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A Localized Thickened Flame Model for Stretched Premixed Flame of Hydrogen and Hydrocarbon Fuels

by
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Pursuing a Ph.D. is an odyssey. It began at 0% and now stands at 14.0625% of my life, and this dissertation traces the journey. The perfectly consistent results presented in these pages, paradoxically, prove that as a record of the journey, it is imperfect. Therefore, I stay a bit from the rigid scientific logic and allow myself a bold deviation here.

I am stubborn and often lost my way in hesitation and overthinking, but my supervisor, Prof. Hiroshi Terashima, broke through the fog, teaching me how to think firmly and guiding me toward concrete goals. I often lacked confidence, second-guessing every idea, but Prof. Nobuyuki Oshima guided me through analogies and broader connections, helping me see problems from fresh and unexpected perspectives. I tended to fixate on what was incomplete at every stage, but Prof. Yusuke Takahashi taught me to embrace imperfection, move forward with it, and continue building nonetheless. I am a solitary person, but my friends and the members of Computational Fluid Mechanics Laboratory accompanied me, Ms. Yoshie Shirai, our secretary, supported me, and my girlfriend believed in and stood by me. I may not have been a dutiful child, but I constantly feel the care and concern of my parents.

Before reaching the end of this journey, I noticed it has not been as smooth or beautiful as I once imagined; at times I hesitated and struggled. But every step has been part of the scenery, and every flower and blade of grass has carried its own meaning.

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Contents

<i>List of Figures</i>	7
<i>List of Tables</i>	11
1 Introduction	13
1.1 Combustion's Vital Role in the Net-Zero Energy Transition	13
1.1.1 Environmental and Energy Decision	13
1.1.2 The Transitional Significance of Combustion	14
1.1.3 Advancement in New Combustion Technology Research	15
1.2 Combustion Computational Fluid Dynamics at Present	16
1.2.1 Difficulty of the Direct Numerical Simulation for Combustion	16
1.2.2 Prevalent Combustion Model Accounting Finite-Rate Chemistry	17
1.2.3 Thickened Flame Model	18
1.2.4 Challenge in Modeling the Stretched Premixed Flame	18
1.3 Thickened Flame Model for Stretched Premixed Flame	19
1.4 Research Objective	20
1.5 Thesis Overview	20
2 Numerical Method	23
2.1 Governing Equation	23
2.1.1 Compressible Navier-Stokes Equations	23
2.1.2 Reaction Kinetics	24
2.1.3 Transport Property	26
2.2 Numerical Scheme	27
2.2.1 Operator-splitting Method	27
2.2.2 Time Integration Scheme of Reaction Kinetics Part	28
2.2.3 Time Integration Scheme for Fluid Dynamics Part	32
3 LTF-S: Localized Thickened Flame Model for Stretched Premixed Hydrogen Flames	39
3.1 Empirical Relationships for Laminar Flame Speed and Flame Thickness	39
3.2 Localized Thickened Flame (LTF) Model	43
3.2.1 LTF Model Implemented Governing Equation	43
3.2.2 Numerical Configuration of Cylindrical Flame Propagation	45
3.3 Development of the LTF-S Model	47
3.3.1 Construction of the Unresolved Stretched Component	47

3.3.2	Designing the Functions of α and β	49
3.3.3	Markstein Length Ratio	51
3.3.4	Evaluation of the Local Stretch Rate	53
3.3.5	Extinction Stretch Rate	55
3.3.6	Comments on Non-dimensional Paramters	56
3.4	Validation with a Cylindrically Propagating Flame	56
3.4.1	Numerical Configuration	56
3.4.2	Grid Convergence	57
3.4.3	Validation of the LTF-S Model	58
4	Flame-Vortex Interaction	63
4.1	Numerical Configuration of the Flame-Vortex Interaction	63
4.1.1	Initial Steady Flame Condition	63
4.1.2	Introduction of a Single Euler Vortex	65
4.1.3	Numerical Configuration	66
4.1.4	Grid Convergence	66
4.2	Result and Discussion	68
4.2.1	Flame Deformation during Flame-Vortex Interaction	68
4.2.2	Result of $u_{cv} = 0.1$, and $1s_u^0$	69
4.2.3	Result of $u_{cv} = 10s_u^0$	70
5	Extension of LTF-S Model to Hydrocarbon Fuel	81
5.1	Validation of LTF-S by Premixed CH_4 and C_3H_8 Flame	81
5.1.1	Numerical Configuration	81
5.1.2	Markstein Length Ratio for CH_4 and C_3H_8	83
5.1.3	Sensitivity of A	84
5.1.4	Validation of the LTF-S Model for Premixed $\text{C}_3\text{H}_8/\text{Air}$ Flames	86
5.2	Perforated-plate Burner Flame	88
5.2.1	Numerical Configuration	88
5.2.2	Result and Discussion	89
5.2.3	Comment on the Distinct Stretch Components	95
6	Conclusion and Future Work	97
6.1	Conclusion	97
6.2	Future Work	98
A	Physical Understanding on Stretched Thickened Flame	99
A.1	1D Unstretched Flame	99
A.2	2D Cylindrical Outwardly Propagating Flame	100
A.3	Quasi-one-dimensional Stagnation Flame	101
	<i>References</i>	105

List of Figures

3.1	Structure of one-dimensional non-stretched premixed flame.	41
3.2	Schematic of a cylindrical outwardly propagating flame.	46
3.3	Flame speed against stretch rate (left) and the evolution of the flame location (right) in a cylindrical flame propagation problem. The lines in the left figure, obtained by a linear least-square fit, are used to extract the Markstein length from the simulation results.	47
3.4	Relationship between Markstein length and flame thickness ratios in a cylindrical flame propagation problem. ($R^2 = 0.97$)	53
3.5	Relationship between Markstein length and flame thickness ratios in a cylindrical flame propagation problem. The results are obtained using a TF model [31–33] where constant thickening factors are used.	54
3.6	Determination of extinction stretch rate.	56
3.7	Flame resolution confirmation of the cylindrical outwardly propagating flame.	58
3.8	Evolution of the flame location (along the x -axes in Fig.3.2) for different grid sizes.	59
3.9	Comparisons of flame speed s and flame location R_f obtained with DNS, LTF, and LTF-S models in a cylindrical flame propagation problem. In the left figure, the lines drawn using a linear least-squares fit represents the relationship between flame speed and stretch rate.	60
3.10	Sequential distributions of temperature, $1 + \chi$, and $1 + \psi$ along $y = 0$ in Fig. 3.2	60
3.11	Effects of grid sizes on stretched flame speed s and flame location R_f in the LTF-S model. In the left figure, the lines drawn using a linear least-squares fit represent the relationship between flame speed and stretch rate.	61
3.12	Comparison of the flame speed s against stretch rate for various equivalence conditions in a cylindrical flame propagation problem. In the figures, the lines drawn using a linear least-squares fit represent the linear relationship between flame speed and stretch rate. Thermo-diffusive (TD) instabilities arise after the linear evolution phase, when $Le < 1$. The TD phase is excluded from the results and discussions in this study.	62
4.1	Schematic of a flame-vortex interaction.	64
4.2	The converged steady flame locations for grids of DNS, LTF, and LTF-S.	64
4.3	Mapping of the vortex conditions onto the turbulent combustion diagram (adapted from [16])	66

4.4	Initial vorticity distribution for the vortex conditions of $u_{cv} = 0.1, 1.0$, and $10s_u^0$. ($\Delta x = 40 \mu\text{m}$)	68
4.5	Grid resolution confirmation for the vortex conditions of $u_{cv} = 0.1, 1.0$, and $10s_u^0$	68
4.6	Grid resolution confirmation for the premixed stiochiometric H_2/Air . ($u_{cv} = 10s_u^0$).	69
4.7	Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 0.1s_u^0$. The thin lines represent the streamlines.	72
4.8	Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 1s_u^0$. The thin lines represent the streamlines.	73
4.9	Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 10s_u^0$. The thin lines represent the streamlines.	74
4.10	Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 0.1s_u^0$	75
4.11	Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 1s_u^0$	76
4.12	Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 10s_u^0$	77
4.13	Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 0.1s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.	78
4.14	Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 1s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.	78
4.15	Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 10s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.	79
4.16	Stretch components distributions of LTF-S model at $t^* = 2.5$ for $u_{cv} = 10s_u^0$	79
4.17	Distributions of the LTF-S model parameters χ and ψ at $t^* = 2.5$ for $u_{cv} = 10s_u^0$	80
5.1	Relationship between the Markstein length and flame thickness ratios in a cylindrical flame propagation problem.	83
5.2	Relationship between the Markstein length and flame thickness ratios in a cylindrical flame propagation problem for the premixed hydrogen and air flames. These results acquired by using two sizes, $\Delta x = 0.016$, and 0.032 cm , with $C_\chi = 400$	84
5.3	Sensitivity of the proportional constant in Eq. (3.84) on the prediction of the stretched burning velocity.	85
5.4	Comparison of the burning velocity s against stretch rate for various equivalence conditions in a cylindrical flame propagation problem. In the figures, the lines drawn using a linear least-squares fit represent the linear relationship between burning velocity and stretch rate. The results of DNS is simulated by a open-source flame solver, Ember. The two-dimensional simulaions of the LTF and LTF-S models use the grid size $\Delta x = 0.032 \text{ cm}$	87
5.5	Schematic of the two-dimensional perforated burner adapted from Kornilov 2009 [90]. ($L = 30 \text{ mm}$, $D = 3 \text{ mm}$, $W = 2 \text{ mm}$, and $P = 1 \text{ mm}$)	88

5.6	Comparison of the experimental and simulated distributions of Y_{OH} . The gray-colored portion is the experimental chemiluminescence picture by Konilov et al.[90].	90
5.7	The temperature distributions of the stable perforated-plate flames of DNS, LTF, and LTF-S for $\text{C}_3\text{H}_8/\text{Air}$ under $\phi = 1.0$. (The white streamlines are presented in the upper half, and the black temperature iso-contours are displayed in the lower half.)	91
5.8	The temperature distributions of the stable perforated-plate flames of DNS, LTF, and LTF-S for $\text{C}_3\text{H}_8/\text{Air}$ under $\phi = 1.2$. (The white streamlines are presented in the upper half, and the black temperature iso-contours are displayed in the lower half.)	92
5.9	Comparison of the global consumption rate for DNS, LTF, and LTF-S. . . .	93
5.10	Comparison of burning velocity s_u against stretch rate K for DNS, LTF, and LTF-S. (Different colors indicate the simulation results extracted from distinct isothermal contours.)	94
5.11	Comparison of the flame iso-contour ($T = 1200$ K) for DNS, LTF, and LTF-S. ($\phi = 1.0$)	94
5.12	The stretch components along the iso-temperature lines ($T = 1200$ K) for C_3H_8 under $\phi = 1.2$	95
5.13	The stretch components along the flame normal direction for the cylindrical outwardly propagating flame for H_2/Air under $\phi = 1.0$. (G is the normalized temperature $G = \frac{T-T_u}{T_b-T_u}$)	95
A.1	Conceptual description of the flame response to stretch in the presence of the non-equiffusion effect for a two-dimensional outwardly propagating flame. . .	100
A.2	Conceptual description of the flame response to stretch in the presence of the non-equiffusion effect for a quasi one-dimensional stagnation flame.	102

List of Tables

2.1	Numerical schemes summary	29
3.1	The laminar flame speeds s^0 and Markstein Lengths $\mathcal{L}_{DNS}$ used in the simulations of the LTF-S model.	57
4.1	Verification of grid convergence for resolving the vortex.	67
5.1	Summary of the parameters. The laminar burning velocity s_u^0 , the flame thickness δ^0 , and the adiabatic flame temperature T_{ad} are calculated by Cantera. The Markstein length is calculated using Ember. The C_χ shown here is used for the simulation of LTF-S model.	82
5.2	Summary of the parameters of H ₂ /air for different initial temperatures ($T_u = 400$ and 500 K).	85

Chapter 1

Introduction

1.1 Combustion's Vital Role in the Net-Zero Energy Transition

1.1.1 Environmental and Energy Decision

The global agenda is dominated by the need to address the severe consequences of climate change and ensure energy security. This dual challenge requires an unprecedented shift towards sustainable energy systems, with international and national policy decisions driving technological development.

The Climate Crisis and Global Response

The main driver of the energy transition is the urgent need to mitigate risks associated with rising global temperatures. The extensive combustion of fossil fuels has significantly elevated atmospheric concentrations of Greenhouse Gases (GHGs), primarily carbon dioxide (CO₂). This prompts the Greenhouse Effect, leading to observable increases in the frequency and intensity of natural disasters, including extreme heatwaves, intense storms, frequent floods in Asia and America, and prolonged droughts in Europe. This affects food safety and energy supplies, alters global economic activities, and damages local ecosystems.

In the *Paris Agreement* (2015), the international communities have achieved the core goal: To hold the increase in the global average temperature to well below 2°C above pre-industrial levels and pursue efforts to limit the temperature increase to 1.5°C [1]. The agreement requires parties to peak global GHG emissions as soon as possible and achieve a balance between anthropogenic emission sources and removal sinks in the second half of this century, a state known as Net-Zero Emissions [1].

Global and Regional Commitment

To meet the ambitious 1.5°C target, global emissions must be reduced by approximately 45% by 2030 (relative to 2010 levels), necessitating worldwide Net-Zero Emissions by around 2050 [2]. The European Union (EU) enshrined its target to achieve climate neutrality (net-zero emissions for all GHGs) by 2050 into law via *the European Climate Law* (Regulation (EU)

2021/1119), making it legally binding for all member states [3]. China has pledged to strive for Carbon Peaking before 2030 and work hard to achieve Carbon Neutrality before 2060 [4]. Japan has instituted specific political and legislative frameworks to align with global climate goals, heavily emphasizing carbon-free fuels [5]. H_2 and NH_3 are positioned as crucial zero-emission fuels in Japan’s national energy strategy. The Ministry of Economy, Trade and Industry (METI) developed the *Green Growth Strategy Through Achieving Carbon Neutrality in 2025* to direct Japan’s climate actions. It utilizes two trillion green innovation fund (through NEDO) to support R&D and commercialization, focusing intensely on H_2 and NH_3 [5].

1.1.2 The Transitional Significance of Combustion

Despite the goal of widespread electrification and reliance on renewable energy, combustion remains critical to the energy system, playing a vital role during the transition due to its reliability, high energy density, and compatibility with existing infrastructure [6].

CO₂ Emissions from Combustion

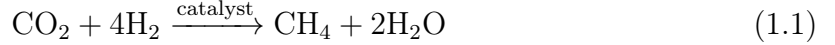
Currently, the burning of fossil fuels accounts for approximately 80% of the world’s primary energy supply and is the source of the majority of global energy-related CO₂ emissions [7]. Specifically, the energy sector (power generation, industry, and transport) is responsible for over 75% of global anthropogenic GHG emissions [7]. This dependence fundamentally contradicts Net-Zero targets, making the decarbonization of combustion processes essential. The transition necessitates mitigating the significant volume of CO₂ produced by the world’s installed capacity of gas turbines, steam generators, and internal combustion engines (ICEs).

Combustion’s Role in the Phase Transition

Combustion-based power generation is valued for its dispatchability and power density, offering immediate, on-demand energy to stabilize grids reliant on variable renewables (solar and wind). This inertia in the existing energy system necessitates a phased approach where established combustion technology is rapidly re-purposed to utilize low- or zero-carbon fuels:

1. **Hydrogen (H_2):** H_2 is a primary focus because it is a carbon-free fuel. Its combustion primarily yields water vapor, producing virtually no CO₂ [8]. H_2 is viewed as a long-term solution for sectors difficult to electrify, like high-temperature industrial processes and large-scale, flexible power generation (e.g., gas turbines). The application of H_2 faces challenges due to its low energy density (by volume) and high reactivity, which complicate storage, transport, and combustion stability, requiring specialized burner and system designs [8].
2. **Synthetic Hydrocarbon Fuels (e-CH₄, e-Diesel):** These fuels are synthesized by combining captured CO₂ (from direct air capture or industrial sources) with green hydrogen (H_2) derived from renewable electricity, often via the Sabatier reaction (to

produce CH₄) or Fischer-Tropsch synthesis (to produce longer-chain hydrocarbons like jet fuel or diesel).



Although the combustion of these fuels releases CO₂, this carbon can be captured resulting in a net-zero carbon cycle. e-fuels are strategic for decarbonizing sectors where high energy density is essential and electrification is challenging, such as aviation (e-jet fuel) and existing road or marine transport (e-diesel). For the existing combustion infrastructures (ICEs, jet engines, and gas turbines) using the fossil fuels, the e-fuels can act as a "drop-in" displacement with minimal or no modifications, facilitating a rapid transition.

3. **Ammonia** (NH₃): NH₃ is increasingly explored as an H₂ carrier for easier storage and transport as a liquid compared to H₂, and as a direct fuel source [9]. It contains no carbon, making it a zero-CO₂ fuel. NH₃ is also a strategic fuel for decarbonizing the maritime transport sector and for large-scale co-firing in coal power plants, actively pursued in Japan [5]. However, NH₃ combustion is challenging due to its low burning velocity and the introduction of nitrogen into the combustion process, leading to the potential fuel NO_x formation and ammonia slip [9].

1.1.3 Advancement in New Combustion Technology Research

The transition to zero-carbon fuels necessitates a paradigm shift in combustion system design. Future combustors must achieve high efficiency and operational flexibility while meeting increasingly stringent emission standards for non-CO₂ pollutants. This development relies heavily on advanced modeling and computational support.

Stringent Emission Requirement

While the primary goal of the energy transition is CO₂ mitigation, the use of hydrogen and synthetic fuels significantly alters the pollutant landscape, shifting the focus to Nitrogen Oxides (NO_x). Regulatory bodies often require NO_x concentrations from stationary gas turbines to remain below 25 ppm. (This is a universal value based on the standards of Japan, the EU, and China [10–12].)

Hydrogen has high diffusivity, wide flammability limits, and rapid laminar burning velocity (> 2 m/s versus ≈ 0.4 m/s for CH₄), leading to elevated combustion temperatures. These high temperatures strongly enhance the Zeldovich mechanism (thermal NO_x formation), resulting in substantial thermal NO_x production. Pure H₂ flames in conventional burners can readily generate NO_x concentrations above 200 ppm [8]. To limit peak temperatures and curb NO_x emissions, modern gas turbines use Lean Premixed (LP) combustion. In this approach, fuel mixes with excess air upstream of the reaction zone to achieve a lean equivalence ratio ($\phi < 0.6$), keeping flame temperature below the critical 1850 K threshold for intense thermal NO_x formation [8]. For synthetic hydrocarbon fuels (e-CH₄, e-C₃H₈), it is essential to maintain high energy density while limiting soot formation and reducing emissions of carbon monoxide CO and unburnt hydrocarbons.

High-Fidelity Computational Fluid Dynamics of Combustion System

The optimization of advanced, high-efficiency, low-emission combustion systems relies on predictive modeling and real-time control, with Computational Fluid Dynamics (CFD) as the primary tool for generating accurate simulation data. High-fidelity CFD approaches, such as Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES), are essential for resolving the flow and combustion processes that govern the pollutant formation and operational stability. These methods enable engineers to verify combustor performance, to predict fuel-dependent stable (flame holding) and unstable combustion regimes (extinction, flashback, and blow-off), to model and reduce NO_x formation in lean hydrogen flames, to analyze combustion instabilities arising from thermo-acoustic interactions within the combustor, and to explore and clarify the underlying physics of these phenomena.

