of the RFM counterflow being on the Kolmogorov scale, subject to far-field strain rates and with a uniform vorticity magnitude across it, means that

it would be physically inconsistent to use the β -PDF to slice out a portion of the domain. From first principles, it makes much more sense to set the RFM scalar boundary conditions consistently with the mixture and temperature (or enthalpy) in a given RANS or LES cell. Obviously, these scalars vary greatly through the global scale, and thus a matrix of RFM scalar boundary conditions is necessary to cover the range of possible mixtures. The question then becomes, given mass fractions and temperature (or enthalpy) in a mean or resolved flow cell, what are the appropriate scalar boundary for the flamelet? The basic issue with varying the scalar boundary conditions is that unless inflows are either chemically-inert or in chemical equilibrium at the given boundary temperature, reactions will occur at the boundary, preventing a quasi-steady numerical solution. This is especially problematic if the inflows are partially-premixed, and unfortunately, is still a problem if the boundary composition is a pure fuel or oxidizer at elevated temperature. For example, with pure CH_4 above $\sim 1800\text{ K}$, dissociation will convert a non-negligible portion of CH_4 to CH_3 , H_2 , and H , while decreasing the temperature. In reality, the flamelet inflows should correspond to the mixture indicated by the RANS or LES cell, and the dissociation problem would be mitigated by a finite time evaluation of the flamelet. This introduces the consideration of unsteady flamelets which has been considered for the RFM using one-step-kinetics [64]; however, it is not the present topic. As of writing this dissertation, the boundary condition question is still open; however, speculation on scalar closure ideas is presented in the following sections.

5.3.1 Scaling Scalar Gradients

In comparison to velocity gradients, scalar gradients have far less literature describing magnitude changes across the turbulence spectrum. As discussed in prior chapters, theory exists for the governing equations of non-reacting scalars; however, little literature covers reacting scalars. In general, an equation governing a non-reacting scalar is invalid for a reacting scalar because the non-reacting scalars are only convected and diffused, which makes their

gradients rather smooth, non-intermittent, and near isotropic. Reacting scalars, however, are also created and destroyed, which introduces sharp gradients and intermittency. Therefore, this section develops a scaling procedure under the assumption that a conserved scalar, such as mixture fraction or Shvab-Zeldovich variables, may be used. While differences between molecular diffusivities, thermal diffusivity, and kinematic viscosity are important on the laminar flamelet scale, they are inconsequential on larger scales because the turbulent diffusivity is of much higher magnitude. This property of the inertial sub-range of the turbulent cascade allows the creation of various conserved scalars which generally follow the same scaling relations.

Consider the non-reacting conserved scalar, $F = \bar{F} + F'$, where $\bar{F}$ is the mean and F' is the fluctuation. The variance is defined as $g \equiv \overline{F'^2}$. Half of the dissipation rate of this scalar is $\epsilon_g = D|\nabla F'|^2$. Elghobashi [170] proposes a transport equation for g (in which F is the mixture fraction) for the case of steady, non-premixed combustion, in cylindrical combustion chambers and found trend-correct agreement with experimental data. However, this work identified, but did not account for differences in time scales between velocity and scalar fields. Later, Newmann et al. [36] and Elghobashi and Launder [37] proposed a two-equation model for g and ϵ_g , in similar fashion to the $k - \epsilon$ model for the turbulence kinetic energy and turbulence kinetic energy dissipation rate, whereby both time scales have sink terms in the ϵ_g equation. They found good agreement with experimental data of decaying homogeneous turbulence away from solid boundaries. In this way, we are stretching the assumptions. If these equations are taken to be valid for a reacting flow, g and ϵ_g can be computed by the RANS or LES code. Assuming the dissipation rate of the scalar quantity is the same through the inertial range, then the scalar gradient on the Kolmogorov scale may be approximated.

Alternatively, if the fluctuation of the conserved scalar on the Kolmogorov scale, F'_κ is assumed to scale similarly to velocity where $k = \frac{1}{2}\overline{u'_i u'_i}$, then $F'^2_\kappa/g \approx u'^2_\kappa/k \approx (\nu\epsilon)^{1/2}/k$

and $|F'_\kappa| \approx (\nu\epsilon)^{1/4}(g/k)^{1/2}$. Therefore, the magnitude of the gradient of F'_κ on the Kolmogorov scale is $|\nabla F'_\kappa| \approx |F'_\kappa|/\delta_\kappa \approx (\epsilon/\nu)^{1/2}(g/k)^{1/2}$ where relations for the Kolmogorov length $\delta_\kappa = (\nu^3/\epsilon)^{1/4}$ and velocity $u'_\kappa = (\nu\epsilon)^{1/4}$ from Pope [2] were used. Furthermore, if the kinematic viscosity of the fluid and the diffusivity associated with F are assumed to be equal, then $\epsilon_g \approx \epsilon g/k$. It may be necessary to add a constant in the prior expression based on empirical findings but this has not been investigated. Anyway, this train of thought bypasses the need for a conservation equation for ϵ_g as ϵ_g is related to g , ϵ , and k algebraically. In either case, g and ϵ_g along with k and ϵ are calculated by the RANS or LES code. For the moment, we will use the later of the two versions and assume that the scalar gradients are in the direction associated with compressive strain as shown by [115–119]. Then the scalar gradient on the Kolmogorov scale is given by Eq. 5.34, and a constant could be multiplied in if necessary.