1.2 Combustion Computational Fluid Dynamics at Present

In the context of the rapid transition toward a carbon-neutral society, the increasing demand for high-fidelity and high-efficiency numerical combustion prediction necessitates precise modeling of complex transient combustion phenomena, including ignition, extinction, pollutant formation, and turbulence–combustion interactions in complex combustor geometries. Consequently, *detailed chemical kinetics simulations considering finite-rate chemistry become increasingly important.*

However, many commonly used models either treat detailed reaction kinetics only partially or neglect them altogether. As a result, the predictive accuracy and computational efficiency of combustion CFD strongly depend on the combustion model adopted, and existing approaches are generally capable of capturing only limited aspects of transient combustion behavior.

1.2.1 Difficulty of the Direct Numerical Simulation for Combustion

The applicability of combustion CFD with finite-rate chemistry is limited by the following factors:

1. *Numerous conservation equations*: In addition to the governing equations for fluid flow, separate transport equations must be solved for each reactive species. For detailed chemical-kinetic mechanisms (e.g., long-chain hydrocarbon fuels with over 1000 reactions), this significantly increases the overall computational cost of the simulation.
2. *Stiff ordinary differential equations (ODEs) for reaction kinetics*: The wide disparity in characteristic time scales for different chemical reactions necessitates a very small time step Δt on the CFD solver to maintain numerical stability. Furthermore, as with the first limitation, the dimension of the Jacobian matrix scales with the square of the number of species, which substantially degrades the efficiency of implicit time-integration schemes.
3. *Resolution of the premixed flame front*: The premixed flame front constitutes a thin reaction zone separating unburned and burned gases. In this zone, chemical reactions produce steep gradients in scalar fields (e.g., species mass fractions and temperature).

For example, the laminar flame thickness of a premixed H_2 –air flame is approximately 0.1 mm and further decreases at elevated pressures (the operating condition in ICEs and the industry gas turbines). Thus, combustion CFD simulations must employ a very fine spatial discretization to resolve this narrow reaction layer. This small spatial interval, on the other hand, requires a small spatial interval to meet the stable criteria for time integration. The small spatial and temporal intervals make DNS prohibitive.

1.2.2 Prevalent Combustion Model Accounting Finite-Rate Chemistry

Corresponding to the above difficulty:

1. Reduced scalar methods: The flamelet approach (Flamelet Progress-Variable approach (FPV) [13], Flamelet Generated Manifold (FGM) [14], the G -equation method [15–17], and the surface density equation [18] all work by simplifying the governing equations for reactive scalars (such as progress variable or mixture fraction). In doing so, they decouple the flame dynamics from the full reactive scalar equations and thus avoid directly resolving detailed chemical kinetics. To characterize the flame structure, these approaches rely on one-dimensional flame calculations, which provide the key flame variables (e.g. scalar profiles in flame-aligned coordinates, or effective diffusion coefficients and reaction rates).
2. Skeletal kinetic mechanisms: Optimized global reaction mechanisms [19–21] and analytically reduced chemistries (ARCs) [22–24] decrease the number of reactions and species included in the detailed kinetic scheme, while preserving important flame characteristics such as laminar burning velocity and ignition delay time. By doing this, they reduce both the number of species conservation equations that must be solved and the dimensionality of the Jacobian matrix associated with the reactive ODE system.
3. Large-Eddy Simulation (LES): Classifying LES itself as a combustion model is not accurate, since it is fundamentally a turbulence modeling strategy. LES applies a spatial filter of width Δ to separate the flow field into grid-resolved (GS) and sub-grid (SGS) components. This can lower the computational cost by approximately a factor of $Re_\Delta^{9/4}$, where Re_Δ is the subfilter Reynolds number [25, 26]. The characteristic flame thickness nevertheless remains much smaller than the LES filter size. Therefore, additional turbulent combustion modeling approaches, including those mentioned above, are required to close the filtered chemical source terms and thus enable the simulations of combustion in practical-scale burners. Several sub-grid scale models have been proposed for combustion LES with finite-rate chemistry, such as the probability density function (PDF) approach [27] and conditional moment closure (CMC) [28]. In the context of non-premixed flames, some studies have directly coupled detailed chemical kinetics with LES [29, 30], assuming sufficiently fine grids so that the interaction between reactions and high-frequency SGS fluctuations can be neglected. For premixed flames, however, the propagating flame front exhibits very steep spatial gradients, which on one hand demand extremely small temporal and spatial resolutions for direct integration

of chemical kinetics, and on the other hand interact with sub-grid scale turbulence, causing wrinkling and folding of the flame front that remain unresolved at the filter width Δ . Consequently, models are required that can represent the additional SGS flame surface area or the effective thickening of the flame.

1.2.3 Thickened Flame Model

Another prevalent method to address the thin premixed flame fronts is the *thickened flame* (TF) model. [31–33] In this approach, the flame thickness is artificially enlarged to a scale at which the flame’s chemical kinetics can be directly resolved on the computational grid. The thickening is implemented by increasing the diffusion coefficient (along with the thermal conductivity and viscosity), while simultaneously reducing the species production rates so that the laminar burning velocity remains unchanged. Because both the temporal and spatial characteristic scales of the flame ($\delta_L \rightarrow F\delta_L$, $\tau = F\delta_L/s_u^0 \rightarrow F\tau$) are extended, the TF model accelerates computations by permitting a significantly larger time step Δt , as the grid spacing Δx can be coarsened in proportion to the thickened flame width without violating the CFL stability condition. Furthermore, an efficiency function [33–35] has been introduced to model the subgrid-scale (SGS) interaction between turbulence and chemistry, with the goal of recovering the local turbulent burning velocities that are otherwise reduced by flame thickening in TF models (to realize the effective thickening of the turbulent flame). Several dynamic TF models [34, 36] have been proposed that confine the thickening effect to the flame region, thereby preventing any influence of thickening on the transport properties of the fluid outside this region.

1.2.4 Challenge in Modeling the Stretched Premixed Flame

Due to non-equidiffusion and preferential diffusion effects, flame stretch alters the local distribution of chemical species, which can either attenuate or enhance combustion intensity, as reflected in the burning velocity and flame temperature. The stretch rate arises from flow non-uniformity, flame curvature, and flame unsteadiness [37–39]. Therefore, it is straightforward to associate stretch effects with flame instabilities (diffusion-thermal and hydrodynamic instabilities) and with turbulent flames, since the locally stretched flame front in these phenomena. The principal objective of the aforementioned combustion models is to represent complex turbulent combustion fields. In such flows, turbulent mixing is far more efficient than molecular diffusion. As a result, the validation of combustion models for stretched flame conditions has frequently been neglected, and the majority models [13] assumes a unity Lewis number approximation, $Le = 1$.

The renewed focus on flame stretch is driven, on one hand, by the growing adoption of lean-burn engine technology aimed at reducing NO_x emissions [8, 40]. Lean premixed conditions generally correspond to non-unity Lewis, which makes stretch effects particularly pronounced. A key motivation on the other hand is the growing utilization of H_2 for combustion control and safety purposes. Under lean conditions, the positive (negative) stretch intensifies (suppress) the burning velocity, which can trigger thermo-diffusive (TD) instabilities. These instabilities can greatly intensify the burning rate, promoting flame flashback, posing a risk of engine damage, and potentially causing explosive accidents.

Recent combustion models increasingly account for stretch effects. Ojien et al. [41] derived the Strong Stretch Flamelet Equations (SSFE) to incorporate stretch terms into the reduced scalar (flamelet) equation formulated in flame coordinates. Scholtissek et al. [42] proposed a self-contained solution method in composition space that explicitly represents the influence of stretch on each term in the flamelet equations, which are closed via a gradient equation. This approach has been applied to study thermo-diffusive (TD) instabilities by Wen [43] and to analyze arbitrary combinations of strain and curvature effects on flames by Botter et al. [44]. Mukundakumar et al. [45] have modified the control-variable diffusion flux to represent preferential diffusion. These flamelet-based methods require a look-up table (flamelet library) that provides flame-state variables (T , ρ , Y_i , etc.) as functions of reduced scalars (such as progress variable and mixture fraction). As a result, extending the dimensionality of these libraries becomes necessary.

1.3 Thickened Flame Model for Stretched Premixed Flame

Recent researches have shown that the thickened flame exhibits a higher sensitivity to stretch than the corresponding non-thickened flame, which results in inaccurately predicted stretched burning velocities. Several modifications [46–49] have proposed have proposed modifications to TF models to restore the propagation speed of stretched flames affected by flame thickening. Popp et al. [46] demonstrated, using a stagnation flow flame system under the unity Lewis number condition, that a thickening factor emerges in the convection term of the governing equation during the thickening operation. This thickening factor alters the global strain rate in the convection term, resulting in an unphysical reduction in the consumption speed of strained flames. To address this, they introduced a strain correction factor in the diffusion term to retrieve the correct consumption speed of strained flames. Poncet et al. [47, 49] proposed a TF-based model that accounts for both strain and curvature effects. They introduced a model parameter in the diffusion coefficient to ensure the correct flame response to stretching effects. This parameter was initially determined using a spherical curved flame problem, maintaining the Markstein length under flame thickening consistent with the reference value. The model employed a Lewis number correction approach proposed by Volpiani et al. [35]. Following the Lewis number modification approach [35], [47], Detomaso et al. [48] developed a stretched TF model for handling various stretch conditions, including high stretch conditions near flame extinction limits. They applied different thickening factors to the thermal conductivity, diffusion coefficient, and production rate of species to match flame properties. An optimization function was also introduced to determine the slope of stretched burning velocities against the stretch rate over a wide range of stretch conditions. Flamelet-based models also address the adverse effects of flame thickening on stretched flames. Proch and Kempf [50] introduced strain effects in their flamelet-generated manifolds approach, modifying the reaction rates using the local strain rate to achieve the correct consumption speed. Han et al. [51] incorporated a mapping variable in their flamelet-generated manifolds approach to characterize strained flame structures.

1.4 Research Objective

The present study aims to improve TF models for simulating premixed flames under stretching effects, leveraging their ease of implementation into the reactive Navier–Stokes equations with finite-rate chemistry. This study proposes a novel TF-based model for simulating premixed flames under stretching effects. This study uses a previously developed dynamic TF approach, the localized thickened flame (LTF) model, as its foundation. In contrast to conventional TF models for stretched flames—which adjust flame transport properties through a Lewis number correction [46–49] to recover the stretched burning velocity—this work reconstructs the "flame-unresolved" terms in the LTF framework based on the resolved stretch rate. In this way, the "unresolved" stretch effects neglected by flame thickening are incorporated. These unresolved terms are formulated to accurately represent the propagation speed of stretched flames under thickening without incorporating a Lewis number correction. Thus, the proposed model retains a property of the original TF model [31–33], preserving primary non-dimensional parameters of flow fields. This property distinguishes the proposed model from existing TF models for stretched flames.

1.5 Thesis Overview

The purpose of this study is to develop a combustion model that includes detailed reaction kinetics in order to accurately and reliably predict the dynamics of the stretched premixed flames. The model is intended to overcome the constraints that the extremely small temporal and spatial scales of premixed flame fronts place on the computational grid and on the time-integration step size, to accelerate the speed of numerical simulations of combustion.

Chapter 1 describes the research background, the current state of research, and the objectives of this study.

Chapter 2 provides a detailed description of the governing equations for reacting flows that account for detailed chemical kinetics, as well as the numerical methods for solving these equations.

Chapter 3 describes the concept of the LTF model, its validation results, and the main focus of this chapter: the development of the extended LTF-S model, and its validation results. We have firstly validate this LTF model using two-dimensional outwardly propagating premixed cylindrical flame of H_2 /air. The results show that, for stretched flames with thickening, the sensitivity of the flame propagation speed to stretch is affected leading to an incorrectly predicted propagation speed. The sensitivity is also known as the Markstein length. The Markstein length ratio found to a linear relationship with the thickening factor. To achieve accurate prediction of the burning velocity of thickened flames under stretch, this study proposed a new LTF-S model (LTF model for stretched flames) by introducing a new model parameter $1 + \psi$. This model parameter allows to restore the sensitivity of the thickened flame to stretch basing on the local stretch rate, and thereby corrects the burning velocity of the thickened flame. Compared with the LTF model, the new LTF-S model, while still using a thickened flame front to reduce computational cost, is able to accurately reproduce the reference DNS flame propagation speed.

Chapter 4 further verifies the predictive accuracy of the LTF-S model when dealing with

more complex combustion scenario, the flame-vortex interaction. This numerical configuration includes both the straining of the vortex acting on the flame and the curvature effects caused by flame deformation. The LTF-S model successfully reproduces the detailed flame shape during vortex–flame interaction and quantitatively yields the identical fuel consumption rate obtained from the reference DNS results.

Chapter 5 further applies the new LTF-S model to the hydrocarbon fuels, specifically methane and propane. The results identify that the universal proportionality coefficient of $A = 0.5$ exists and this finding renders the LTF-S model highly flexible and easy-to-use model for the combustion simulations. Finally, the LTF-S model is implemented on a practical combustor, namely a perforated plate burner. The new LTF-S model accurately captures both the local and overall combustion behavior in this system.

Chapter 6 concludes this study by introducing the development of a stretched premixed flame model for reactive flow simulations that includes detailed chemical kinetics, and by outlining potential future directions for this line of research.

Chapter 2

Numerical Method

2.1 Governing Equation

2.1.1 Compressible Navier-Stokes Equations

The governing equations are the compressible Navier-Stokes equations including the mass conservation equations for i -th chemical species and the equation of state of thermally perfect gas. The governing equations are written as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (2.1)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + p \boldsymbol{\delta} - \boldsymbol{\tau}) = 0, \quad (2.2)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p) \mathbf{u} - \boldsymbol{\tau} \cdot \mathbf{u} + \mathbf{q}] = 0, \quad (2.3)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot (\rho Y_i \mathbf{u} - \mathbf{d}_i) = \dot{\omega}_i, \quad (2.4)$$

$$p = \rho R \sum_{i=1}^N \frac{Y_i}{M_i} T, \quad (2.5)$$

where, ρ , p , E ($= \rho e + \frac{1}{2} \rho \mathbf{u} \mathbf{u}$), T , and R denote the density, pressure, total energy, temperature, and universal gas constant, respectively. e is the internal energy per unit mass. The operator $\otimes$ represents the Kronecker product. $\mathbf{u}$, $\boldsymbol{\tau}$, $\mathbf{q}$, and $\boldsymbol{\delta}$ are the velocity vector, viscous stress tensor, heat flux vector, and unit tensor, respectively. Y_i , $\mathbf{d}_i$, M_i , and $\dot{\omega}_i$ represent the mass fraction, diffusion vector, molar mass, and production rate of i -th chemical species. N is the total number of chemical species.

The viscous stress tensor $\boldsymbol{\tau}$, the heat flux vector $\mathbf{q}$, and the diffusion vector $\mathbf{d}_i$ are evaluated as follows,

$$\boldsymbol{\tau} = \mu \left[2\mathbf{S} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \boldsymbol{\delta} \right], \quad (2.6)$$

$$\mathbf{q} = -\kappa \nabla T - \sum_{i=1}^N h_i \mathbf{d}_i, \quad (2.7)$$

$$\mathbf{d}_i = -\rho D_i \nabla Y_i, \quad (2.8)$$

where, μ and κ denote the viscosity and thermal conductivity of the mixture. h_i and D_i represent the total enthalpy and diffusion coefficient of the i -th species. $\mathbf{S}$ is the symmetric shear strain tensor, and is evaluated as follows,

$$\mathbf{S} = \frac{1}{2} \left[\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right]. \quad (2.9)$$

2.1.2 Reaction Kinetics

This study considered the detailed chemistry involving N species and M reactions. The reactions in a general form can be represented by

$$\sum_{i=1}^N v'_{i,j} \Theta_i \Leftrightarrow \sum_{i=1}^N v''_{i,j} \Theta_i, \quad (j = 1, \dots, M), \quad (2.10)$$

where Θ_i is the symbol of the i -th species. $v_{i,j}$ is the stoichiometric coefficient of the i -th species for the j -th reaction. The superscripts $'$ and $''$ of $v_{i,j}$ indicate the forward and reverse coefficients, respectively.

Thus, the production rate $\dot{\omega}_i$ can be written as a sum of the rate of progress variable for all reactions involving the i -th species,

$$\dot{\omega}_i = \sum_{j=1}^M \dot{\omega}_{i,j} = M_i \sum_{j=1}^M v_{i,j} Q_j, \quad (i = 1, \dots, N), \quad (2.11)$$

where,

$$v_{i,j} = v''_{i,j} - v'_{i,j}, \quad (2.12)$$

and Q_j is the rate of progress variable of the j -th reaction,

$$Q_j = k_{f,j} \prod_{i=1}^N [\Theta_i]^{v'_{i,j}} - k_{r,j} \prod_{i=1}^N [\Theta_i]^{v''_{i,j}}. \quad (2.13)$$

In the above equation, $[\Theta_i]$ is the molar concentration of the i -th species, $k_{f,j}$ and $k_{r,j}$ are the forward and reverse rate constants of the j -th reaction. In general, the forward rate constants $k_{f,j}$ are assumed to follow the Arrhenius equation,

$$k_{f,j} = A_j T^{\beta_j} \exp -\frac{Ea_j}{RT}, \quad (2.14)$$

where A_j , β_j , and Ea_j are the pre-exponential factor, temperature exponent, and the activation energy of the j -th reaction. For the reverse rate constant $k_{r,j}$, in the thermal systems, it is related to the $k_{f,j}$ and the equilibrium constant,

$$k_{r,j} = \frac{k_{f,j}}{K_{c,j}}, \quad (2.15)$$

where $K_{c,j}$ is the equilibrium constant in concentration units. Since the thermodynamic properties in pressure units more easily determine the equilibrium constants, $K_{c,j}$ can be evaluated as follows,

$$K_{c,j} = K_{p,j} \left(\frac{p}{RT} \right)^{\sum_{i=1}^N v_{i,j}}, \quad (2.16)$$

where the equilibrium constants $K_{p,j}$ are obtained with the following equation,

$$K_{p,j} = \exp \left(\frac{\Delta S_j^0}{R} - \frac{\Delta H_j^0}{RT} \right), \quad (2.17)$$

where ΔS_j^0 represents the difference of the standard-state entropy (or standard entropy of reaction) between the reactants and the products when the reactants completely change to products in the j -th reaction. Together with the standard enthalpy of reaction ΔH_j^0 , they are evaluated as

$$\frac{\Delta S_j^0}{R} = \sum_{i=1}^N v_{i,j} \frac{S_i^0}{R}, \quad (2.18)$$

$$\frac{\Delta H_j^0}{RT} = \sum_{i=1}^N v_{i,j} \frac{H_i^0}{RT}, \quad (2.19)$$

where S_i^0 and H_i^0 are the standard-state molar entropy and the standard-state molar enthalpy (specific values) of the i -th species as a function of temperature.

$$S_i^0(T) = S_i^0(T_{ref}) + \int_{T_{ref}}^T \frac{C_{p,i}^0(T)}{T} dT, \quad (2.20)$$

$$H_i^0(T) = H_i^0(T_{ref}) + \int_{T_{ref}}^T C_{p,i}^0(T) dT, \quad (2.21)$$

where $C_{p,i}^0$ is the standard-state molar heat capacity of the i -th species at constant pressure as a function of temperature. To effectively calculate thermodynamic data (without handling large datasets or time-consuming table-lookup algorithms), the data is stored as a polynomial in T . The NASA 7-coefficient polynomial parameterization [52] is used to compute $C_{p,i}^0 (= C_{V,i}^0 + R)$, H_i^0 , and S_i^0 .

$$\frac{C_{p,i}^0(T)}{R} = a_{0,i} + a_{1,i}T + a_{2,i}T^2 + a_{3,i}T^3 + a_{4,i}T^4, \quad (2.22)$$

$$\frac{S_i^0(T)}{R} = a_{0,i} \ln T + a_{1,i}T + \frac{a_{2,i}}{2}T^2 + \frac{a_{3,i}}{3}T^3 + \frac{a_{4,i}}{4}T^4 + a_{6,i}, \quad (2.23)$$

$$\frac{H_i^0(T)}{RT} = a_{0,i} + \frac{a_{1,i}}{2}T + \frac{a_{2,i}}{3}T^2 + \frac{a_{3,i}}{4}T^3 + \frac{a_{4,i}}{5}T^4 + \frac{a_{5,i}}{T}. \quad (2.24)$$

To improve the accuracy, two different sets of polynomials are used for high and low temperatures, separated by a switch temperature (usually $T = 1000$ K). The reason is that the heat capacity increases with temperature, as the molecule's translational, rotational, and vibrational degrees of freedom are successively excited. (One set of the polynomials could not fit all the data well, leading to a large calculation error.)

2.1.3 Transport Property

The molecular transport processes - *heat conduction*, *viscosity*, and *diffusion* - are caused by the movements of molecules due to the gradients of the corresponding physical properties [53]. The temperature, velocity, and concentration gradients cause the transport of heat, momentum, and mass, respectively. The thermal conductivity κ , viscosity μ , and diffusion coefficient D_i of a multi-component gas are evaluated using a mixture-averaged model as follows.

Thermal Conductivity:

$$\kappa = \frac{1}{2} \left[\sum_i^N X_i \kappa_i + \left(\sum_i^N \frac{X_i}{\kappa_i} \right)^{-1} \right], \quad (2.25)$$

Viscosity:

$$\mu = \frac{1}{2} \left[\sum_i^N X_i \mu_i + \left(\sum_i^N \frac{X_i}{\mu_i} \right)^{-1} \right], \quad (2.26)$$

Diffusion Coefficient:

The diffusion of a compound i into the mixture of the other compounds M .

$$D_i = D_i^M = (1 - Y_i) \left(\sum_{j \neq i} \frac{X_j}{D_{i,j}} \right), \quad (2.27)$$

where X_i and Y_i are the fraction of the i -th species in mole and mass bases, respectively. $D_{i,j}$ is the binary diffusion coefficient between the i -th and the j -th species. The specific coefficients - κ_i , μ_i and $D_{i,j}$ - for each species are modeled based on the kinetic theory by assuming the particles of the gas components are rigid spheres.

$$\kappa_i = \frac{25}{32} \frac{\sqrt{\pi m_i k T}}{\pi \sigma_i^2 \Omega_i^{(2,2)*}} \frac{c_V}{m_i}, \quad (2.28)$$

$$\mu_i = \frac{5}{16} \frac{\sqrt{\pi m_i k T}}{\pi \sigma_i^2 \Omega_i^{(2,2)*}}, \quad (2.29)$$

$$D_{i,j} = \frac{3}{8} \frac{\sqrt{\pi \frac{2m_i m_j}{m_i + m_j} k T}}{\pi \sigma_{ij}^2 \Omega_{ij}^{(1,1)*} T_{ij}^*} \frac{1}{\rho}, \quad (2.30)$$

where m_i is the mass of the particle (atom or molecule), $k(= R/N_A)$ is the Boltzmann constant, T is the absolute temperature, σ_i is the particle diameter ($\sigma_{ij} = (\sigma_i + \sigma_j)/2$), and $c_V(= C_V/N_A)$ is the molecular heat capacity. $\Omega^{(1,1)*}$ and $\Omega^{(2,2)*}$ (accounting for the diffusion of a substance within a fluid and for the viscosity of a substance, respectively) are the collision integrals of a reduced temperature $T^*(= kT/\epsilon)$. N_A is Avogadro's constant, and ϵ is the well depth of the Lennard-Jones 6-12 potential model.

Practically, more convenient formulations are used.

$$\kappa_i = 8.323 \cdot 10^{-4} \frac{\sqrt{T/M_i}}{\sigma_i^2 \Omega_i^{(2,2)*}} \left[\frac{\text{J}}{\text{m} \cdot \text{K} \cdot \text{s}} \right], \quad (2.31)$$

$$\mu_i = 2.6693 \cdot 10^{-8} \frac{\sqrt{M_i T}}{\sigma_i^2 \Omega_i^{(2,2)*}} \left[\frac{\text{kg}}{\text{m} \cdot \text{s}} \right], \quad (2.32)$$

$$D_{i,j} = 2.662 \cdot 10^{-9} \frac{\sqrt{\frac{1}{2} \frac{M_i M_j}{M_i + M_j} T^3}}{p \sigma_{ij}^2 \Omega_i^{(1,1)*} T_{ij}^*} \left[\frac{\text{m}^2}{\text{s}} \right], \quad (2.33)$$

Note the units listed in the above three equations: T in the unit of K, M_i in the unit of g/mol, and σ in the unit of nm, therefore, the coefficients of each equation involve unit conversions. Additionally, the thermal conductivity κ_i and viscosity μ_i are proportional to $\sqrt{T}$, while the diffusion coefficients $D_{i,j}$ are also a function of pressure and are proportional to $T^{3/2}$ and $1/p$.

2.2 Numerical Scheme

In this study, the two-dimensional compressible Navier-Stokes equations are numerically solved by a FORTRAN code [54], and the CHEMKIN-II library [55] is used to calculate the thermodynamic properties and transport coefficients. The numerical methods for solving the governing equations are discussed in the following section.

2.2.1 Operator-splitting Method

For the reacting flows with detailed chemistry, the governing equations (the transport equations for energy and chemical species) are large, nonlinear, and highly stiff. To calculate the conservation variables (or primary variables), the fully coupled method is computationally prohibitive due to the large number of coupled multi-geometry equations, the increasing number of species, and the increasing number of implicit matrix solves, where high-order differencing approximates the spatial derivatives. In contrast, the operator-splitting method divides the governing equation into several parts to capture the physics processes. This allows the use of an optimal scheme to solve different parts, and it is possible to avoid the expensive matrix operations.

The present work used the Strang splitting scheme [56, 57] to solve the governing equations of the reacting flow effectively. This scheme separates the stiff chemical reaction term from the (non-stiff) convection and diffusion terms. The discretized transport equations of energy and chemical species can be written in the following general form.

$$\frac{\partial \mathbf{Q}}{\partial t} = \mathbf{C}(\mathbf{Q}) + \mathbf{D}(\mathbf{Q}) + \mathbf{R}(\mathbf{Q}), \quad (2.34)$$

where $\mathbf{Q}$ is the vector of the solution vector, and it is a function of time t . $\mathbf{C}$, $\mathbf{D}$, and $\mathbf{R}$ are the convection, diffusion, and the reaction terms, respectively. The splitting scheme

Algorithm 1 The operator-splitting method.

Require: Q^0 , N_{max}

```

1:  $n \leftarrow 1$ 
2: while  $n \leq N_{max}$  do
3:    $\Delta t_{CFD}^n$  { $\Delta t$  of the  $n$ -th time step}
4:   {Step 1: Sub-time-integration of the reaction part}
5:    $\Delta t_{chem} \leftarrow 0$ 
6:   while  $\Delta t_{chem} < \Delta t_{CFD}^n$  do
7:      $\Delta t^*$  { $\Delta t^*$  of the sub-integration}
8:      $Q^* \leftarrow Q^0 + R(Q^0) \cdot \Delta t^*$ 
9:      $\Delta t_{chem} \leftarrow \Delta t_{chem} + \Delta t^*$ 
10:     $Q^* \leftarrow Q^0$ 
11:  end while
12:  {Step 2: Sub-time-integration of the fluid part}
13:   $Q^{n+1} \leftarrow Q^* + [C(Q^*) + D(Q^*)] \cdot \Delta t_{CFD}^n$ 
14:  {Step 3: Replacement of initial condition for the next time step}
15:   $n \leftarrow n + 1$ 
16:   $Q^0 \leftarrow Q^{n+1}$ 
17: end while

```

solves the following sub-time-integration of the reaction kinetics and the fluid dynamics parts sequentially.

$$\frac{\partial Q^*}{\partial t} = R(Q^*), \quad (2.35)$$

$$\frac{\partial Q^{**}}{\partial t} = C(Q^{**}) + D(Q^{**}), \quad (2.36)$$

The algorithm, based on a simple explicit time integration method, is listed in the Algorithm 1.

This study numerically solves the sound-speed-based compressible Navier-Stokes equations using the operator-splitting method. The schemes for different sub-time-integrations are listed in Table 2.1. The following sections give detailed descriptions of those schemes.

2.2.2 Time Integration Scheme of Reaction Kinetics Part

When integrating the reaction kinetics part, the fluid is assumed stationary, and the reactive mixture at each grid point advances under adiabatic, constant-volume conditions. Thus, Eqn. (2.35) can be deduced into the following ordinary differential equations (ODEs) from the transport equations of chemical species and energy.

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i}{\rho} = c_i - d_i, \quad (2.37)$$

Reaction Kinetics Part	
Time integration	ERENA [58]
Fluid Dynamics Part	
Numerical flux	HLLC[59]
High order	3rd-order MUSCL [60] (w/ minmod limiter)
Viscous / Convection / Diffusion terms	2nd-order central difference
Time integration	TVD 3rd-order RK [61]

Table 2.1: Numerical schemes summary

$$\frac{dT}{dt} = -\frac{1}{\rho c_v} \sum_{i=1}^N e_i \dot{\omega}_i, \quad (2.38)$$

c_v is the mean specific heat capacity at constant volume. e_i is the internal energy of the i -th species. (All the previous variables are in mass-based units.) c_i and d_i are the creation and the destruction rates (in the unit of s^{-1}) of the i -th species, and they are evaluated from a special form for the reaction rate,

$$\dot{\omega}_i = \dot{C}_i - \dot{D}_i. \quad (2.39)$$

Together with the Eqn. (2.11) and Eqn. (2.13), i -th species' reaction and destruction rates (basing on mass unit) can be derived:

$$\dot{C}_i = M_i \sum_{j=1}^M v'_{i,j} k_{r,j} \prod_{i=1}^N [\Theta_i]^{v''_{i,j}} + M_i \sum_{j=1}^M v''_{i,j} k_{f,j} \prod_{i=1}^N [\Theta_i]^{v'_{i,j}}, \quad (2.40)$$

$$\dot{D}_i = M_i \sum_{j=1}^M v'_{i,j} k_{f,j} \prod_{i=1}^N [\Theta_i]^{v'_{i,j}} + M_i \sum_{j=1}^M v''_{i,j} k_{r,j} \prod_{i=1}^N [\Theta_i]^{v''_{i,j}}. \quad (2.41)$$

(Note: $c_i = \dot{C}_i/\rho$ and $d_i = \dot{D}_i/\rho$.)

A characteristic time of a species could be defined as $\tau_i = Y_i/d_i$. Inside the reactive ODEs (Eqn. (2.37) and Eqn. (2.38)), there is a large difference between the fast and slow characteristic times of the species. This difference leads to the system having a large degree of stiffness, namely, the ratio of the largest and smallest (in magnitude) negative eigenvalues of the Jacobian.

To solve those ODEs, some implicit methods, like VODE [62], can use a relatively large time step size Δt . However, for simulation of the compressible CFD, the Δt_{CFD} becomes very small (e.g. 10^{-8} s), due to the sound speed based Courant-Friedrichs-Lewy (CFL) condition. This small time size makes the stiffness less severe. Instead, the implicit method becomes computationally expensive due to the Jacobin matrix generation and the LU factorization. On the other hand, for the simple explicit method, e.g., the explicit Euler method, a small time size $\Delta t < \min(\tau_i)$ is needed to get a stable numerical solution; this means the time size of the reacting CFD will be restricted by the shortest τ_i . Considering the characteristic time of flow is greater than that of chemical reaction, we adopt a fast and robust Jacobian-free integration

method, known as the extended robustness-enhanced numerical algorithm (ERENA) [58], to effectively acquire the numerical solution of the reactive ODEs.

ERENA: Extended Robustness-Enhanced Numerical Algorithm

ERENA [58] explicitly solves Eqn. (2.37) based on the quasi-steady-state assumption (QSSA). Although large Δt can be used to avoid the stiffness of the ODEs of detailed chemistry, numerical instabilities are induced by the errors in the mass conservation. ERENA uses the Lagrange multiplier method to robustly avoid these instabilities by correcting Δt to limit the error below a threshold value ϵ .

An exact solution of Eqn. (2.37) could be used to approximate Y_i^{n+1} by assuming c_i and τ_i are constant (or vary slowly) over a time scale Δt . (the QSSA [63])

$$Y_i^{n+1} = Y_i^n \exp\left(-\frac{\Delta t^n}{\tau_i^n}\right) + c_i^n \tau_i^n \left[1 - \exp\left(-\frac{\Delta t^n}{\tau_i^n}\right)\right]. \quad (2.42)$$

The above equation is unconditionally stable even using a large $\Delta t > \tau_i$. However, the total mass of the chemical species is poorly conserved, as $\sum_{i=1}^N Y_i^{n+1} \neq 1$. To overcome this disadvantage, ERENA solves the following optimization problem.

$$\begin{cases} \text{minimize} & Z(Y_i^*, Y_i^{n+1}) \\ \text{subject to} & \sum_{i=1}^N Y_i^{n+1} = 1 \end{cases} \quad (2.43)$$

where Y_i^* is the mass fraction of the i -th species predicted by the QSSA method. The arbitrary function Z uses the summation of the weighted squared residuals. Using the Lagrange multiplier method, the above optimization problem is expressed as follows.

$$\sum_{i=1}^N \frac{1}{2\eta_i} (Y_i^{n+1} - Y_i^*)^2 + \lambda \left(\sum_{i=1}^N Y_i^{n+1} - 1 \right) = \epsilon, \quad (2.44)$$

where η_i is an arbitrary weighted value of the i -th species, λ is the Lagrange multiplier, and ϵ is an auxiliary function of λ and Y_i^{n+1} . By solving $\frac{\partial \epsilon}{\partial \lambda} = 0$ and $\frac{\partial \epsilon}{\partial Y_i^{n+1}} = 0$ ($N + 1$ conditions in total), an optimal solution could be acquired as follows,

$$Y_i^{n+1} = Y_i^* + \frac{\eta_i}{\sum_{i=1}^N \eta_i} \left(1 - \sum_{i=1}^N Y_i^* \right) \xrightarrow{\eta_i=Y_i} \frac{Y_i^*}{\sum_{i=1}^N Y_i^*}, \quad (2.45)$$

and

$$\lambda = \frac{1 - \sum_{i=1}^N Y_i^*}{\sum_{i=1}^N \eta_i} \xrightarrow{\eta_i=Y_i} \frac{1 - \sum_{i=1}^N Y_i^*}{\sum_{i=1}^N Y_i^*}. \quad (2.46)$$

The Algorithm 2 demonstrates the process of how ERENA integrates the ODEs when it is implemented into a CFD solver. In this study, a user-specified threshold value $\epsilon = 1.0 \times 10^{-7}$ is used to limit the error and to refine the time size. (At Step 4 of the Algorithm 2, users may slightly increase Δt^* to let the algorithm find a larger time size instead of continuing to use the smallest one.)

Note that ERENA can also be applied to other integration methods to solve the reactive ODEs numerically.

Algorithm 2 Extended Robustness-Enhanced Numerical Algorithm (ERENA).

Require: Δt_{CFD} , ϵ , Δt_{min}

- 1: $\Delta t_{chem} \leftarrow 0$
 - 2: $\Delta t^* \leftarrow \Delta t_{CFD}$
 - 3: **while** $\Delta t_{chem} < t_{CFD}$ **do**
 - 4: {Step 1: Y_i^* predicted by the QSSA method using Δt^* }
 - 5: $c_i^n \leftarrow c(Y_i^n)$
 - 6: $\tau_i^n \leftarrow \frac{Y_i^n}{d(Y_i^n)}$
 - 7: $Y_i^* \leftarrow Y_i^n \exp\left(-\frac{\Delta t^*}{\tau_i^n}\right) + c_i^n \tau_i^n \left[1 - \left(-\frac{\Delta t^*}{\tau_i^n}\right)\right]$
 - 8: {Step 2: Criteria for the mass conservation}
 - 9: $\lambda \leftarrow \frac{1 - \sum_{i=1}^N Y_i^*}{\sum_{i=1}^N Y_i^*}$
 - 10: **if** $|\lambda| > \epsilon$ **then**
 - 11: $\Delta t^* \leftarrow \max(\epsilon \Delta t^*, \Delta t_{min})$ {Correction of Δt^* }
 - 12: **else**
 - 13: $Y_i^{n+1} \leftarrow \frac{Y_i^*}{\sum_{i=1}^N Y_i^*}$
 - 14: $T^{n+1} \leftarrow T^n - \frac{\sum_{i=1}^N e_i^n (Y_i^{n+1} - Y_i^n)}{\rho c_v^n}$
 - 15: **end if**
 - 16: {Step 3: Sub-integration fulfillment}
 - 17: $Y_i^n \leftarrow Y_i^{n+1}$
 - 18: $T^n \leftarrow T^{n+1}$
 - 19: $\Delta t_{chem} \leftarrow \Delta t_{chem} + \Delta t^*$
 - 20: {Step 4: Δt^* adjustment}
 - 21: $\Delta t^* \leftarrow \min(\Delta t^*, \Delta t_{CFD} - \Delta t_{chem})$
 - 22: **end while**
-

2.2.3 Time Integration Scheme for Fluid Dynamics Part

Governing Equations in the Conserved Form

In dealing with the fluid dynamics part, the production term is assumed to be zero. Thus, the governing equation could be written in a general form with $\dot{\omega}_i = 0$. (Eqn. (2.36))

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{E}_C}{\partial x} + \frac{\partial \mathbf{F}_C}{\partial y} = \frac{\partial \mathbf{E}_D}{\partial x} + \frac{\partial \mathbf{F}_D}{\partial y}, \quad (2.47)$$

The column vectors are indicated as follows.

$$\mathbf{Q} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho Y_1 \\ \vdots \\ \rho Y_N \end{pmatrix}, \mathbf{E}_C = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (E + p)u \\ \rho u Y_1 \\ \vdots \\ \rho u Y_N \end{pmatrix}, \mathbf{F}_C = \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (E + p)v \\ \rho v Y_1 \\ \vdots \\ \rho v Y_N \end{pmatrix}, \mathbf{E}_D = \begin{pmatrix} 0 \\ \tau_{xx} \\ \tau_{yx} \\ \beta_x \\ d_{1,x} \\ \vdots \\ d_{N,x} \end{pmatrix}, \mathbf{F}_D = \begin{pmatrix} 0 \\ \tau_{xy} \\ \tau_{yy} \\ \beta_y \\ d_{1,y} \\ \vdots \\ d_{N,y} \end{pmatrix}, \quad (2.48)$$

and

$$\beta_x = \tau_{xx} + \tau_{xy} - q_x, \quad (2.49)$$

$$\beta_y = \tau_{yx} + \tau_{yy} - q_y, \quad (2.50)$$

where $\mathbf{Q}$ is the solution vector, $\mathbf{E}$ and $\mathbf{F}$ are the flux vectors. The subscripts C and D of the flux vector represent the "convective" and the "diffusive" terms, respectively.