$$\left. \frac{dF}{dy} \right|_\kappa \approx \left(\frac{\epsilon}{\nu} \right)^{1/2} \left(\frac{g}{k} \right)^{1/2} \quad (5.34)$$

We assume the average value of the conserved scalar across the flamelet scale is taken to be equal to the local mean value on the integral scale; $F_\kappa \approx \bar{F}$ then the flamelet boundary values for F_κ are calculated by extrapolating the average value, $\bar{F}$, to $\pm\infty$ via the gradient $dF/dy|_\kappa$ times some integer number of Komogorov lengths as shown in Eq. 5.35. This is a first-order Taylor expansion of the conserved scalar.

$$F_{\kappa,+\infty} = \bar{F} + \left. \frac{dF}{dy} \right|_\kappa N\delta_\kappa \quad F_{\kappa,-\infty} = \bar{F} - \left. \frac{dF}{dy} \right|_\kappa N\delta_\kappa \quad (5.35)$$

The best choice for N is an ongoing area of research; however, we lean toward the lowest value possible for two reasons. First, the RFM is by definition a Kolmogorov-scale model and in general the reaction zone is smaller than the Kolmogorov scale; therefore, going to $\pm\delta_\kappa/2$ should in theory be far enough away to obtain Dirichlet scalar boundary conditions. Secondly, although F is normalized to vary in some confined range, $0 \rightarrow 1$ if $F = Z$, the

Taylor expansion in Eq. 5.35 is not limited to any range, which means that there is a maximum value of N for which $F_{\kappa,+\infty}$ and $F_{\kappa,-\infty}$ are obtained within their allowed range. If N exceeds this maximum (which is dependent on the local magnitude of the gradient), then the boundary values for F will not be physical; e.g., $Z < 0$, $Z > 1$, $Y_m < 0$, $Y_m > 1$. These cases would then require some ad hoc correction, which we would like to avoid. In a cursory testing of this method using Shvab-Zeldovich variables, mass fractions were routinely found outside of their physical range.

Once the values of the conserved scalar are known for the two flamelet inflows, they must be converted to mass fractions and temperature or enthalpy. There are a few paths here. If Shvab-Zeldovich variables are used to form F , then the mass fractions and enthalpy can be backed out relatively easily; however, this will not work for a multi-step chemical kinetics formulation which is one of the primary motivations for using a flamelet model. If one accepts a one-step chemistry approach, then this would be valid and the flamelet model would still allow inclusion of finite-rate chemistry effects, which is the other primary motive for use. If multi-step chemistry is desired, then it would be better to use the mixture fraction as the conserved scalar; however, this suffers from the differential diffusion problem discussed in Sec. 2.4.3 and Sec. 3.4.4-3.4.5 and does not distinguish between products and reactants for the boundary conditions. Regardless of the chemical kinetics, the extrapolation of scalar boundary conditions guarantees that practically all flamelet inflows will be complex mixtures including products at elevated temperature, not pure fuel and pure oxidizer at the global inflow temperatures, and some of these will be partially-premixed mixtures.

This poses two more two issues in solving the RFM governing equations. First, the mesh is tricky. Pure diffusion flames only have central gradients, which means that fine mesh is only necessary near the stagnation point, and the domain is rather small. Together, these attributes result in a relatively low number of required mesh points which make the numerical solution fast and, in practice, stable. However, if premixed or partially-premixed

mixtures exist for the inflows, a triple flame will likely result, having separate lean or rich premixed flames that burn out from the stagnation point. There is no way to know a priori where these flames will stabilize, which means that a complex adaptive mesh refinement algorithm is necessary. Furthermore, the domain size increases substantially because many premixed flames will stabilize far from the stagnation point; i.e., while a diffusion flame may be solved on a domain of a few Kolmogorov lengths, a premixed flame may stabilize at $10\delta_\kappa - 100\delta_\kappa$. This results in many hundreds or thousands more mesh points and much longer computation times. This also raises the physical issue that a premixed flame stabilized far from the stagnation point is well outside of the Kolmogorov eddy where the RFM is designed to operate. Therefore, even if it were numerically simple to solve these triple flames, the output would be inconsistent with the physical domain of applicability of the RFM.