General Transformation of the Governing Equation

The partial differential equations are solved using the finite difference method in the computational domain (the generalized coordinate system) with uniformly distributed spatial intervals. The general form of the governing equation (Eqn. (2.47)) describes the flow phenomenon in the physical domain (the Cartesian coordinate system in this case). Thus, we need to transform the independent variables of the physical domain (x, y) to those of the computational domain (ξ, η) . (This study assumes the coordinates are unchanged with time. Thus, the transformation of time t is irrelevant.)

The variables of the general coordinate system are expressed as,

$$\begin{cases} \xi = \xi(x, y), \\ \eta = \eta(x, y). \end{cases} \quad (2.51)$$

The following matrix form gives the inverse transformation (from general to physical coordinates).

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} x_\xi & x_\eta \\ y_\xi & y_\eta \end{pmatrix} \begin{pmatrix} d\xi \\ d\eta \end{pmatrix}, \quad (2.52)$$

and the direct transformation (from physical to general coordinates) is expressed as follows,

$$\begin{pmatrix} d\xi \\ d\eta \end{pmatrix} = \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix} = \frac{1}{J} \begin{pmatrix} y_\eta & -x_\eta \\ -y_\xi & x_\xi \end{pmatrix} \begin{pmatrix} dx \\ dy \end{pmatrix}, \quad (2.53)$$

In the above transformation equations, the elements of the coefficient matrix represent the partial derivatives with respect to the subscript variable (e.g. $x_\xi = \partial x / \partial \xi$). The Jacobian determinant J is expressed as follows,

$$J \equiv \frac{\partial(x, y)}{\partial(\xi, \eta)} \equiv \begin{vmatrix} x_\xi & y_\xi \\ x_\eta & y_\eta \end{vmatrix} = x_\xi y_\eta - y_\xi x_\eta \quad (2.54)$$

The contravariant velocity components (U, V), the velocity components perpendicular to the ξ and η direction, are evaluated as,

$$\begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}. \quad (2.55)$$

Thereafter, the transformed governing equations (Eqn. (2.47)) can be written as,

$$\frac{\partial \hat{\mathbf{Q}}}{\partial t} + \frac{\partial \hat{\mathbf{E}}_C}{\partial x} + \frac{\partial \hat{\mathbf{F}}_C}{\partial y} = \frac{\partial \hat{\mathbf{E}}_D}{\partial x} + \frac{\partial \hat{\mathbf{F}}_D}{\partial y}, \quad (2.56)$$

$$\hat{\mathbf{Q}} = \frac{1}{J} \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \\ \rho Y_1 \\ \vdots \\ \rho Y_N \end{pmatrix}, \hat{\mathbf{E}}_C = \frac{1}{J} \begin{pmatrix} \rho U \\ \rho U u + \xi_x p \\ \rho U v + \xi_y p \\ (E + p)U \\ \rho u Y_1 \\ \vdots \\ \rho u Y_N \end{pmatrix}, \hat{\mathbf{F}}_C = \frac{1}{J} \begin{pmatrix} \rho V \\ \rho V u + \eta_x p \\ \rho V v + \eta_y p \\ (E + p)V \\ \rho v Y_1 \\ \vdots \\ \rho v Y_N \end{pmatrix},$$

$$\hat{\mathbf{E}}_D = \frac{1}{J} \begin{pmatrix} 0 \\ \xi_x \tau_{xx} + \xi_y \tau_{xy} \\ \xi_x \tau_{yx} + \xi_y \tau_{yy} \\ \xi_x \beta_x + \xi_y \beta_y \\ \xi_x d_{1,x} + \xi_y d_{1,y} \\ \vdots \\ \xi_x d_{N,x} + \xi_y d_{N,y} \end{pmatrix}, \hat{\mathbf{F}}_D = \frac{1}{J} \begin{pmatrix} 0 \\ \eta_x \tau_{xx} + \eta_y \tau_{xy} \\ \eta_x \tau_{yx} + \eta_y \tau_{yy} \\ \eta_x \beta_x + \eta_y \beta_y \\ \eta_x d_{1,x} + \eta_y d_{1,y} \\ \vdots \\ \eta_x d_{N,x} + \eta_y d_{N,y} \end{pmatrix}.$$

The following sections introduce the scheme to acquire the numerical solution of the above non-linear governing equations. To simple clarify the basic concept of each scheme, the following introduction focus on the one-dimensional simplified form. For the actual two-dimensional solver used in this study, the one-dimensional manipulations are applied to the ξ and η direction in sequence.

To get the conservative variables $\mathbf{U}_i^{n+1}$ on i -th grid points x_i at $n + 1$ time step, we can treat the spatial interval within the fictional boundaries $x_{i-1/2}$ and $x_{i+1/2}$ as a *cell* (or a one-dimensional infinitesimal control volume). Let's call these boundaries the *intercell boundaries*. The grid points x_i are centred between them. The conservative variable $\mathbf{U}_i$ is considered as a *piece-wise* constant (a constant state) inside the cell. Since the variable is discontinuously distributed at the grid points (assuming $\mathbf{U}_{i-1}^n \neq \mathbf{U}_i^n$ and $\mathbf{U}_i^n \neq \mathbf{U}_{i+1}^n$), the solution for the next time step $\mathbf{U}_i^{n+1}$ is determined by solving the Riemann (or shock tube) problem at the intercell boundaries (namely, the Godunov method).

For a conservation equation, an integral form is evaluated by applying Green's theorem on the $x - t$ plane.

$$\oint \mathbf{U} dx + \mathbf{F} dt = 0. \quad (2.57)$$

The first-order upwind Godunov method discretises the above integral form as follows,

$$\mathbf{U}_i^{n+1} = \mathbf{U}_i^n - \frac{\Delta t}{\Delta x} (\mathbf{F}_{i+1/2} - \mathbf{F}_{i-1/2}) \quad (2.58)$$

$$= \mathbf{U}_i^n - \frac{\Delta t}{\Delta x} \left\{ \left[(\mathbf{F}_C)_{i+1/2} - (\mathbf{F}_C)_{i-1/2} \right] + \left[(\mathbf{F}_D)_{i+1/2} - (\mathbf{F}_D)_{i-1/2} \right] \right\} \quad (2.59)$$

Here, $F_{i-1/2}$ and $F_{i+1/2}$ denote the numerical fluxes at the intercell boundaries. The indices C and D represent the *inviscid*/convective (hyperbolic-type) and *viscous*/diffusive (parabolic-type) numerical fluxes, respectively. The Godunov method requires the exact solution of the Riemann problem to construct the numerical fluxes (this involves iteratively solving for p^* and u^* in the fluid motion and sampling the wave-propagation information for classification and piecewise treatment), which increases the computational cost.

This study employs an approximate Riemann solver to efficiently obtain numerical solutions of the governing equations. The Harten–Lax–van Leer–Contact (HLLC) [59, 64] scheme is adopted to construct the inviscid numerical fluxes at intercell boundaries. (The characteristic wave speeds are determined via Roe averaging [65], and Thornber's velocity correction [66] is applied to reduce numerical viscosity in low-Mach-number regions.) To achieve high spatial accuracy, the Monotone Upstream-centered Scheme for Conservation Laws (MUSCL) [60, 64] is used to reconstruct the conservative variables at the intercell boundaries. A quadratic reconstruction yields third-order accuracy in space. A minmod limiter is employed to revert to first-order accuracy and prevent numerical instabilities when discontinuities are detected. For the viscous numerical flux, which has effectively infinite wave speed and no clear propagation direction (isentropic), a second-order central difference scheme is used for its evaluation. Finally, a Total-Variation-Diminishing (TVD) third-order Runge–Kutta method [61] is applied for time integration, ensuring the TVD property of the solution while attaining third-order temporal accuracy.

Harten-Lax-van Leer-Contact (HLLC) Scheme

The approximate-state Riemann solver directly evaluates the numerical intercell flux, thereby bypassing the Godunov method's need for an exact solution of the Riemann problem. In the HLLC scheme [59], the numerical flux at cell interfaces is represented by four constant states, $\mathbf{U}_L$, $\mathbf{U}_{*L}$, $\mathbf{U}_{*R}$, and $\mathbf{U}_R$. These states are separated on the $x-t$ plane by three characteristic wave speeds: a minimum, a maximum, and an intermediate speed ($S_L = u - a$, $S_R = u + a$, and S_* , with $S_L < S_* < S_R$). The region between S_L and S_R on the $x-t$ diagram is referred to as the *star region*. The intermediate wave speed S_* splits this star region into two subregions, associated with $\mathbf{U}_{*L}$ and $\mathbf{U}_{*R}$, which enables the HLLC scheme to accurately resolve the middle waves (such as the contact discontinuity and species convection waves).

The HLLC scheme then determines the numerical flux at the cell interface as follows:

$$\mathbf{F}_{i+1/2}^{HLLC} = \begin{cases} \mathbf{F}_L, & 0 \leq S_L, \\ \mathbf{F}_{*L} = \mathbf{F}_L + S_L (\mathbf{U}_{*L} - \mathbf{U}_L), & S_L \leq 0 \leq S_*, \\ \mathbf{F}_{*R} = \mathbf{F}_R + S_R (\mathbf{U}_R - \mathbf{U}_{*R}), & S_* \leq 0 \leq S_R, \\ \mathbf{F}_R, & S_R \leq 0, \end{cases} \quad (2.60)$$

where the states of the star regions read,

$$U_{*K} = \rho_K \frac{S_K - u_K}{S_K - S_*} \left(\begin{array}{c} 1 \\ S_* \\ v_K \\ \frac{E_K}{\rho_K} + (S_* - u_K) \left[S_* + \frac{p_K}{\rho_K(S_K - u_K)} \right] \\ Y_1 \\ \vdots \\ Y_N \end{array} \right), K = L \text{ or } R. \quad (2.61)$$

The middle wave speed S_* is evaluated as follows:

$$S_* = \frac{p_R - p_L + \rho_L u_L (S_L - u_L) - \rho_R u_R (S_R - u_R)}{\rho_L (S_L - u_L) - \rho_R (S_R - u_R)}. \quad (2.62)$$

To determine the constant states in the star regions for constructing the HLLC numerical flux, it is necessary to identify the maximum and minimum wave speeds. The speed of sound can then be directly computed as

$$a = \sqrt{\frac{\gamma p}{\rho}} \quad (2.63)$$

where $\gamma (= c_p/c_v)$ represents the adiabatic index. S_L and S_R take the values from the minimum and the maximum wave speed,

$$\begin{cases} S_L = \min(u_L - a_L, \tilde{u} - \tilde{a}), \\ S_R = \max(u_R + a_R, \tilde{u} + \tilde{a}), \end{cases} \quad (2.64)$$

where $\tilde{u}$ and $\tilde{a}$ are evaluated using the Roe averaging method [65], as shown below:

$$\tilde{u} = \frac{\sqrt{\rho_L} u_L + \sqrt{\rho_R} u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \quad (2.65)$$

$$\tilde{H} = \frac{\sqrt{\rho_L} H_L + \sqrt{\rho_R} H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}, \quad (2.66)$$

$$\tilde{a}^2 = (\gamma - 1) \left(\tilde{H} - \frac{1}{2} \tilde{u}^2 \right), \quad (2.67)$$

where $H (= (E + p)/\rho)$ is the total enthalpy in mass units.

The HLLC (upwind) scheme employs numerical viscosity to handle supersonic flows and to capture shocks in a stable manner. This artificial viscosity is directly related to the speed

of sound. In low-Mach-number (Ma) flows, however, this viscosity becomes excessively large and suppresses the fluid's kinetic energy. Thornber's velocity correction [66] addresses this by reducing the velocity difference that feeds into the numerical viscosity. In doing so, it preserves the correct scaling of pressure and density fluctuations as Ma decreases, allowing the numerical method to mimic incompressible flow behavior. The velocity jump is then adjusted as follows,

$$u_{L,\text{new}} = \frac{u_L + u_R}{2} + \Phi \frac{u_L - u_R}{2}, \quad (2.68)$$

$$u_{R,\text{new}} = \frac{u_L + u_R}{2} - \Phi \frac{u_L - u_R}{2}, \quad (2.69)$$

$$(2.70)$$

where

$$\Phi = \min \left[1, \max \left(\frac{|\mathbf{u}_L|}{a_L}, \frac{|\mathbf{u}_R|}{a_R} \right) \right]. \quad (2.71)$$

(Note that $|\mathbf{u}|$ is the magnitude of the velocity vector, $|\mathbf{u}| = \sqrt{u^2 + v^2}$.)

Monotone Upstream Centered Scheme for Conservation Law (MUSCL)

MUSCL [60] reconstructs the intercell surface variables ($\mathbf{U}_L, \mathbf{U}_R$) for evaluating numerical flux $\mathbf{F}_{i+1/2}^{HLLC}$ to achieve high-order accuracy.

The Godunov-type method treats variables of a cell as constant piece-wise data, namely, $U(x) = U_i = \text{Const.}$ between the intercell boundaries from $i - 1/2$ to $i + 1/2$. The MUSCL method assumes that the variables are distributed inside the cell with the characteristic state unchanged (U_i conserved). (Here, we assume variable U is one component of $\mathbf{U}$.)

$$U_i = \frac{1}{\Delta x} \int_{i-1/2}^{i+1/2} U(x) dx. \quad (2.72)$$

A piece-wise quadratic reconstruction considering both the linear and curvature effects reads,

$$U(x) = U_i + \frac{1}{\Delta x} (x - x_i) U'_i + \frac{3\kappa}{2(\Delta x)^2} \left[(x - x_i)^2 - \frac{(\Delta x)^2}{12} \right] U''_i, \quad (2.73)$$

where the first and the second derivatives are evaluated by,

$$U'_i = \frac{1}{2} (U_{i+1} - U_{i-1}), \quad (2.74)$$

$$U''_i = U_{i+1} - 2U_i + U_{i-1}. \quad (2.75)$$

The variables on both sides of the intercell surface $i + 1/2$ are extrapolated as

$$\begin{aligned} U_{i+1/2}^L &= U_i + \frac{1}{2} U'_i + \frac{\kappa}{4} U''_i \\ &= U_i + \frac{1}{4} (1 - \kappa) (U_i - U_{i-1}) + \frac{1}{4} (1 + \kappa) (U_{i+1} - U_i) \\ &= U_i + \frac{1}{4} [(1 - \kappa) \Delta_- + (1 + \kappa) \Delta_+]_i, \end{aligned} \quad (2.76)$$

$$\begin{aligned}
U_{i+1/2}^R &= U_{i+1} - \frac{1}{2}U'_{i+1} + \frac{\kappa}{4}U''_{i+1} \\
&= U_{i+1} - \frac{1}{4}(1+\kappa)(U_{i+1} - U_i) - \frac{1}{4}(1-\kappa)(U_{i+2} - U_{i+1}) \\
&= U_{i+1} - \frac{1}{4}[(1-\kappa)\Delta_+ + (1+\kappa)\Delta_-]_{i+1},
\end{aligned} \tag{2.77}$$

where the slopes $\Delta_{\pm}$ are defined by

$$(\Delta_+)_i = U_{i+1} - U_i, \quad (\Delta_-)_i = U_i - U_{i-1}. \tag{2.78}$$

Assuming $\kappa = 1/3$, the above quadratic reconstruction yields the third-order spatial accuracy.

To ensure the Total Variation Diminishing (TVD), the slopes restricted by the minmod limiter are used,

$$\begin{aligned}
\bar{\Delta}_+ &= \text{minmod}(\Delta_+, b\Delta_-) \\
\bar{\Delta}_- &= \text{minmod}(\Delta_-, b\Delta_+) \\
b &= \frac{3-\kappa}{1-\kappa}
\end{aligned} \tag{2.79}$$

The minmod limiter is defined as

$$\text{minmod}(\alpha, \beta) = \text{sgn}(\alpha) \cdot \max\{0, \min[\alpha \text{sgn}(\beta), \beta \text{sgn}(\alpha)]\}. \tag{2.80}$$

The above equation could be interpreted as follows,

$$\text{minmod}(\alpha, \beta) = \begin{cases} \text{sgn}(\alpha) \cdot \min(|\alpha|, |\beta|), & \text{sgn}(\alpha) = \text{sgn}(\beta), \\ 0, & \text{sgn}(\alpha) \neq \text{sgn}(\beta). \end{cases} \tag{2.81}$$

When the slopes (Δ_+ and Δ_-) have different signs (indicating the presence of a shock or a discontinuity), the reconstruction reverts to first-order accuracy to avoid numerical instabilities. ($U_{i+1/2}^L = U_i$, $U_{i+1/2}^R = U_{i+1}$)

Second-order Central Difference Scheme

Compared to the inviscid numerical flux (*hyperbolic*), which requires an upwind scheme to capture the propagation of characteristic waves, the viscous numerical flux (*parabolic*) is simply computed using a second-order central difference scheme, as the perturbation is immediately applied to the entire simulation domain. Here, we rewrite the flux of molecular transport (diffusive) processes in a general form as

$$F_D = D \frac{\partial U}{\partial x}, \tag{2.82}$$

where F_D corresponds to the molecular transport processes of heat conduction, viscosity, and species diffusion, respectively. D and $\partial U/\partial x$ are the corresponding coefficient and the variable gradient. Their values at the intercell surface are built by

$$D_{i+1/2} = \frac{D_{i+1} + D_i}{2}, \tag{2.83}$$

$$\left(\frac{\partial U}{\partial x}\right)_{j+1/2} = \frac{U_{i+1} - U_i}{\Delta x}. \quad (2.84)$$

Therefore, the viscous flux is computed by

$$(F_D)_{i+1/2} = D_{i+1/2} \frac{U_{i+1} - U_i}{\Delta x}. \quad (2.85)$$

This leads to the second-order spatial accuracy in computing the gradients of the viscous fluxes,

$$\frac{(F_D)_{i+1/2} - (F_D)_{i-1/2}}{\Delta x} = \frac{D_{i+1/2} (U_{i+1} - U_i) - D_{i-1/2} (U_i - U_{i-1})}{\Delta x^2}. \quad (2.86)$$

Total-Variation Diminishing (TVD) Third-order Runge-Kutta

This study uses a TVD third-order Runge-Kutta method [61] to achieve high temporal accuracy while maintaining the TVD property, namely, the total variation of the numerical solution is non-increasing in time. An optimal method provided by Gottlieb reads,

$$\begin{aligned} \mathbf{U}^{(1)} &= \mathbf{U}^n + \Delta t \Delta \mathbf{F}(\mathbf{U}^n), \\ \mathbf{U}^{(2)} &= \frac{3}{4} \mathbf{U}^n + \frac{1}{4} [\mathbf{U}^{(1)} + \Delta t \Delta \mathbf{F}(\mathbf{U}^{(1)})], \\ \mathbf{U}^{n+1} &= \frac{1}{3} \mathbf{U}^n + \frac{2}{3} [\mathbf{U}^{(2)} + \Delta t \Delta \mathbf{F}(\mathbf{U}^{(2)})], \end{aligned} \quad (2.87)$$

where the $\Delta \mathbf{F}$ includes all the spatial discretisations and the numerical fluxes evaluated using the preceding schemes. Analytically, for numerically solving Euler equation, this method require the CFL coefficients less than one, $c = \Delta x / (a \Delta t) \leq 1$. In this study, the CFL coefficients are all lower than 0.8.

Chapter 3

LTF-S: Localized Thickened Flame Model for Stretched Premixed Hydrogen Flames

In this chapter, a previously proposed LTF model is evaluated using a stretched flame configuration, namely a cylindrical, outwardly propagating flame (OPF). This assessment shows that the LTF model increases the Markstein length of the flame, causing an exaggerated response to flame stretch. The results demonstrate a linear relationship between the Markstein length ratio and the flame thickening factor. To address the issue of the thickened stretched flame and recover the correct stretch response, an improved LTF-S model is developed. When validated against the same flame configuration, the LTF-S model successfully reproduces the stretched flame speed while preserving the increased flame thickness.

Section 3.2 presents the general concept of the thickened flame models and the governing equations of the LTF formulation. This section provides revised analytical expressions for the flame speed and flame thickness derived from the energy conservation equation, describes the numerical setup for the two-dimensional OPF configuration, and demonstrates the inability of the LTF model to accurately predict stretched burning velocities. Section 3.3 develops the mathematical formulation of the new LTF-S model, which extends the LTF approach to stretched premixed flames, and details the numerical procedure used to compute the local stretch rate required for the LTF-S model parameters. To restrict the model's influence in regimes of intense stretch, an extinction stretch rate is introduced. The LTF-S model is subsequently distinguished with other stretched thickened flame formulations. Finally, simulation results are presented to confirm the predictive accuracy of the LTF-S model.

3.1 Empirical Relationships for Laminar Flame Speed and Flame Thickness

We use two equations—the sensible enthalpy and progress variable equations—to derive empirical relationships for laminar flame speed and thickness:

$$\frac{\partial}{\partial t}(\rho h^s) + \nabla \cdot \left(\rho \mathbf{u} h^s + \rho \sum_{i=1}^N h_i^s Y_i \mathbf{V}_i - \kappa \nabla T \right) = \frac{dp}{dt} - \sum_{i=1}^N h_{f,i}^0 \dot{\omega}_i, \quad (3.1)$$

$$\frac{\partial \rho Y_c}{\partial t} + \nabla \cdot [\rho Y_c (\mathbf{u} + \mathbf{V}_c)] = \dot{\omega}_c. \quad (3.2)$$

Here, $h_{f,i}^0$ and h_i^s denote the standard enthalpy of formation and the sensible enthalpy of the i -th species. (, respectively, where $h_i^s = \int_{T^0}^T c_{p,i} dT$. The sensible enthalpy of the mixture is given by $h^s = \sum_{i=1}^N Y_i h_i^s$. The vector $\mathbf{V}_i$ represents the diffusion velocity of the species i -th species, and $Y_i \mathbf{V}_i = -\rho D_i \nabla Y_i$. The progress variable Y_c is defined as a linear combination of species mass fractions, $Y_c = \sum_{i=1}^N \alpha_i Y_i$, where α_i is a weighting coefficient specific to each species. Analogous to the species conservation formulation, the diffusive flux of the progress variable is given by $Y_c \mathbf{V}_c = \sum_{i=1}^N \alpha_i Y_i \mathbf{V}_i$, and its source term by $\dot{\omega}_c = \sum_{i=1}^N \alpha_i \dot{\omega}_i$. (In practice, choosing the deficient species or the light reactants such that $Y_c = Y_i$ can be convenient.) By taking $C_{p,i} \equiv C_p$ (and therefore $h_i^s \equiv h^s$), the third term in Eq. (3.1) vanishes because the statistically averaged diffusion velocity is zero, i.e., $\sum_{i=1}^N Y_i \mathbf{V}_i = 0$,

$$\sum_{i=1}^N h_i^s Y_i \mathbf{V}_i = h^s \sum_{i=1}^N Y_i \mathbf{V}_i = 0. \quad (3.3)$$

For a one-dimensional, steady, and non-stretched flame, Eq. (3.1) and Eq. (3.2) can be reduced to the following forms:

$$\frac{d}{dx} \left(\rho u C_p T - \kappa \frac{dT}{dx} \right) = -Q \dot{\omega}_c, \quad (3.4)$$

$$\frac{d}{dx} \left(\rho u Y_c - \rho D_c \frac{dY_c}{dx} \right) = \dot{\omega}_c, \quad (3.5)$$

where the source term in the sensible enthalpy equation is expressed as $Q \dot{\omega}_c = \sum_{i=1}^N h_{f,i}^0 \dot{\omega}_i$, with Q denoting the heat of reaction per unit mass of reactant.

We adopt the activation energy asymptotic approximation, assuming that the reaction occurs in a thin reaction zone whose thickness is comparably smaller than that of the preheat zone of the flame. The flame structure basing on the activation energy asymptotic approximation is illustrated by Fig. 3.1. The following boundary conditions can be applied,

$$\left\{ \begin{array}{ll} T = T_u, & \frac{dT}{dx} = 0, \\ \frac{dY_c}{dx} = 0, & \text{at } x = -\infty; \\ T = T_i, & \frac{dT}{dx} = \left(\frac{dT}{dx} \right)_{x_f^-}, \\ \frac{dY_c}{dx} = \left(\frac{dY_c}{dx} \right)_{x_f^-}, & \text{at } x = x_f^-; \\ T = T_b^0, & \frac{dT}{dx} = 0, \\ \frac{dY_c}{dx} = 0, & \text{at } x = x_f^+ \text{ and } x = \infty. \end{array} \right. \quad (3.6)$$

In the preheat zone, the convection term is balanced by the diffusion term, and Eq. (3.4) can be simplified as follows,

$$\frac{d}{dx} \left(\rho u C_p T - \kappa \frac{dT}{dx} \right) = 0. \quad (3.7)$$

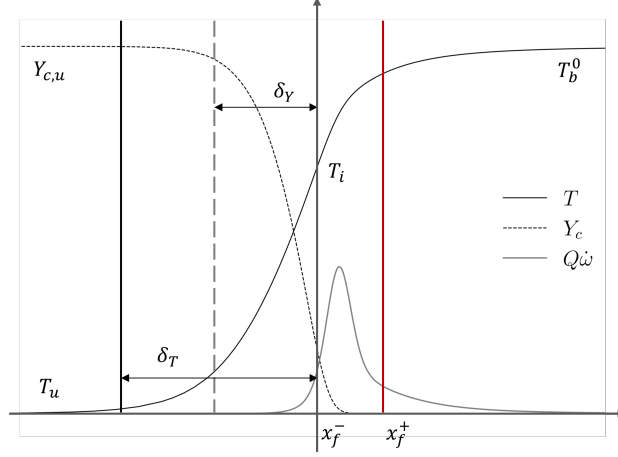


Figure 3.1: Structure of one-dimensional non-stretched premixed flame.

By integrating the above equation across the preheat zone, we obtain

$$\left(\rho u C_p T - \kappa \frac{dT}{dx} \right)_{-\infty}^{x_f^-} = 0, \quad (3.8)$$

$$\left(\frac{dT}{dx} \right)_{x_f} = \frac{\rho u C_p}{\kappa} (T_i - T_u) \simeq \frac{\rho u C_p}{\kappa} (T_b^0 - T_u) \quad (3.9)$$

As the temperature gradient could be also approximated by,

$$\left(\frac{dT}{dx} \right)_{x_f} \approx \frac{T_b^0 - T_u}{\delta_L}, \quad (3.10)$$

By substituting the above equation into Eq. (3.9), a formulation for thermal thickness can be acquired

$$\delta_L = \frac{\kappa}{\rho u C_p}. \quad (3.11)$$

In the reaction zone, convection is neglected, and the diffusion term is taken to be in balance with the source term,

$$\frac{d}{dx} \left(\frac{dT}{dx} \right) = -\frac{Q}{\kappa} \dot{\omega}_c. \quad (3.12)$$

By multiplying $2 \frac{dT}{dx}$ on both sides of the above equation, we obtain a more convenient form,

$$2 \frac{dT}{dx} \cdot \frac{d}{dx} \left(\frac{dT}{dx} \right) = -2 \frac{dT}{dx} \frac{Q}{\kappa} \dot{\omega}_c, \quad (3.13)$$

$$\frac{d}{dx} \left(\frac{dT}{dx} \right)^2 = -2 \frac{dT}{dx} \frac{Q}{\kappa} \dot{\omega}_c. \quad (3.14)$$

Integrating the above equation through the reaction zone (from x_f^- to x_f^+),

$$\left[\left(\frac{dT}{dx} \right)^2 \right]_{x_f^-}^{x_f^+} = -\frac{2Q}{\kappa} \int_{x_f^-}^{x_f^+} \dot{\omega}_c \frac{dT}{dx} dx, \quad (3.15)$$

$$0 - \left[\left(\frac{dT}{dx} \right)_{x_f^-} \right]^2 = -\frac{2Q}{\kappa} \int_{T_i}^{T_b^0} \dot{\omega}_c dT. \quad (3.16)$$

By substituting Eq. (3.9) into the above equation,

$$\left[\frac{\rho u C_p}{\kappa} (T_b^0 - T_u) \right]^2 = \frac{2Q}{\kappa} (T_b^0 - T_i) \dot{\omega}, \quad (3.17)$$

$$\rho u = \sqrt{\frac{2Q\kappa\dot{\omega}(T_b^0 - T_i)}{[C_p (T_b^0 - T_u)]^2}}, \quad (3.18)$$

where $\dot{\omega}$ is the averaged reaction rate.

For the one-dimensional steady non-stretched flame, the laminar burning flux $\rho_u s_u^0 = \rho u$ is conserved inside the flame, thus the lamianr flame speed could be evaluated as

$$s_u^0 = \sqrt{\frac{2Q\kappa\dot{\omega}(T_b^0 - T_i)}{[\rho_u C_p (T_b^0 - T_u)]^2}} \quad (3.19)$$

$$= \sqrt{\frac{2Q(T_b^0 - T_i)}{\rho_u C_p (T_b^0 - T_u)^2}} \sqrt{\alpha \dot{\omega}} \quad (3.20)$$

where $\alpha = \frac{\kappa}{\rho_u C_p}$ is the thermal diffusivity

By substituting Eq. (3.18) into Eq. (3.11), the flame thickness can be determined as follows:

$$\delta_L = \frac{\kappa}{\rho u C_p} = \frac{\kappa}{\rho_u s_u^0 C_p} = \frac{\alpha}{s_u^0} = \sqrt{\frac{\rho_u C_p (T_b - T_u)^2}{2Q(T_b^0 - T_i)}} \sqrt{\frac{\alpha}{\dot{\omega}}} \quad (3.21)$$

Consequently, empirical correlations for the laminar flame speed and flame thickness can be written as follows,

$$s_u^0 \propto \sqrt{\alpha \dot{\omega}} \quad (3.22)$$

$$\delta_L \propto \sqrt{\alpha / \dot{\omega}} \quad (3.23)$$

Combining the Lewis number ($Le_i = \frac{\alpha}{D_i}$) and the Prandtl number ($Pr = \frac{\nu}{\alpha}$), the flame speed also proportional to the species diffusion coefficients and the momentum diffusivity (kinematic viscosity $\nu = \mu/\rho$),

$$s_u^0 \propto \sqrt{Le_i D_i \dot{\omega}}, \quad (3.24)$$

$$\delta_L \propto \sqrt{Le_i D_i / \dot{\omega}}, \quad (3.25)$$

and

$$s_u^0 \propto \sqrt{\nu \dot{\omega} / Pr}, \quad (3.26)$$

$$\delta_L \propto \sqrt{\nu / (\dot{\omega} Pr)}. \quad (3.27)$$

For convenience, we restate these relationships directly using two equivalent expressions in summation form,

$$s_u^0 \propto \sqrt{\alpha \dot{\omega} + D_i \dot{\omega} + \nu \dot{\omega}}, \quad (3.28)$$

$$\delta_L \propto \sqrt{\frac{\alpha}{\dot{\omega}} + \frac{D_i}{\dot{\omega}} + \frac{\nu}{\dot{\omega}}}. \quad (3.29)$$

Note that, in 3.3, the thermal diffusivity α and the kinematic viscosity ν are replaced by the thermal conductivity κ and the viscosity μ , respectively. This is done to ensure consistency with the governing equation used to derive the LTF-S model parameters. (This modification is made purely for clarity.)

3.2 Localized Thickened Flame (LTF) Model

For the combustion CFD with finite rate chemistry, the reaction occurs in a extremely small time scale and cause the steep spatial gradient across the flame fronts. This study employs the thickened flame (TF) concept to overcome the constraints to accelerate the combustion simulations.

3.2.1 LTF Model Implemented Governing Equation

The governing equation with the localized thickened flame model is show as follows,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (3.30)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot [\rho \mathbf{u} \otimes \mathbf{u} + p \boldsymbol{\delta} - (1 + \chi) \boldsymbol{\tau}] = 0, \quad (3.31)$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p) \mathbf{u} - (1 + \chi) \boldsymbol{\tau} \cdot \mathbf{u} + (1 + \chi) \mathbf{q}] = 0, \quad (3.32)$$

$$\frac{\partial \rho Y_i}{\partial t} + \nabla \cdot [\rho Y_i \mathbf{u} - (1 + \chi) \mathbf{d}_i] = \frac{\dot{\omega}_i}{1 + \chi}, \quad (3.33)$$

The viscous and source terms of the equation may be interpreted as

$$\boldsymbol{\tau}_{\text{LTF}} = (1 + \chi) \boldsymbol{\tau} = \mu_{\text{LTF}} \left[2\mathbf{S} - \frac{2}{3} (\nabla \cdot \mathbf{u}) \boldsymbol{\delta} \right], \quad (3.34)$$

$$\mathbf{q}_{\text{LTF}} = (1 + \chi) \mathbf{q} = -\kappa_{\text{LTF}} \nabla T - \sum_{i=1}^N h_i \mathbf{d}_{i,\text{LTF}}, \quad (3.35)$$

$$\mathbf{d}_{i,\text{LTF}} = (1 + \chi)\mathbf{d}_i = \rho D_{i,\text{LTF}} \nabla Y_i, \quad (3.36)$$

$$\dot{\omega}_{i,\text{LTF}} = \frac{\dot{\omega}_i}{1 + \chi}, \quad (3.37)$$

where

$$\mu_{\text{LTF}} = (1 + \chi)\mu, \quad (3.38)$$

$$\kappa_{\text{LTF}} = (1 + \chi)\kappa, \quad (3.39)$$

$$D_{i,\text{LTF}} = (1 + \chi)D_i. \quad (3.40)$$

Thus, when χ is uniform in both time and space, the LTF model collapses to the original TF model [31–33]. The factor $1 + \chi$ can be identified with the flame thickening factor F commonly employed in TF formulations.

The LTF model parameter χ is defined as the following function.

$$\chi = C_\chi \frac{\Delta s_F}{\delta_L} \overline{\sum_{i=1}^3 \left| \frac{\partial^4}{\partial x_i^4} \left(\frac{T}{T_{ad}} \right) \right| \Delta x_i^4}, \quad (3.41)$$

where Δs_F is the grid spacing for resolving a flame. δ^0 and T_{ad} represent a laminar flame thickness and an adiabatic flame temperature for a given condition. x_i refers to the Cartesian coordinates x , y , and z when the subscript i is 1, 2, and 3, respectively. Δx_i is the grid spacing. The overline in Eq. (3.41) denotes a Gaussian filter with a standard deviation of 3.0. The ratio of grid spacing to the laminar flame thickness $\Delta s_F/\delta^0$ ensures that the same number of grid points is used to resolve the flame. C_χ is a user-defined parameter.

While the previous study [36] recommended a C_χ value between 100 and 150 for 1-D planar propagating flames, this study employs a larger value of $C_\chi = 400$. This adjustment is due to the inadequacy of the recommended C_χ value for resolving flames propagating diagonally within a grid cell in simulations using a multi-dimensional Cartesian grid, which led to spurious (grid-induced) flame instabilities. A preliminary study confirmed that, for a 2-D cylindrically propagating flame problem, the flame propagation behaviors were nearly identical between $C_\chi = 300$ and $C_\chi = 400$, with spurious flame instabilities effectively prevented. The fourth-order temperature gradient detects the flame location and localizes the flame thickening effects, and thus, the model was named the localized TF (LTF) model.

Gaussian Filter

To reduce the noise and obtain a smooth function of the fourth-order temperature derivative, a Gaussian filter is applied. The Gaussian filter modifies the input signal by convolution with a Gaussian function, and the one-dimensional Gaussian function is expressed as follows,

$$g(\xi) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\xi^2}{2\sigma^2}}, \quad (3.42)$$

where σ^2 is the variance (σ is the standard deviation). σ decides the filter range and $\sigma = 3$ is used in this study. ξ represents the general coordinates.

To operate the filtering operation, firstly the average of the Gaussian distribution ($g'(\xi_i)$) at the point $\xi = \xi_i$ (the i -th cell (or grid point) in ξ direction) is numerically calculated as follows,

$$g'(\xi_i) = \frac{1}{100} \sum_{N=-50}^{50} \frac{1}{\sqrt{2\pi\sigma^2}} e^{\left[-\frac{1}{2\sigma^2}\left(\xi_i + \frac{N}{100}\right)^2\right]}, \quad (3.43)$$

where the Gaussian function is discretized on 100 points in the cell (49 points each at the left- and right-hand side of the center point). Then, $g'(\xi_i)$ is normalized on the adjacent 39 grid points to get the discretized Gaussian function $g''(\xi_i)$,

$$g''(\xi_i) = \frac{1}{\sum_{i=-19}^{19} g'(\xi_i)} g'(\xi_i) \quad (3.44)$$

Finally, the Gaussian filter is applied to the evaluated distribution $f(x)$,

$$\bar{f}(x) = \int f(x) g''(x - \xi) d\xi. \quad (3.45)$$

In case of multidimensional (2D and 3D) occasions, the filter operation is sequentially applied to each direction of the general coordinates.

3.2.2 Numerical Configuration of Cylindrical Flame Propagation

This study proposes a new LTF model for flames under stretching effects. As indicated in previous studies [46–49], the flame thickening in TF models inhibits a flame response when the flame is stretched (curved or strained). Fig. 3.3 shows the flame speed against the stretch rate and the flame location in a cylindrical H₂/air flame propagation, obtained using the direct numerical simulation (DNS) and LTF model [36]. As shown in Fig. 3.2, a uniformly spaced grid is used for a fine-grid focused region of $|x| \leq 6$ cm and $|y| \leq 6$ cm, while a 10 m $\times$ 10 m large rectangular domain is used to minimize the influence of boundaries where the grid spacing is coarsened towards the outer boundaries. In the fine-grid focused region, a grid size of 20 μ m is used for the DNS, while two coarser uniform grid sizes of 160 μ m and 320 μ m are applied to the LTF model. For the LTF model, $\delta^0 = 0.0379$ cm, $T_{ad} = 2385.7$ K, and $C_\chi = 400$ are used in Eq. (3.41). The whole domain is initially filled with a stoichiometric H₂/air premixed gas of 300 K under 1 atm. The Neumann condition is applied at the outer boundaries. A high-temperature spot of the equilibrium burned gas with a radius of 0.5 cm is introduced in the center of the domain to initiate flame propagation. The temperature and chemical compositions of the equilibrium gas are obtained using the NASA-CEA program [67]. The initial temperature and mass fraction distributions of chemical species between the unburned and burned gas regions are connected using an error function. The UT-JAXA detailed reaction model [68], which consists of 9 species and 34 reactions, is applied.