The second issue pertains to the flamelet table dimension. For a fixed non-dimensional vorticity ω , and fixed S_1 and S_2 combination, the table will have one dimension for S^* (or ϵ), and two dimensions for each scalar property that is allowed to vary in the inflows (one for each of the two boundaries). For a diffusion flame having no fuel on one side, no oxidizer on the other, and a pre-defined vector of products in both inflows, the table has five dimensions: S^* , $T_{-\infty}$, $T_{+\infty}$, $Y_{O,-\infty}$, $Y_{F,+\infty}$. A typical S-curve may have $O(100)$ individual flamelet solutions and if each of the scalars has 10 increments between their minimum and maximum values, the table will have $O(10^5)$ individual flamelet solutions. This is a lot of solutions to compute and would take weeks on a personal computer even with a simple chemical kinetics model. If premixed mixtures are allowed for the inflows, the dimension would increase $100\times$ to $O(10^7)$ individual solutions. Furthermore, reactions at the boundaries will be an issue if there are products, radicals, and reactants at the boundary which are not in chemical equilibrium, so this method does not work even if the necessary computational resources were available.

5.3.2 Criteria for Practical Scalar Boundary Conditions

With the issues identified in the prior section in mind, a scalar coupling procedure that is ideal in the practical sense would have the following features: 1) gradients multiplied by $N\delta_\kappa$ are not used because N is arbitrary and case dependent, which causes flamelet boundary conditions to be un-physical; 2) Shvab-Zeldovich variables are not used because they do not allow for detailed chemical kinetics; 3) mixture fraction is not used because it does not allow for differential diffusion and cannot distinguish between products and reactants; 4) premixed, partially-premixed, or any other thermodynamic state producing significant reactions at the flamelet boundaries are avoided so that a numerical solution is possible. These criteria motivated ideas for other scalar coupling procedures.

5.3.3 Cell-averaged Scalar Boundary Conditions

One method which allows for varying scalar boundary conditions while ensuring that reactions do not disturb the boundaries is to assume that inflow mixtures are given enough time to reach equilibrium on larger scales, thereby requiring the RFM to solve diffusion flames only. This is done via a 0-D equilibration of the boundary mixture. This assumption is numerically convenient; however, it ignores all finite-rate effects of the inflows. Turbulence can induce flame stretch and curvature, which alter partially-premixed flames and cause extinction. Thus, if this method were pursued, a better treatment of partially-premixed flames would be desired, which would likely yield a hybrid model in which a partially-premixed flamelet model accounts for the boundary mixture and then feeds the output to the RFM. However, since the RFM is designed for globally non-premixed flows, and a hybrid model is beyond the scope of this work, we explore this highly simplified version of the coupling procedure as an “investigation of concept,” accepting that the premixed flame treatment ignores finite-rate effects.

To reduce the dimensionality of the flamelet table, only two scalar inputs are used: $Y_{O,I}$ and $Y_{F,I}$. These are the mass fractions of O_2 and primary fuel in the RANS or LES cell, respectively. Given $Y_{O,I}$ and $Y_{F,I}$, a piecewise function is used to determine the RFM scalar boundary conditions, $Y_{O,L}$ and $Y_{O,R}$ which are the O_2 mass fractions of the left and right inflows, and $Y_{F,L}$ and $Y_{F,R}$ which are the primary fuel mass fractions of the left and right inflows. This is shown in Table 5.1. Here, primary fuel means the global fuel; e.g. CH_4 for methane-oxygen combustion. Since $Y_{O,L} + Y_{F,L}$ and $Y_{O,R} + Y_{F,R}$ generally will not sum to one, the remaining mass fractions are filled with $\vec{Y}_{P,I}$, which is a pre-determined vector of product mass fractions. The product vector could be primary products; e.g., CO_2 , H_2O , and CO , or could be computed from stoichiometric equilibrium of the global fuel and oxidizer inflows. This way, if a mean or resolved-scale cell contains products, the flamelet inflows will also contain products of similar proportion and enthalpy; however, they will be equilibrated before entering the counterflow domain. The multiplication by two in many cells of the table is necessary to preserve the ratio of fuel, oxidizer, and products, when splitting the singular RANS or LES cell values into the binary counterflow inflows.

Table 5.1: Mass Fraction Boundary Conditions

$Y_{m,I}$	$Y_{O,I} \leq 0.5; Y_{F,I} \leq 0.5$		$Y_{O,I} \leq 0.5; Y_{F,I} > 0.5$		$Y_{O,I} > 0.5; Y_{F,I} \leq 0.5$	
side	Left	Right	Left	Right	Left	Right
Y_O	$2Y_{O,I}$	0	$2Y_{O,I}$	0	1	$2Y_{O,I} - 1$
Y_F	0	$2Y_{F,I}$	$2Y_{F,I} - 1$	1	0	$2Y_{F,I}$
$\Sigma \vec{Y}_P$	$1 - Y_{O,L}$	$1 - Y_{F,R}$	$1 - Y_{F,L} - Y_{O,L}$	0	0	$1 - Y_{F,R} - Y_{O,R}$

Mass fraction boundary conditions. For each of the three combinations of mean or resolved flow fuel and oxidizer mass fraction, the left and right flamelet boundary mass fractions are given.