In Fig. 3.3, the flame speed and stretch rate are evaluated as follows:

$$s_u = \frac{\rho_b}{\rho_u} \frac{dR_f}{dt} \quad (3.46)$$

$$K = \frac{1}{A} \frac{dA}{dt} = \frac{1}{R_f} \frac{dR_f}{dt} \quad (3.47)$$

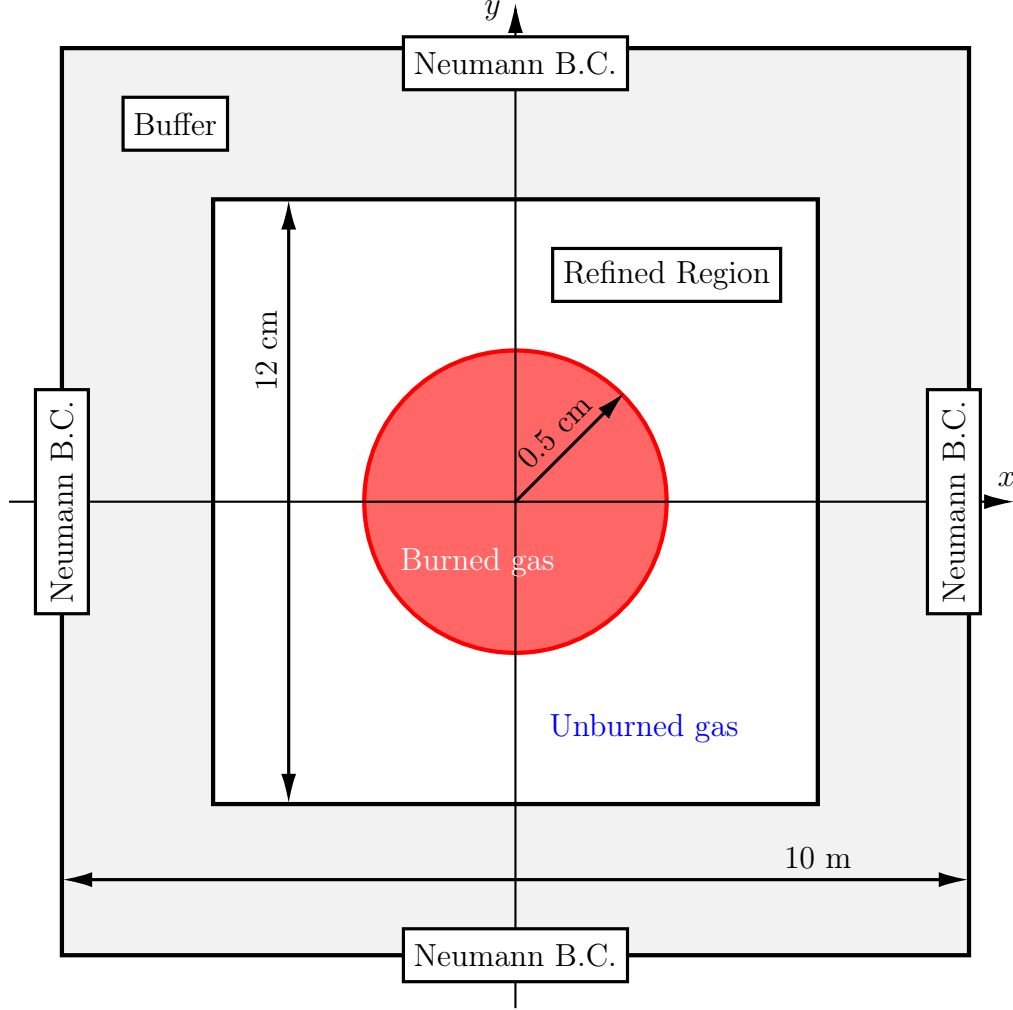


Figure 3.2: Schematic of a cylindrical outwardly propagating flame.

where ρ_b and ρ_u represent the unburned and burned gas densities, respectively. The area of the cylindrical flame front can be evaluated by $A = 2\pi R_f \Delta l$ where $\Delta l (= 1.0)$ is the unit length. R_f is the radial position of the propagating flame, which is determined by averaging three flame positions specified by the iso-temperature contours of 1200, 1400, and 1600 K.

$$R_f = \frac{R_{1000K} + R_{1200K} + R_{1400K}}{3} \quad (3.48)$$

Note that a line is drawn to represent the relationship between flame speed and stretch rate. This line is used to extract the Markstein length from the simulation results. A linear least-squares fit is applied to the data where the flame propagates steadily, with the value at $K = 0$ fixed for the unstretched flame speed.

The results show that the LTF model, which predicts accurate flame speeds for planar flames [36], simulates the lower flame speeds than the DNS solution under stretching conditions. Thus, it is demonstrated the flame thickening hinders the flame's proper response when it is stretched. The DNS results in Fig. 3.3 also illustrate that the flame speed and stretch rate

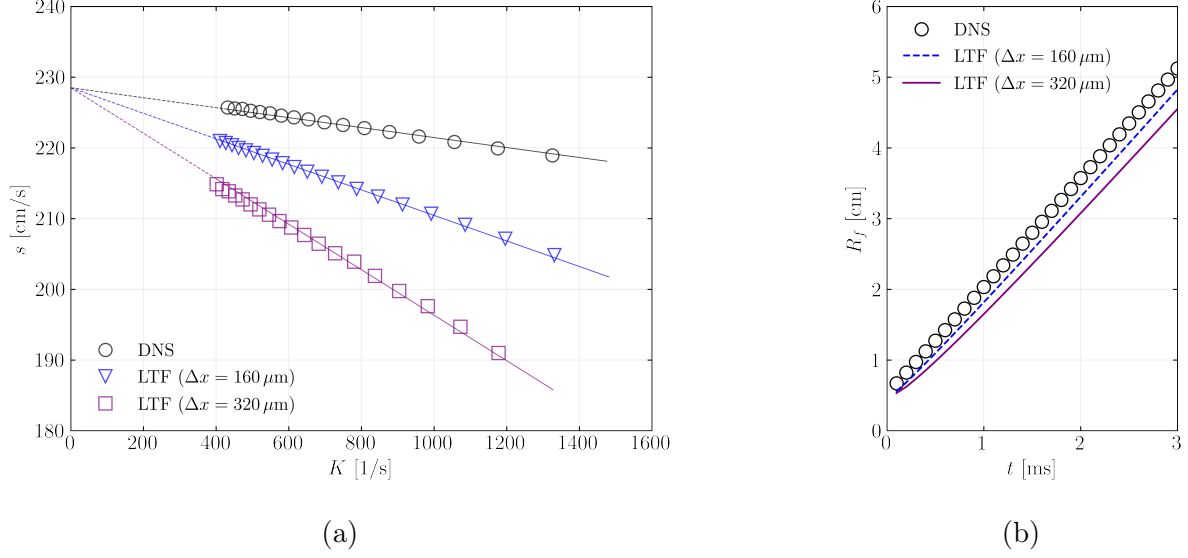


Figure 3.3: Flame speed against stretch rate (left) and the evolution of the flame location (right) in a cylindrical flame propagation problem. The lines in the left figure, obtained by a linear least-square fit, are used to extract the Markstein length from the simulation results.

exhibit a linear relationship from the steady stages of the propagation. Note that the initial transient phase, where nonlinear behaviors appear, have been removed from the results. The duration of the initial transient is within 0.5 ms. Therefore, the flame speed under stretching effects may be described as follows:

$$s_u = s_u^0 - \mathcal{L}_u K \quad (3.49)$$

where s_u^0 is the (laminar) unstretched flame speed, and $\mathcal{L}_u$ is the Markstein length. The relationship in Eq. (3.49) has been widely accepted for representing the stretching effects on flame speeds under weak stretching conditions [15, 69–71]. Considering that the Markstein length may be proportional to the flame thickness [37, 72], the flame speed simulated with TF models may be described as follows:

$$s_{u,\text{TF}} = s_u^0 - F \mathcal{L}_u K \quad (3.50)$$

where F is a flame thickening factor in TF models. Eq. (3.50) indicates that the flame speed under stretching effects is influenced by flame thickening (with the negative slope increasing for positive F values), consistent with the LTF results in Fig. 3.3.

3.3 Development of the LTF-S Model

3.3.1 Construction of the Unresolved Stretched Component

From the previous section, the LTF model thickened flame could not predict the correct flame speed. Here, we further introduce new components in the LTF modeled governing equations

to account for the unresolved stretch effect omitted by the LTF thickened flame. So that, the speed of stretched flames can be retrieved even under flame thickening.

$$\dot{\omega}_{i,\text{LTF-S}} = \dot{\omega}_{i,\text{LTF}} + \dot{\omega}_i^{\text{stretch}}, \quad (3.51)$$

$$\mu_{\text{LTF-S}} = \mu_{\text{LTF}} + \mu^{\text{stretch}}, \quad (3.52)$$

$$\kappa_{\text{LTF-S}} = \kappa_{\text{LTF}} + \kappa^{\text{stretch}}, \quad (3.53)$$

$$D_{i,\text{LTF-S}} = D_{i,\text{LTF}} + D_i^{\text{stretch}}, \quad (3.54)$$

where the LTF modeled terms are based on the directly resolved components and could be written as,

$$\dot{\omega}_{i,\text{LTF-S}} = \dot{\omega}_i + \left(-\frac{\chi}{1+\chi} \right) \dot{\omega}_i + \dot{\omega}_i^{\text{stretch}}, \quad (3.55)$$

$$\mu_{\text{LTF-S}} = \mu + \chi\mu + \mu^{\text{stretch}}, \quad (3.56)$$

$$\kappa_{\text{LTF-S}} = \kappa + \chi\kappa + \kappa^{\text{stretch}}, \quad (3.57)$$

$$D_{i,\text{LTF-S}} = D_i + \chi D_i + D_i^{\text{stretch}}. \quad (3.58)$$

Similarly, we here assume that the unresolved part for stretched flame can be constructed using the directly resolved part $\dot{\omega}_i$ and a newly introduced arbitrary function α as follows:

$$\dot{\omega}_i^{\text{stretch}} = \alpha \dot{\omega}_i \quad (3.59)$$

Then, the LTF-S modeled production rate of species in Eq. (3.51) is obtained as follows:

$$\begin{aligned} \dot{\omega}_{i,\text{LTF-S}} &= \dot{\omega}_{i,\text{LTF}} + \dot{\omega}_i^{\text{stretch}} \\ &= \left(1 - \frac{\chi}{1+\chi} + \alpha \right) \dot{\omega}_i \end{aligned} \quad (3.60)$$

In a similar fashion to the production rate of species, the LTF-S modeled diffusion coefficient (Eq. (3.58)) can be written by considering the unresolved part for the stretched flame $D_i^{\text{stretch}} = \beta D_i$ with a new function β , we derive the LTF-S modeled diffusion coefficient as follows:

$$\begin{aligned} D_{i,\text{LTF-S}} &= D_{i,\text{LTF}} + D_i^{\text{stretch}} \\ &= (1 + \chi + \beta) D_i \end{aligned} \quad (3.61)$$

Likewise, similar to the LTF model discussed in Eqs. (3.56) to (3.58), the LTF-S modeled thermal conductivity and viscosity are obtained as

$$\kappa_{\text{LTF-S}} = (1 + \chi + \beta) \kappa \quad (3.62)$$

and

$$\mu_{\text{LTF-S}} = (1 + \chi + \beta) \mu \quad (3.63)$$

respectively.

To determine the functions α and β for the unresolved parts of stretched flames, we first introduce a constraint that the flame is thickened by a factor of $1 + \chi$ as in the TF models

[31–33] for unstretched flames. Since the flame thickness may be approximately proportional to the square root of $D_i/\dot{\omega}_i$, $\kappa/\dot{\omega}_i$, and $\mu/\dot{\omega}_i$ according to [15], incorporating the unresolved parts yields the flame thickness δ given by

$$\begin{aligned}\delta &\propto \sqrt{\frac{D_i}{\dot{\omega}} + \frac{\kappa}{\dot{\omega}} + \frac{\mu}{\dot{\omega}}} \\ &= \sqrt{\frac{1 + \chi + \beta}{1 - \frac{\chi}{1 + \chi} + \alpha}} \sqrt{\frac{D_i}{\dot{\omega}} + \frac{\kappa}{\dot{\omega}} + \frac{\mu}{\dot{\omega}}}\end{aligned}\quad (3.64)$$

Therefore, a following condition is imposed for the functions α and β :

$$\sqrt{\frac{1 + \chi + \beta}{1 - \frac{\chi}{1 + \chi} + \alpha}} = 1 + \chi \quad (3.65)$$

and then the above equation yields a relationship

$$\beta = (1 + \chi)^2 \alpha \quad (3.66)$$

Another constraint for the functions α and β relates to the flame speed. The flame speed may be proportional to the square root of $D_i\dot{\omega}_i$, $\kappa\dot{\omega}_i$, and $\mu\dot{\omega}_i$ according to [15] (while this assumption may be ambiguous, the results of this study demonstrate its validity in modeling the flame speed). Therefore, introducing the unresolved parts gives the flame speed s_u as follows:

$$\begin{aligned}s_u &\propto \sqrt{D_i\dot{\omega}_i + \kappa\dot{\omega}_i + \mu\dot{\omega}_i} \\ &= \sqrt{(1 + \chi + \beta) \left(1 - \frac{\chi}{1 + \chi} + \alpha\right)} \sqrt{D_i\dot{\omega}_i + \kappa\dot{\omega}_i + \mu\dot{\omega}_i}\end{aligned}\quad (3.67)$$

Then, substituting Eq. (3.66) into the above equation yields

$$s_u \propto [1 + (1 + \chi)\alpha] \sqrt{D_i\dot{\omega}_i + \kappa\dot{\omega}_i + \mu\dot{\omega}_i} \quad (3.68)$$

Thus, it is interpreted that the unresolved parts can control the flame speed with the factor $[1 + (1 + \chi)\alpha]$ shown in Eq. (3.68). The flame speed can vary depending on the value of $(1 + \chi)\alpha$. The following section will discuss how to construct the function α and thus β to predict the correct speed of stretched flames under flame thickening.

3.3.2 Designing the Functions of α and β

In this study, we apply the theoretical equation for the speed of stretched flames of Eq. (3.49) to determine the functions α and β . Therefore, the model proposed in this study is primarily designed for flame speeds under weak stretching conditions, and the prediction accuracy may decrease under strong stretching condition, particularly near extinction, where Eq. (3.49) becomes invalid. A correct flame speed under stretching effects can be obtained with

$$s_u = s_u^0 - \mathcal{L}_u K \quad (3.69)$$

where $\mathcal{L}_u$ is a correct Markstein length, which can be obtained from experiments, analyses, or DNS solutions. In the LTF model, the flame speed under stretching effects can also be described as follows:

$$s_{u,\text{LTF}} = s_u^0 - \mathcal{L}_{u,\text{LTF}} K \quad (3.70)$$

where note that generally $\mathcal{L}_u \neq \mathcal{L}_{u,\text{LTF}}$ and thus $s_u \neq s_u^0$ because of flame thickening.

In Eq. (3.70), we consider modifying the Markstein length by introducing a function ε to retrieve the correct stretched flame speed. Thus, a modified flame speed s_ε can be written as follows:

$$\begin{aligned} s_\varepsilon &= s_u^0 - (\mathcal{L}_{u,\text{LTF}} + \varepsilon) K \\ &= s_{u,\text{LTF}} - \varepsilon K \\ &= \left(1 - \frac{\varepsilon K}{s_{u,\text{LTF}}}\right) s_{u,\text{LTF}} \end{aligned} \quad (3.71)$$

Considering the condition that the modified flame speed matches with the correct stretched flame speed ($s_\varepsilon = s_u$) provides a condition for ε as follows:

$$\varepsilon K = (\mathcal{L}_u - \mathcal{L}_{u,\text{LTF}}) K \quad (3.72)$$

Then, substituting Eq. (3.72) into (3.71) gives

$$\begin{aligned} s_\varepsilon &= \left[1 - \frac{(\mathcal{L}_u - \mathcal{L}_{u,\text{LTF}}) K}{s_{u,\text{LTF}}}\right] s_{u,\text{LTF}} \\ &= \left[1 + \frac{(\mathcal{L}_{u,\text{LTF}} - \mathcal{L}_u) K}{s_u^0 - \mathcal{L}_{u,\text{LTF}} K}\right] s_{u,\text{LTF}} \end{aligned} \quad (3.73)$$

where note that $s_{u,\text{LTF}}$ in the bracket is only replaced with Eq. (3.73) with (3.70) for convenience. Equation. (3.73) is interpreted that the flame speed obtained with an employed grid ($s_{u,\text{LTF}}$) can be modified with a factor $(1 + \psi)$ where

$$\psi = \frac{(\mathcal{L}_{u,\text{LTF}} - \mathcal{L}_u) K}{s_u^0 - \mathcal{L}_{u,\text{LTF}} K} \quad (3.74)$$

Finally, comparing Eq. (3.73) with Eq. (3.68) provides the function α as follows:

$$1 + (1 + \chi)\alpha = 1 + \psi \quad \rightarrow \quad \alpha = \frac{\psi}{1 + \chi} \quad (3.75)$$

and the function β in Eq. (3.66) is

$$\beta = (1 + \chi)\psi \quad (3.76)$$

Using the function α and β , the LTF-S modeled production rate of species in Eq. (3.51) and the transport properties in Eqs. (3.58) (3.53), and (3.52) are obtained as follows:

$$\dot{\omega}_{i,\text{LTF-S}} = \frac{1 + \psi}{1 + \chi} \dot{\omega}_i \quad (3.77)$$

$$D_{i,\text{LTF-S}} = (1 + \chi)(1 + \psi) D_i \quad (3.78)$$

$$\kappa_{\text{LTF-S}} = (1 + \chi)(1 + \psi) \kappa \quad (3.79)$$

$$\mu_{\text{LTF-S}} = (1 + \chi)(1 + \psi) \mu \quad (3.80)$$

The term $(1 + \psi)$ retrieves the deviation of stretched flame speed caused by flame thickening. Here, it is interesting to note that the term $(1 + \psi)$ may correspond to the efficiency function adapted in some TF-based models [46–49], which accounts for flame wrinkling effects on turbulent flame speeds under flame thickening. Further, note that the flame is thickened with the factor $(1 + \chi)$, as in TF-based models, owing to the constraint introduced in Eq. (3.65). Therefore, this derivation establishes a general approach to flame modeling based on flame thickening. Hereafter, the proposed model in Eqs. (3.77) to (3.80) may be referred to as the LTF-S model: LTF model for stretched flames.

To determine the function ψ in Eq. (3.74), the unstretched flame speed (s_u^0), the correct Markstein length ($\mathcal{L}_u$), and the Markstein length of the LTF model ($\mathcal{L}_{u,\text{LTF}}$) are needed, respectively. The unstretched flame speed s_u^0 can be readily obtained, for example, using Cantera [73]. The target Markstein length $\mathcal{L}_u$ may be obtained from experimental data [74, 75], theoretical expressions [37, 72, 76, 77], and even numerical simulations [78–80]. Note that, since the Markstein length can vary across experiments, theories, and simulations, the choice of the target Markstein length depends on the user’s discretion. If reliable experimental, theoretical, and numerical values (such as DNS) are not accessible, we may suggest using open-source 1-D solvers, such as Ember [81], for cost-effective computations to obtain Markstein lengths. Although the results are not shown here, we confirmed a good agreement between the Markstein lengths obtained from our in-house DNS and those from Ember in an H₂/air cylindrical flame problem. Furthermore, regarding the dimensionality, Giannakopoulos [80] demonstrated that the Markstein length is independent of flame geometries, suggesting that the Markstein lengths for both 3-D spherical and 2-D cylindrical flames are identical. Therefore, the target Markstein length obtained from 2-D simulations is applicable to 3-D simulations.

On the other hand, the Markstein length of LTF is only obtained from simulations using the LTF model. Thus, the following section will discuss a strategy for constructing the function ψ .

3.3.3 Markstein Length Ratio

The Markstein length obtained using the LTF model ($\mathcal{L}_{u,\text{LTF}}$) is influenced by numerical factors, such as grid size or user-defined parameter C_χ . For instance, altering the grid size influences the Markstein length predicted by the LTF model (refer to Fig. 3.3). Therefore, $\mathcal{L}_{u,\text{LTF}}$ must be adjusted based on the specific grid sizes used for each simulation, and consequently, the formulation in Eq. (3.74) may not be practical. Hence, here we rewrite Eq. (3.74) as follows:

$$\psi = \frac{\left(\frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_u} - 1\right) K}{s_u^0 - \mathcal{L}_u \frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_u} K} \quad (3.81)$$

where the ratio of $\mathcal{L}_{u,\text{LTF}}$ to $\mathcal{L}_u$ is named the Markstein length ratio. Theoretical studies [37, 72, 82] indicate that the Markstein length is linearly proportional to the flame thickness:

$$\mathcal{L} = \delta_L f(Le, Ze, \theta) \quad (3.82)$$

where f is an arbitrary function, Ze is the Zel’dovich number and θ is the expansion factor defined as $\theta = \rho_b/\rho_u$. For instance, Law [82] derived the form of the function f using a

counter-flow premixed flame as follows:

$$f = \frac{Ze}{2} \left(1 - \frac{1}{Le} \right) \quad (3.83)$$

Considering the influence of flame thickening ($\mathcal{L}_{u,\text{LTF}} = \delta_{\text{LTF}} f(Le, Ze_{\text{LTF}}, \theta)$; note that Le and θ are not affected by flame thickening in the proposed model), the Markstein length ratio may be generally expressed as follows:

$$\frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_u} = A \frac{\delta_{\text{LTF}}}{\delta_L} + B \quad (3.84)$$

where A and B are expected to be arbitrary constants, and $\delta_{\text{LTF}}/\delta_L$ may be denoted as the flame thickness ratio. As the thickening factor approaches unity, the Markstein length ratio approaches unity as well. Therefore, we have $B = 1 - A$ and then Eq. (3.84) yields

$$\frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_u} = A \frac{\delta_{\text{LTF}}}{\delta_L} + (1 - A) \quad (3.85)$$

Fig. 3.4 illustrates the relationship between the Markstein length and flame thickness ratios in a cylindrical H₂/air flame propagation problem described in Section 2.4. The correct Markstein length and flame thickness were obtained from the DNS solutions: $\mathcal{L}_u = \mathcal{L}_{u,\text{DNS}}$ and $\delta_L = \delta_{\text{DNS}}$, respectively. The simulations using the LTF model are performed across a wide range of conditions and parameters, including the equivalence ratios of 0.5 to 2.0, grid sizes of 160 μm to 320 μm , and user-defined parameters C_χ of 300 to 800. The thermal thickness is used to estimate the flame thickness ratio. The result in Fig. 3.4 shows that the Markstein length and flame thickness ratios have a linear relationship for a wide range of conditions and parameters, and a linear fitting gives a proportional constant of $A = 0.579$. Therefore, the Markstein length ratio can be obtained as follows:

$$\frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_{u,\text{DNS}}} = 0.579 \frac{\delta_{\text{LTF}}}{\delta_{\text{DNS}}} + 0.421 \quad (3.86)$$

Further, as the flame thickness ratio may correspond to the thickening factor $\delta_{\text{LTF}}/\delta_{\text{DNS}} \approx (1 + \chi)$ in the LTF model [36], the Markstein length ratio can be approximately determined in simulations as follows:

$$\frac{\mathcal{L}_{u,\text{LTF}}}{\mathcal{L}_{u,\text{DNS}}} = 0.579(1 + \chi) + 0.421 \quad (3.87)$$

Having Eq. (3.87), the function ψ in Eq. (3.81) and the LTF-S modeled quantities can be determined. In simulations, the Markstein length ratio is considered a spatial variable. Note that when $\chi = 0$, i.e., the flame is fully resolved on an employed grid, the LTF-S model is automatically deactivated with $\mathcal{L}_{u,\text{LTF}}/\mathcal{L}_{u,\text{DNS}} = 1$ and thus $\psi = 0$. Then, the original DNS equations are recovered.

Figure 3.5 presents the relationship between the Markstein length ratio and thickening factor obtained using the TF models [31–33], in which spatially constant thickening factors (χ is constant) are applied. The result indicates an almost linear relationship with $A \approx 1$ and thus

$$\frac{\mathcal{L}_{u,\text{TF}}}{\mathcal{L}_{u,\text{DNS}}} \approx \frac{\delta_{\text{TF}}}{\delta_{\text{DNS}}} \approx 1 + \chi \quad (3.88)$$

Here, it is important to note that Eq. (3.88) indicates that the value of the function f in Eq. (3.82) is not significantly affected by flame thickening. This implies that $Ze \approx Ze_{LTF}$ in Eq. (3.82), or it may suggest that Ze number is not relevant to the Markstein length. Consequently, the proportional constant A is determined by the localization of flame thickening introduced in the LTF model. Thus, if other dynamic thickening approaches were applied, the proportional constant in Eq. (3.85) would change depending on how the thickening factor is introduced in flame regions [46]. However, determining the proportional constant A is not particularly time-consuming, as pre-computations using TF-based models (which do not include stretching effects) can be performed at low computational cost with significantly fewer grid points. Given the arbitrariness of A , we conducted a sensitivity analysis of A on the prediction of stretched flame speed, which is presented in Section 5.1. The determination of the Markstein length ratio is a key feature specific to the proposed model. It should be noted that existing TF-based models for stretched flames [48, 49] also incorporate similar elements to account for the effect of flame thickening on stretch. For example, the S-TF model [48] introduces an optimization function, denoted as X_0 , while the model developed by Poncet et al. [49] employs a correction parameter, γ . Both X_0 and γ may play a role similar to that of the Markstein length ratio in predicting stretched flame propagation.

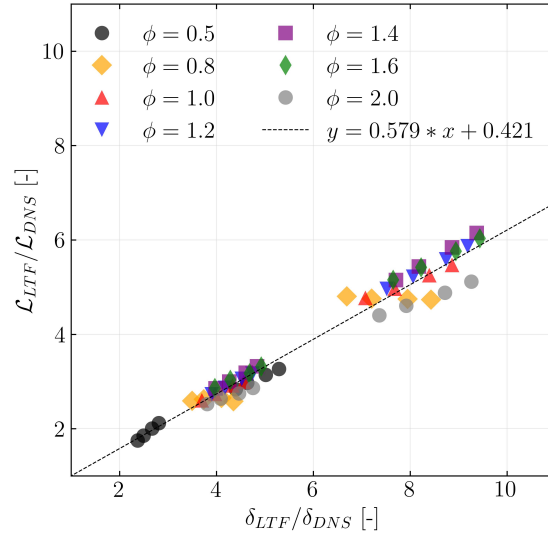


Figure 3.4: Relationship between Markstein length and flame thickness ratios in a cylindrical flame propagation problem. ($R^2 = 0.97$)

3.3.4 Evaluation of the Local Stretch Rate

In the simulations using the LTF-S model, the stretch rate needs to be obtained on an employed grid. The stretch rate [18, 26, 83] can be generally evaluated using

$$K = \nabla \cdot \mathbf{u} - \mathbf{n} \cdot (\mathbf{n} \cdot \nabla) \mathbf{u} + s_d (\nabla \cdot \mathbf{n}) \quad (3.89)$$

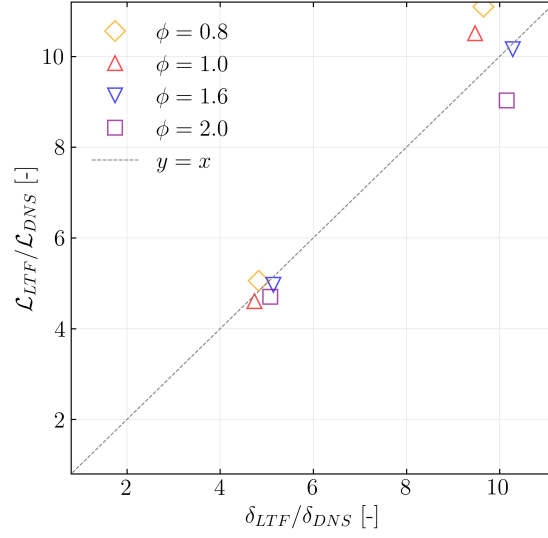


Figure 3.5: Relationship between Markstein length and flame thickness ratios in a cylindrical flame propagation problem. The results are obtained using a TF model [31–33] where constant thickening factors are used.

where $\mathbf{n}$ is the unit vector normal to the flame front pointing towards the unburned gas and $\mathbf{u}$ is the velocity vector of the flow. The displacement speed s_d is defined by

$$s_d = (\mathbf{V}_f - \mathbf{u}) \cdot \mathbf{n} \quad (3.90)$$

where $\mathbf{V}_f$ is the velocity vector of the flame.

The flame front can be represented as an iso-contour of the temperature distributions, and the propagation of the flame front is described by a level-set equation:

$$\frac{\partial \phi}{\partial t} + \mathbf{V}_f \cdot \nabla \phi = 0 \quad (3.91)$$

where the variable ϕ is defined as a non-dimensional temperature,

$$\phi = \frac{T - T_u}{T_{ad} - T_u} \quad (3.92)$$

and T_u is the temperature of the unburned gas. The local gradient of ϕ defines the normal vector

$$\mathbf{n} = -\frac{\nabla \phi}{|\nabla \phi|} \quad (3.93)$$

and substituting for $\nabla \phi$ into Eq. (3.91) gives the speed of the flame front

$$\mathbf{V}_f \cdot \mathbf{n} = \frac{1}{\nabla \phi} \frac{\partial \phi}{\partial t} \quad (3.94)$$

which is used in Eq. (3.90). The time derivative is evaluated using the first-order Euler time integration method.

3.3.5 Extinction Stretch Rate

In simulations, the stretch rate calculated using Eq. (3.89) may exhibit numerical wiggles due to its discretization on coarse grids. To mitigate potential instabilities caused by numerical wiggles, we introduce an extinction stretch rate (ESR). The justification for using ESR may lie in the fact that the proposed LTF-S model relies on the linear relationship between flame speed and stretch rate in Eq. (3.49), which does not hold under strong stretching conditions near extinction. A nonlinear relation between flame speed and stretch rate [84–86] is given as

$$\left(\frac{s_u}{s_u^0}\right)^2 \ln \left(\frac{s_u}{s_u^0}\right)^2 = -\frac{2\mathcal{L}_u K}{s_u^0} \quad (3.95)$$

Thus, the stretch rate is expressed as

$$K = -\frac{s_u^0}{2\mathcal{L}_u} \left(\frac{s_u}{s_u^0}\right)^2 \ln \left(\frac{s_u}{s_u^0}\right)^2. \quad (3.96)$$

Given the laminar flame speed and Markstein length, the maximum stretch rate is determined, as illustrated in Fig. 3.6. The maximum stretch rate corresponds to the extinction stretch rate (ESR), denoted as K_{ext} .

In simulations, we impose a limit on the stretch rate as

$$K < K_{ext}. \quad (3.97)$$

A analytical solution of K_{ext} can be acquired by derivative of Eq. (3.96), $\frac{dK}{ds_u} = 0$.

$$\begin{cases} \frac{s_u}{s_u^0} = 0, & K = 0 \text{ (omitted)}, \\ \left(\frac{s_u}{s_u^0}\right)^2 = e^{-1}, & K = \frac{s_u^0}{2e\mathcal{L}_u} = K_{ext}. \end{cases} \quad (3.98)$$

From this equation, because the laminar flame speed s_u^0 is positive, the sign of K_{ext} is determined by the Markstein length $\mathcal{L}_u$. (If $\mathcal{L}_u$ is negative, the flame will be extinguished under negative stretch, and the opposite holds for positive $\mathcal{L}_u$.) Another possible limiting criterion can be defined using the Karlovitz number, $Ka = \delta^0 K / s_u^0$. When $Ka = 1$, the characteristic time scale of the flow becomes comparable to the chemical time scale, leading to flame extinction. For a negative Markstein length, the limiter can be specified as $K_{ext} < K < s_u^0 / \delta^0$. For a positive Markstein length, it can be defined as $-s_u^0 / \delta^0 < K < K_{ext}$, or more simply as $K < K_{ext}$, since negative strain is conditionally stable and the effect of negative curvature (an unburnt pocket surrounded by burnt gases) will consume the remaining reactants. Furthermore, the stretch rate is only introduced to a flame region to avoid numerical instabilities. The flame region is found by

$$|\nabla\phi| > \frac{0.01}{\min(\Delta x, \Delta y, \Delta z)} \quad (3.99)$$

where the coefficient 0.01 is determined from numerical experiments using a coefficient range from 0.005 to 0.04. The results using 0.01, 0.02, and 0.04 show almost similar prediction accuracy for the flame speed in a cylindrically propagating flame. The stretch rate is finally

filtered by a Gaussian filter with a standard deviation of 3.0 to remove high-frequency fluctuations in the distribution of the stretch rate. We note that Eq. (3.99) and the Gaussian filter are introduced for numerical stability rather than for physical modeling. These techniques are applied solely for calculating the stretch rate and can also be used in the calculation of stretch rates in other TF-based models.

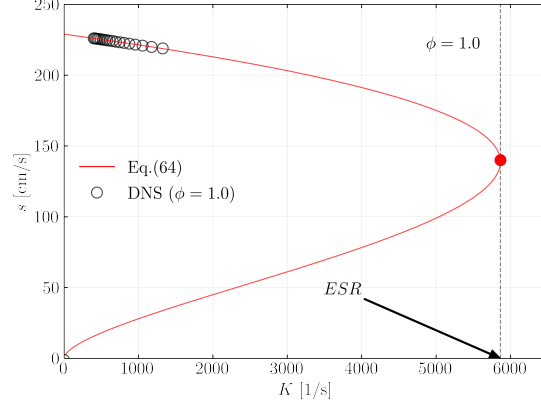


Figure 3.6: Determination of extinction stretch rate.

3.3.6 Comments on Non-dimensional Parameters

TF-based models for stretched flame have been proposed in some previous studies [46–49]. The most recent models are based on modifications to the Lewis number. These modifications are attributed to the theoretical relationship $\mathcal{L}_u \propto \delta_L(Le - 1)$ [26, 72], and the constraint that the Markstein length is preserved under flame thickening. The TF models [31–33] maintain the original Reynolds (if the flame thickness is used as a spatial scale), Prandtl, Schmidt, and thus Lewis numbers under flame thickening. On the other hand, for example, the S-TF model [48] modifies the primary non-dimensional numbers, such as the Reynolds, Prandtl, and Schmidt numbers, due to the modification of the Lewis number. The proposed LTF-S model maintains the concept of the original TF model: as in Eqs. (3.78) to (3.80), the Prandtl, Schmidt, and thus Lewis numbers are preserved while the Reynolds number is only modified with the factor $1 + \psi$. The preservation may be a superior feature of the LTF-S model, compared to the existing TF-based models for stretched flames. Note that a very recent study [87] extends TF-based modeling with the Lewis number correction to address issues related to thermo-diffusive instability.

3.4 Validation with a Cylindrically Propagating Flame

3.4.1 Numerical Configuration

The first validation case of the LTF-S model is a two-dimensional (2-D) cylindrically propagating premixed H₂/air flame. The computational conditions are described in Section 2.4.

ϕ [-]	s^0 [cm/s]	$\mathcal{L}_{DNS}$ [cm]	δ^0 [cm]	T_{ad} [K]	ESR [1/s]	C_χ [-]
0.5	53.823	-0.02565	0.0459	1646.7	5100 (Liang, 2023)	400
0.8	168.514	0.00334	0.0365	2184.8	5630.976	
1.0	228.504	0.00702	0.0371	2385.7	4781.870	
1.2	269.770	0.00773	0.0358	2367.0	5746.567	
1.4	293.013	0.00828	0.0346	2286.6	5666.091	
1.6	302.016	0.00956	0.0342	2206.6	5048.050	
2.0	293.321	0.01239	0.0347	2060.5	3827.247	

Table 3.1: The laminar flame speeds s^0 and Markstein Lengths $\mathcal{L}_{DNS}$ used in the simulations of the LTF-S model.

Here, five different equivalence ratio conditions ($\phi=0.5, 0.8, 1.0, 1.4, 2.0$) are simulated for validation, covering both $Le < 1$ and $Le > 1$ conditions. Note that Comer et al. [88] indicated that the response of TF-based models to extinction caused by stretching effects varies depending on whether $Le < 1$ or $Le > 1$. The effective Lewis numbers [77] for each condition are listed in Table 3.1. We compare the results from the DNS, LTF, and LTF-S models. It is worth mentioning that the DNS solutions are obtained using a grid size $\Delta x = \Delta y = 0.002$ cm for the region of $|x| \leq 6$ cm and $|y| \leq 6$ cm, while the LTF and LTF-S use a larger grid size $\Delta x = \Delta y = 0.016$ cm. To determine the factor ψ in the LTF-S model, the unstretched flame speed (s_u^0), the correct Markstein length ($\mathcal{L}_u$), and the Markstein length ratio ($\frac{\mathcal{L}_{u,LTF}}{\mathcal{L}_u}$) are needed. The unstretched flame speed and correct Markstein length are preliminarily determined using DNS, and the values are listed in Table 3.1. Table 3.1 also shows the parameters used in the LTF and LTF-S models. On the other hand, the Markstein length ratio is determined using χ in simulations, as described in Eq. (3.87), which is consistently applied across all cases.

3.4.2 Grid Convergence

To establish reference DNS data for validating the LTF-S model, the flame resolution for a stoichiometric H_2 /air mixture is assessed by comparing simulations performed on four grid spacings ($\Delta x = 20, 40, 80, 160 \mu m$). (Grid convergence was verified only for this premixed gas condition, because the flame thickness is smallest near the stoichiometric state.)

The corresponding results are presented in Fig. 3.7. The temporal evolution of the flame location (along the x -axes in Fig. 3.2) is shown in Fig. 3.8. For the coarser grids, $\Delta x = 0.008$ and 0.016 cm, non-physical instabilities develop on the circular flame front, causing artificially rapid propagation in Fig. 3.8. In contrast, for the finer grids, $\Delta x = 0.002$ and 0.004 cm, the flame front remains smooth and the corresponding flame position histories coincide. It is noted that instabilities also appear for $\Delta x = 0.002$ cm at later times. The fact that these instabilities arise earlier for $\Delta x = 0.004$ cm indicates that $\Delta x = 0.002$ cm provides sufficient flame resolution and is therefore suitable for use as the reference solution in the model validation. (A finer grid with $\Delta x = 0.001$ cm was not pursued due to its prohibitive computational cost. However, in the next chapter (4.1.4) we have verified the flame resolution is converged at $\Delta x = 0.002$ cm through the flame-vortex interaction.)