Next, the temperatures of the left and right inflows must be determined. This is done using a weighted average of the amount of fuel, oxidizer, and products. The oxidizer, fuel, and product temperatures are assumed to be at $T_{O,I}$, $T_{F,I}$, and $T_{P,I}$, respectively. Thus, once the left and right flamelet inflow mass fractions are determined, their temperatures can be

determined as shown in Table 5.2. The temperature of the RANS or LES cell could also be used as the boundary temperature; however, doing so adds another table dimension.

Table 5.2: Temperature Boundary Conditions

$Y_{O,I} \leq 0.5; Y_{F,I} \leq 0.5$		$Y_{O,I} \leq 0.5; Y_{F,I} > 0.5$		$Y_{O,I} > 0.5; Y_{F,I} \leq 0.5$	
Left	Right	Left	Right	Left	Right
$Y_{O,L}T_{O,I} + Y_{P,L}T_{P,I}$	$Y_{F,R}T_{F,I} + Y_{P,R}T_{P,I}$	$Y_{O,L}T_{O,I} + Y_{F,L}T_{F,I} + Y_{P,L}T_{P,I}$	$T_{F,I}$	$T_{O,I}$	$Y_{O,R}T_{O,I} + Y_{F,R}T_{F,I} + Y_{P,R}T_{P,I}$

Temperature boundary conditions. For each of the three combinations of mean or resolved flow fuel and oxidizer mass fraction, the left and right flamelet boundary temperatures are given.

Once the raw boundary conditions for the left and right inflows are determined, the partially-premixed mixtures are removed via conserved enthalpy equilibration. For this demonstration, the sequences of $Y_{F,I}$ and $Y_{O,I}$ were chosen to vary from 0.0 to 1.0 in 21 increments. For constant values of S_1 , S_2 , ω , and pressure, the resulting flamelet table has only three input dimensions: S^* , $Y_{F,I}$, and $Y_{O,I}$. The heat release rate of this formulation is shown in Fig. 5.2 for CH_4/O_2 combustion using a 12-species version of the FFCM-1 mechanism [127]. The global fuel and oxidizer temperatures are $T_{F,I} = 300 \text{ K}$ and $T_{O,I} = 1000 \text{ K}$ and the product vector $\vec{Y}_{P,I}$ and temperature $T_{P,I}$ are computed from stoichiometric CH_4/O_2 equilibrium beginning from the mass-weighted initial temperature.

While equilibrating the boundary conditions is likely too great an assumption for an accurate coupled simulation, these figures do illustrate a few important points. For cases in which the inflows mimic classical flamelets; i.e., substantial fuel on the fuel side and substantial oxidizer on the oxidizer side, classical behavior is observed. Specifically, HRR increases with strain rate until the extinction limit is reached. This is most obvious for $Y_{O,I} = 0.4, 0.5$, and 0.6 . Secondly, HRR magnitude and extinction limits differ substantially with different inflow mixtures. Cases with low temperatures, substantial non-premixed fresh reactants, and low radical pools in the inflows tend to have high HRR magnitudes and extinction limits

(classical behavior). However, cases with higher temperatures and higher radical pools with fewer fresh reactants have lower HRR magnitudes and often no extinction limit within the S^* range over which the flamelets were computed. Note that this occurs both when there are significant products in the mean flow cell ($\Sigma \vec{Y}_{P,I}$ is high) and when the raw, pre-equilibrium boundary mixtures constitute partially-premixed flames ($Y_{O,I} > 0.5$ or $Y_{F,I} > 0.5$). This second situation is especially evident for the $Y_{O,I} = 0.4$ plot when $Y_{F,I} = 0.55$. Since $Y_{F,I} > 0.5$, the oxidizer boundary mixture contains 10% fuel by mass, which when equilibrated, produces high temperature ox-rich products that feed a central diffusion flame. The tendency for these cases to have lower HRR magnitudes and no extinction limit is because fuel oxidation requires long residence times, resulting in extinction, while radical recombination reactions happen quickly and can therefore tolerate extreme strain rates. As the radical recombination reactions are primarily between hydrogen and oxygen, water becomes the major product produced under extreme strain rates while hydrocarbons do not react. The dominance of radical recombination over hydrocarbon oxidation is shown in all sub-figures for curves of $Y_{F,I}$ which are non-zero up to the maximum S^* value. These cases are better described as boundary-stabilized reaction zones rather than classical combustion because they do not require a self-sustaining central diffusion flame to continue releasing heat. The cases showing extinction do so because there is a diffusion flame between low enthalpy fuel-rich and ox-rich streams which must provide its own heat to burn. When the residence time gets too short, the fuel-oxidation pathways shut off and the flame goes extinct. While the equilibrium treatment of boundary mixtures is not appropriate for a coupled simulation, these figures and findings suggest that flamelet models which do not account for high enthalpy radical pools in the inflow mixtures may under-predict HRR and species production in combustors that stabilize flames via recirculated high-enthalpy products. Furthermore, DNS data of non-premixed flames indicates that under high strain rates, fuel and oxidizer do not react, yet mixing still occurs. When the partially-premixed mixture then gets convected to a region of lower strain rate or local strain rate decreases due to fluctuating turbulent

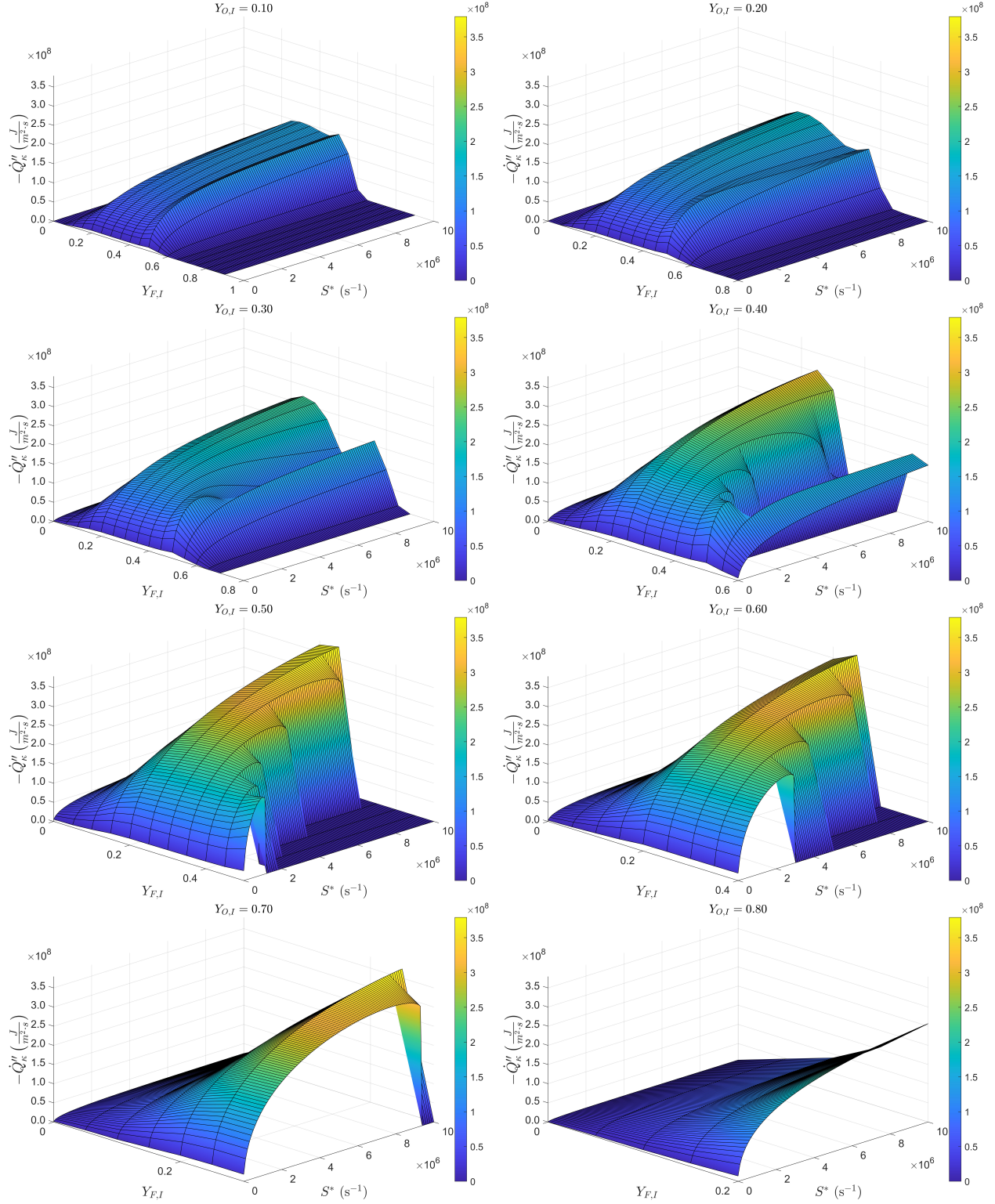


Figure 5.2: Integrated heat release rate (HRR or $-\dot{Q}''_{\kappa}$) as a function of CFD cell fuel and oxidizer mass fractions, $Y_{F,I}$ and $Y_{O,I}$.

intensity, that unburned partially-premixed mixture may react, suggesting variable scalar inflows to the flamelet model may better predict turbulent reacting flows.

5.3.4 Fixed Scalar Boundary Conditions

Due to the complications of variable mixture and enthalpy boundary conditions, a simpler and lower-dimensional coupling approach may be useful in some scenarios. In keeping with the classical flamelet approach, the RFM boundary conditions could be set according to the global fuel and oxidizer inflow conditions. Every flamelet would then be a diffusion flame between pure fuel at $T_{F,I}$ (the global fuel inflow temperature) and pure oxidizer at $T_{O,I}$ (the global oxidizer inflow temperature). To account for areas in which there is little to no flammable mixture, a scale factor could be multiplied into the flamelet output so that *each flamelet is a canonical, Kolmogorov-scale, counterflow diffusion flamelet representing only the unburned fuel and oxidizer present in the cell*. In this way, the RANS or LES cell composition would determine how much of the canonical flamelet HRR and SPR are fed back to the RANS or LES source terms. The reactant scale factor f should be jointly-based on the cell mass fractions of fuel and oxidizer to ensure that heat and products are only produced when fuel and oxidizer are both present. With ν_c being the stoichiometric mass ratio, the reactant scale factor is given by Eq. 5.36 and would then be multiplied into Eqs. 5.32-5.33 as shown below in Eqs. 5.37-5.38.

$$f = \min(\nu_c Y_{F,I}, Y_{O,I}) \quad (5.36)$$

$$\dot{Q}_{CFD}''' = f \frac{1}{\delta_\kappa} \dot{Q}_\kappa'' = \frac{1}{(\nu^3/\epsilon)^{1/4}} \dot{Q}_\kappa'' \quad \left(\frac{J}{m^3 \cdot s} \right) \quad (5.37)$$

$$\dot{\omega}_{m,CFD}''' = f \frac{1}{\delta_\kappa} \dot{\omega}_{m,\kappa}'' = \frac{1}{(\nu^3/\epsilon)^{1/4}} \dot{\omega}_{m,\kappa}'' \quad \left(\frac{kg}{m^3 \cdot s} \right) \quad (5.38)$$

Depending on the range of temperatures experienced by the fluid, a flamelet boundary temperature limit may be required to prevent dissociation at the inlets. This is to avoid gradients at Dirichlet boundaries which constitute ill-posed numerical problems. This can also be avoided via equilibration of the boundary conditions prior to solving the flamelet; however, doing so ignores finite-rate effects. The issue of gradients at the boundaries frequently arises when the oxidizer is pure O_2 because the maximum temperatures of RANS or LES cells are then likely to exceed the reactant dissociation temperatures, regardless of the fuel choice. This issue is unlikely to arise in situations where the oxidizer is substantially diluted or the mixture is sufficiently rich or lean such that the maximum cell temperatures are below the fuel and oxidizer dissociation temperatures. Examples of HRR, S-curve surfaces, and SPR are given in Fig. 5.3 and Fig. 5.4 with pure O_2 as the left inflow mixture and pure CH_4 as the right inflow mixture. The boundary condition temperature range is kept below 1800 K to avoid substantial dissociation at the boundaries.

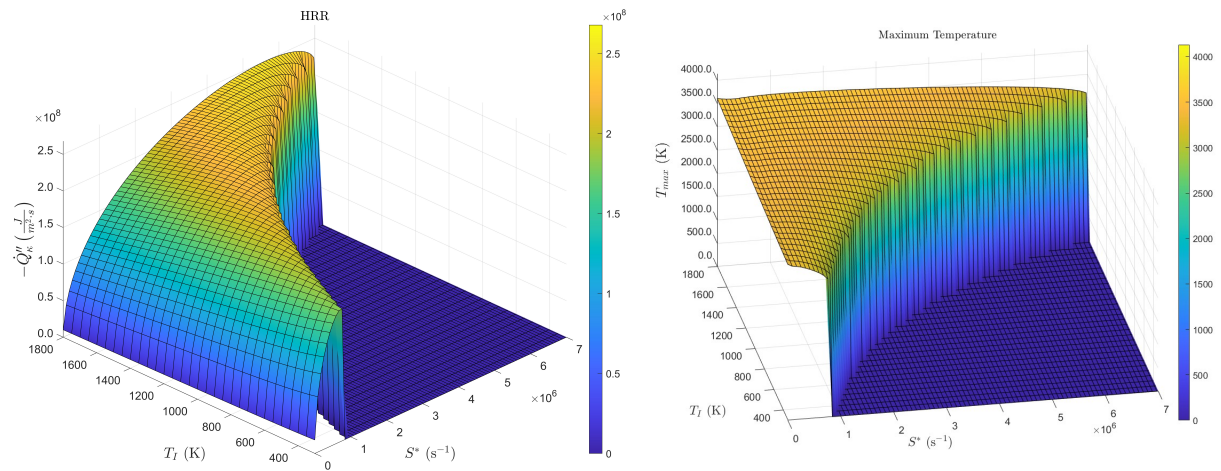


Figure 5.3: Integrated heat release rate (HRR or $-\dot{Q}''_{\kappa}$) and maximum temperature as a function of CFD cell temperature, T_f .

It is evident from Figs. 5.3-5.4 in contrast to Fig. 5.2 that varying the flamelet boundary temperatures alone produces significantly different behavior in maximum HRR, maximum temperature, SPR, and extinction limits. Except in cases where boundary temperatures are high enough to cause dissociation, this method of varying the boundary temperatures in accordance with the CFD cell temperature while keeping inflow mixtures fixed, provides

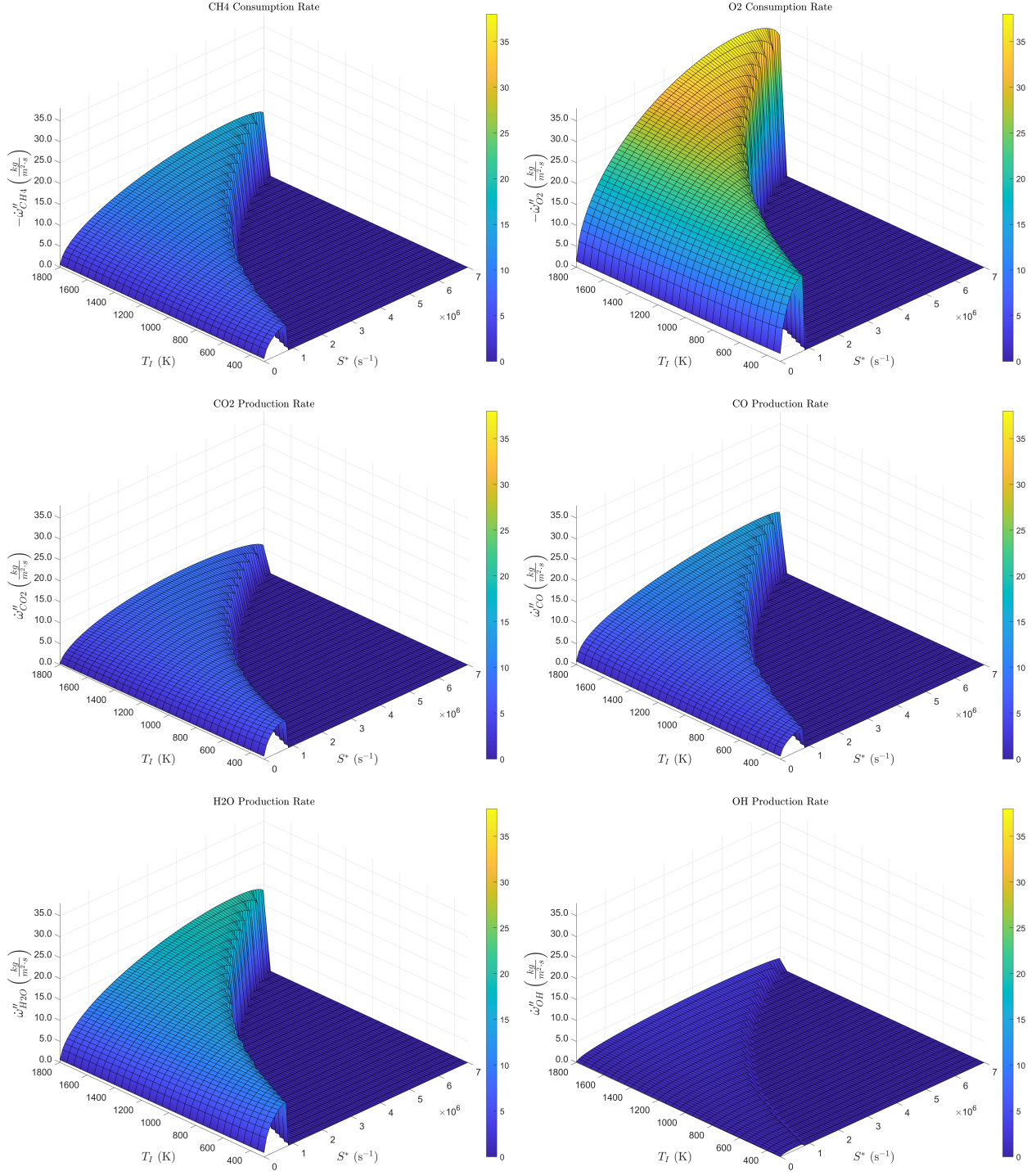


Figure 5.4: Integrated species production and consumption rates (SPR or $\pm \dot{\omega}_{m,\kappa}''$) as a function of CFD cell temperature, T_I .

a straightforward pathway to couple the CFD cell thermodynamic state with the flamelet boundary conditions. While there is a clear issue for cases with high cell temperatures, this

method may perform well in practical jet engine combustors where mixtures are kept lean in order to avoid turbine thermal fatigue and mitigate NOx formation.

Chapter 6

Conclusions

The Rotational Flamelet Model (RFM) is a novel chemistry closure method for RANS and LES simulation of non-premixed, turbulent reacting flows. Non-premixed flows typically have high Damköhler numbers, which indicate that heat release rates (HRR), and species production rates (SPR), are rate-limited by mixing rather than by chemical reaction rates. Therefore, the RFM is based on the supposition that the dominant portions of HRR and SPR occur on the smallest turbulent length scales (Kolmogorov scales) because these scales are subjected to the highest mixing rates. DNS studies of non-premixed turbulent reacting flows indicate that Kolmogorov velocity gradients are asymmetric and highly rotational, with the vorticity magnitude being on the same order as the major compressive strain rate. Prior flamelet models have assumed planar-symmetric or axisymmetric velocity gradients without rotation, and frequently solve the flamelet equations without momentum equations or detailed molecular transport. The RFM improves flamelet modeling by explicitly accounting for asymmetric velocity gradients and vorticity in the momentum equations, without a necessity to invoke any assumptions about constant thermo-physical properties, molecular diffusion rates, or Lewis numbers. Through the inclusion of vorticity and asymmetric velocity gradients, flamelet extinction limits are shown to increase by up to 43.5% for

the various fuel/oxidizer combinations tested. Overall, the RFM introduces vital physics to counterflow-based flamelets, leading to a wholistic description of flammability limits in terms of all sub-grid velocity gradients.

The RFM has been used to compute flamelet solutions for a variety of fuel/oxidizer combinations, including $\text{H}_2\text{-N}_2/\text{O}_2$, JP-5/Air, and CH_4/O_2 , and in all cases, shows that the inclusion of vorticity in the momentum equations creates a centrifugal effect that extends flammability limits appreciably. Non-premixed flames rely on diffusion to produce a flammable mixture, which when burning, provides enough heat for the flame to sustain itself. The diffusion, preheat, and reaction processes require finite time to occur, and thus when the strain rate in the fluid exceeds a critical threshold, the residence time in the flame zone decreases to the point where the flame cannot self-sustain, and extinction occurs. In order for a RANS or LES simulation to accurately predict combustion phenomena and engine performance metrics such as peak temperature, hot/cold streaks, flame standoff, lean-blowout, extinction and re-ignition, combustion instabilities, thrust, power, efficiency, and pollutant formation, the flamelet closure model must accurately quantify the extinction limit, HRR, and SPR across the range of possible conditions. The RFM does this via an explicit calculation of the sub-grid fluid structure. Specifically, flamelets are parameterized by far-field strain rates with a uniform vorticity magnitude over the domain, allowing the solution (subject to the full set of governing equations) to conform to the boundary conditions and determine the local flame structure. Vorticity creates a centrifugal acceleration that reduces the flame-local strain rate, and thereby increases the flammability limit. This also causes a reduction in mass flux that results in a reduction in HRR and SPR for a given asymptotic strain rate S^* . The extension of the flammability limit also results in the HRR and SPR source terms being active through a larger S^* range and having a higher maximum magnitude. When applied to a coupled CFD + RFM simulation, these differences are expected to result in higher strain rate pockets of the resolved or mean flow field experiencing heat release, while the same regions using an irrotational flamelet model would be extinct.

Asymmetry of the velocity gradients also allows for two different general vortex geometries: stretched vortex layers, which have a single inflow axis and binary outflow axes, and stretched vortex tubes, which have binary inflow axes and a single outflow axis. The degree and type of asymmetry modifies the centrifugal effect. In the stretched vortex layer case, when the strain rate aligned with the vorticity vector is higher than the rotational plane outflow strain rate ($S_2 > S_1 > 0$), flammability limits are further extended. In the converse situation ($S_1 > S_2 > 0$), flammability limits are extended to a lesser degree, but are still higher than the irrotational case. In the stretched vortex tube cases ($S_2 > 0$, $S_1 < 0$), an opposite trend is observed in which flammability limits increase with larger S_1 (less negative S_1) and smaller (positive) S_2 .

The second aspect of this dissertation is the creation of a new mechanical CFD-flamelet coupling procedure. The coupling procedure follows first-principles turbulence scaling rules between the large and small scales. As the length scales decrease, the velocity gradients increase, and a method is needed to quantify the Kolmogorov velocity gradients given RANS or LES quantities. The viscous dissipation of turbulence kinetic energy acts at rate ϵ within the viscous sub-range where the flamelet lives. As ϵ is also a primary modeled quantity in unresolved turbulent CFD, it provides such a coupling. Given ϵ and a choice of non-dimensional modeling coefficients, the three far-field principal strain rates and vorticity magnitude that the flamelet is subjected to are given. The HRR and SPR of the flamelet are then determined via a full solution of the RFM governing equations. This approach avoids coupling via flame-local quantities and creation of progress variables and scalar dissipation rates for which closures are less substantiated in turbulence cascade theory.

The final section of this work speculated on ideas regarding scalar CFD-flamelet coupling. Although this is still an active area of investigation, it is apparent that varying mixtures, temperatures, and/or enthalpies in the flamelet inflows significantly alters flammability limits, HRR, and SPR. This is a proper area for future study.

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