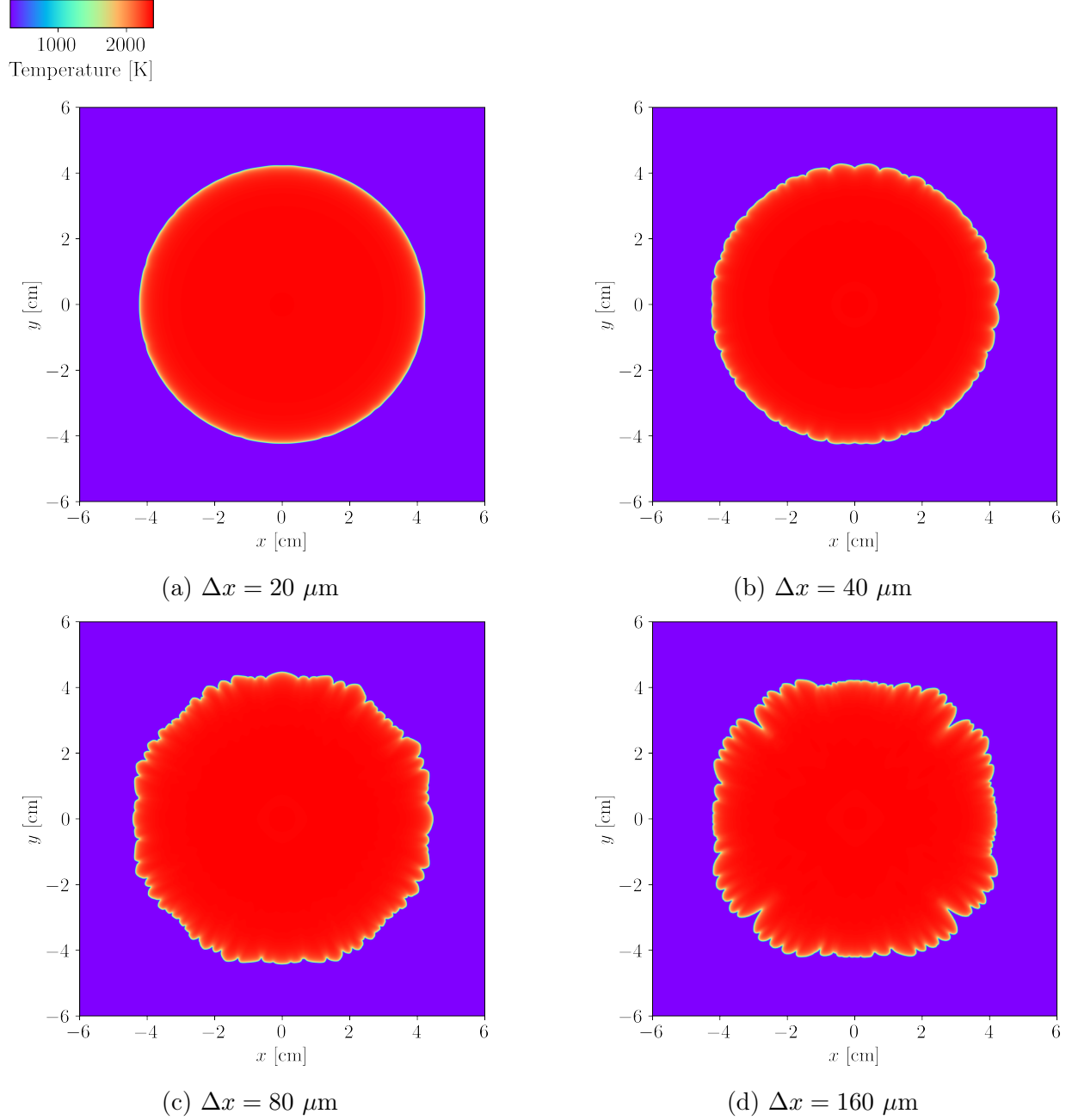


Figure 3.7: Flame resolution confirmation of the cylindrical outwardly propagating flame.

3.4.3 Validation of the LTF-S Model

Figure 3.9 shows the stretched flame speed against the stretch rate and flame location for the stoichiometric condition ($\phi = 1.0$) obtained with the DNS, LTF, and LTF-S models. The DNS, LTF, and LTF-S results all show that the flame speed and stretch rate have a linear relationship when $K < 1400 \text{ s}^{-1}$, i.e, the flame steadily propagates, and the flame speed converges to the unstretched flame speed (s_u^0) at $K = 0$. Note that the initial transient phase, where nonlinear behaviors appear, have been removed from the results and discussions, as

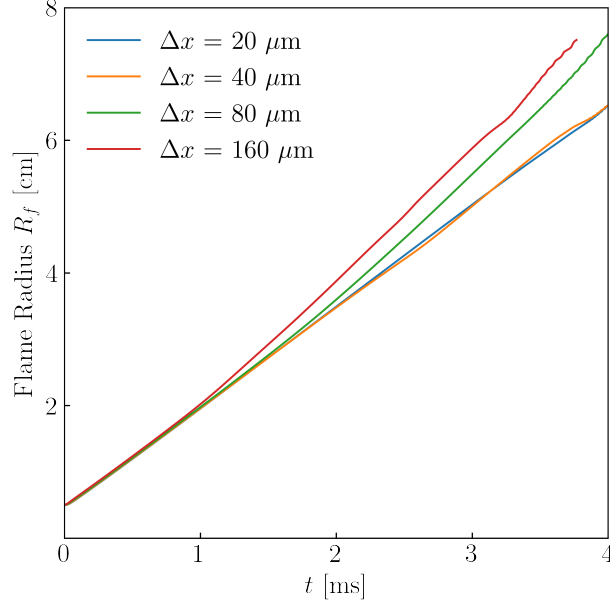


Figure 3.8: Evolution of the flame location (along the x -axes in Fig.3.2) for different grid sizes.

the LTF model relies on the linear relationship between the stretched flame speed and strain rate. The duration of the initial transient is typically within 0.5 ms, except for 2.0 ms in the $\phi = 0.5$ case. Since the flame thickening increases the Markstein length as discussed in Section 2.4, the LTF model overestimates the stretching effect on the flame speed, providing lower flame speeds than the DNS solutions. In contrast, the LTF-S model successfully retrieves the stretched flame speed with an almost identical Markstein length to the DNS solutions. Figure 3.10 displays the sequential distributions of the temperature, $1 + \chi$, and $1 + \psi$. It is observed that the thickening factor $1 + \chi$ is localized in the flame region. The maximum value of $1 + \chi$ remains almost constant, while the maximum value of $1 + \psi$ decreases as the stretch rate decreases. While the values of $1 + \psi$ are two orders of magnitude smaller than those of $1 + \chi$, the results suggest that these small values play a crucial role in accurately capturing the stretching effects on the flame speed.

Figure 3.11 compares the results of the LTF-S model obtained using three grid sizes. The LTF-S model demonstrates nearly identical behavior across three different grid sizes. Even with the coarsest grid size of 0.032 cm, the result with the LTF-S model agrees well with the DNS solution using 0.002 cm. In contrast, as already shown in Fig. 3.3, the prediction capability of the LTF model [36] for stretched flames is significantly influenced by grid resolution.

Figure 3.12 shows the comparison results for the other equivalence ratio conditions. Note that only for $\phi = 0.5$, the flame speed shows a positive response to the stretch rate, accompanied by a negative Markstein length. The flame speeds with the LTF-S model agree well with those predicted by the DNS for all equivalence ratio conditions, demonstrating the applicability of the LTF-S model and confirming the validity of the derived Markstein length ratio in Eq. (3.87) across a wide range of conditions.

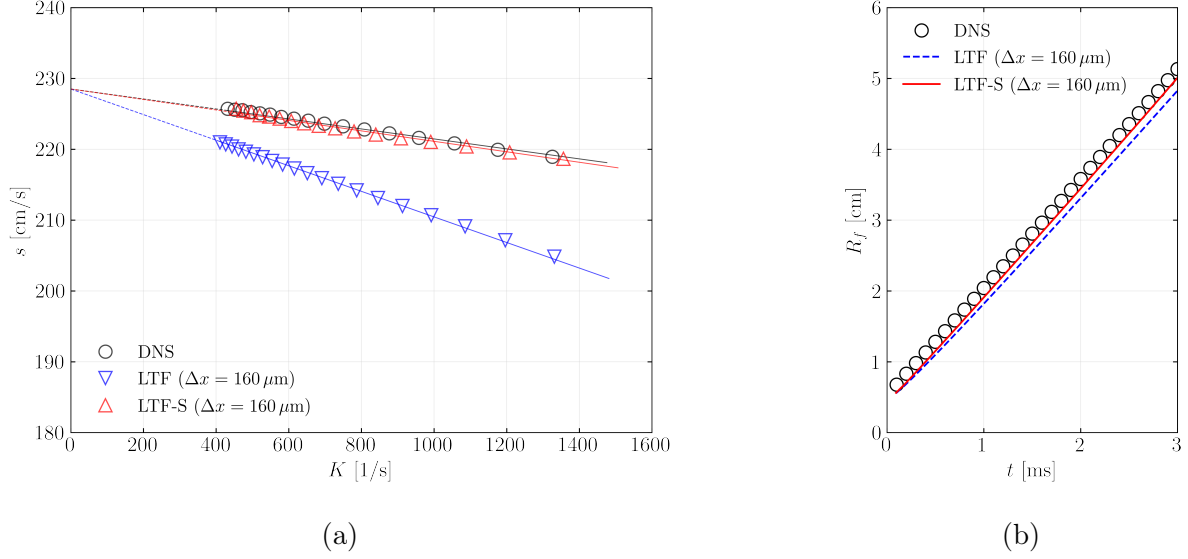


Figure 3.9: Comparisons of flame speed s and flame location R_f obtained with DNS, LTF, and LTF-S models in a cylindrical flame propagation problem. In the left figure, the lines drawn using a linear least-squares fit represents the relationship between flame speed and stretch rate.

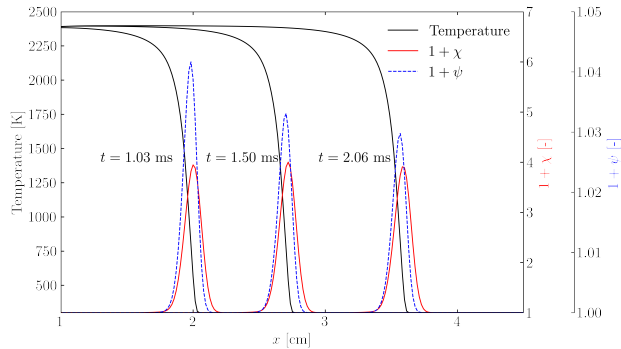
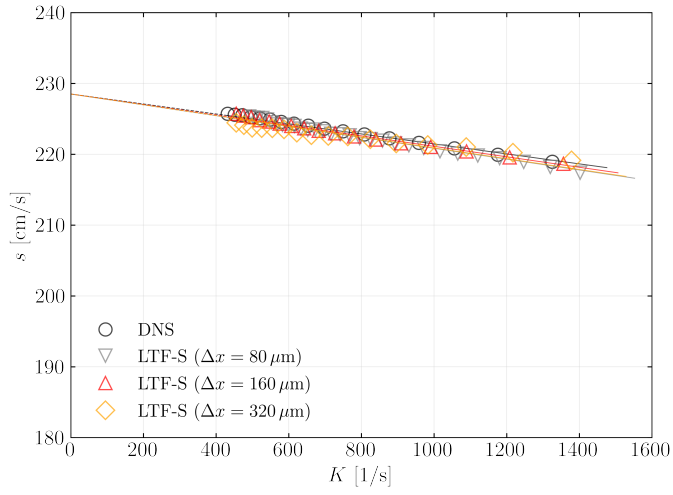
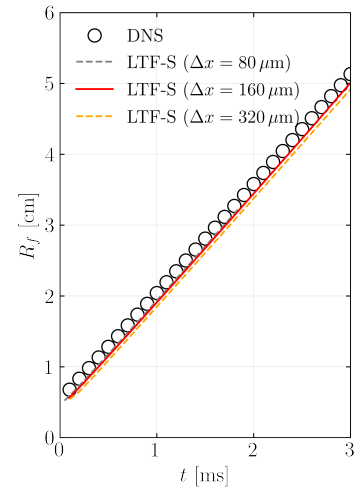


Figure 3.10: Sequential distributions of temperature, $1 + \chi$, and $1 + \psi$ along $y = 0$ in Fig. 3.2

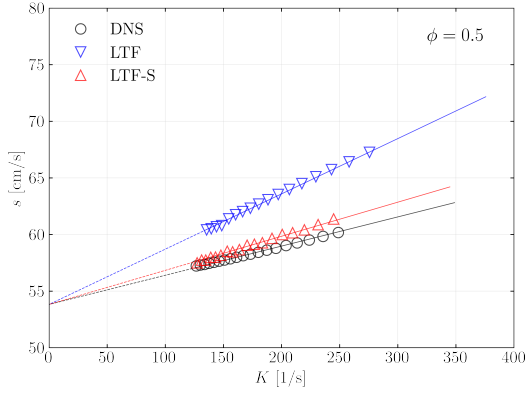


(a)

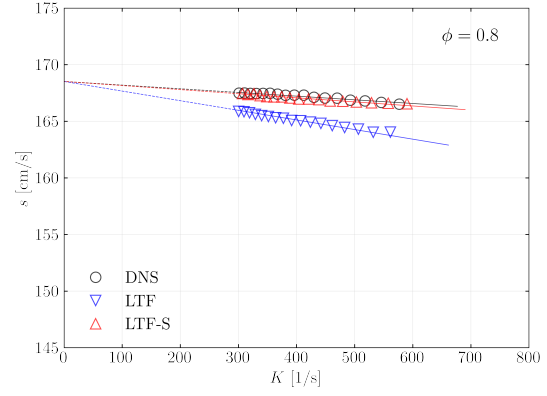


(b)

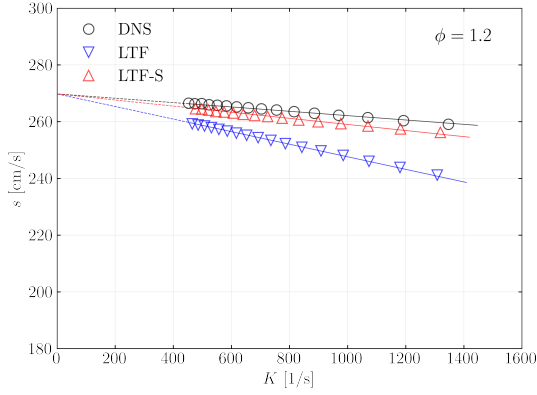
Figure 3.11: Effects of grid sizes on stretched flame speed s and flame location R_f in the LTF-S model. In the left figure, the lines drawn using a linear least-squares fit represent the relationship between flame speed and stretch rate.



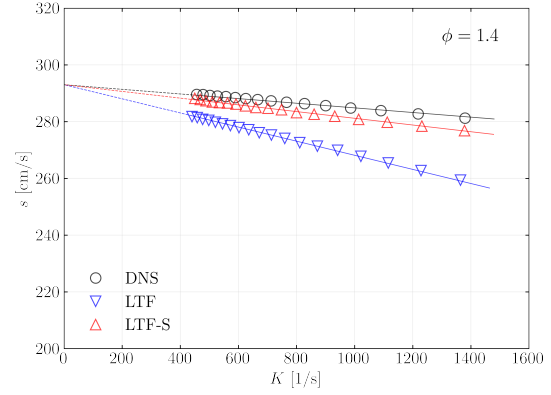
(a) $\phi = 0.5$



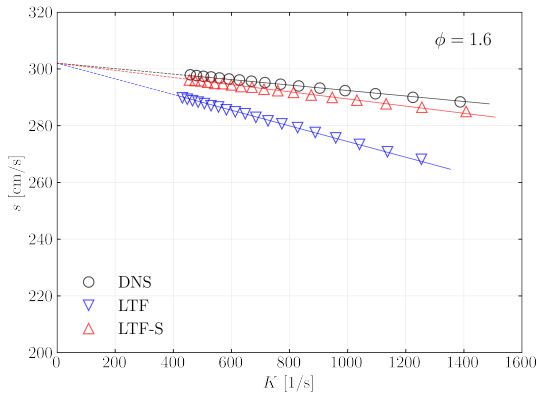
(b) $\phi = 0.8$



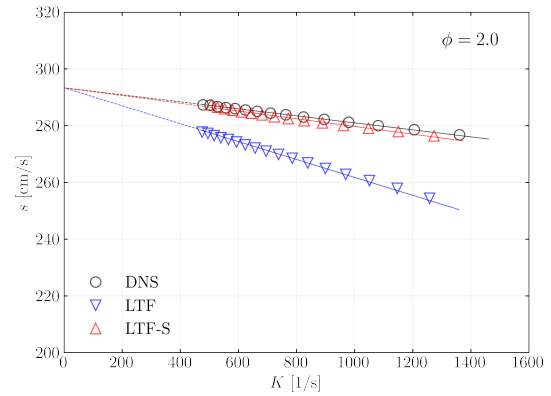
(c) $\phi = 1.2$



(d) $\phi = 1.4$



(e) $\phi = 1.6$



(f) $\phi = 2.0$

Figure 3.12: Comparison of the flame speed s against stretch rate for various equivalence conditions in a cylindrical flame propagation problem. In the figures, the lines drawn using a linear least-squares fit represent the linear relationship between flame speed and stretch rate. Thermo-diffusive (TD) instabilities arise after the linear evolution phase, when $Le < 1$. The TD phase is excluded from the results and discussions in this study.

Chapter 4

Flame-Vortex Interaction

For the second validation case, a canonical flame–vortex interaction configuration [33] is examined. This configuration incorporates both strain and curvature effects on the flame dynamics (i.e., the stretch components), thereby providing a more comprehensive assessment of the LTF-S model. A schematic representation of the flame–vortex interaction problem is presented in Fig. 4.1.

4.1 Numerical Configuration of the Flame-Vortex Interaction

4.1.1 Initial Steady Flame Condition

A stoichiometric H_2/air premixed mixture at 300 K and 1 atm was considered.

A non-stretched, one-dimensional planar flame was initialized at $x = 0$ cm, with the premixed stoichiometric H_2/air at $T = 300$ K entering the domain at the laminar burning velocity s_u^0 determined by Cantera (see Table 3.1). Dirichlet boundary conditions were imposed on the temperature field and on the mass fractions of all chemical species, while a Neumann boundary condition was prescribed for the pressure. Neumann boundary conditions were also applied at the outlet. The burned and unburned gases were initialized on the left- and right-hand sides of $x = 0$ cm, respectively. The temperature and composition of the burned gas were obtained from Cantera calculations for the stoichiometric H_2/air mixture. An error-function profile was employed to smoothly connect the burned and unburned regions and thereby initialize the flame structure. In this configuration, the isotherm at $T = 1200$ K was used as an indicator of the flame position. Figure 4.2 shows the converged flame positions, which are slightly shifted from $x = 0$ cm. On the DNS grid, the steady flame location converges to $x_{\text{init}} = -0.0474$ cm, while on the grid used for LTF and LTF-S it converges to $x_{\text{init}} = -0.0076$ cm. To ensure identical timing of the flame–vortex interaction, the initial vortex centers are placed $4R_v$ upstream of these misaligned initial flame positions. To remove the misalignment in the simulation results, the flame locations in the DNS, LTF, and LTF-S datasets were aligned a posteriori by shifting the coordinate system ($x_{\text{shifted}} = x - x_{\text{init}}$) based on the position of the $T = 1200$ K isotherm during post-processing.

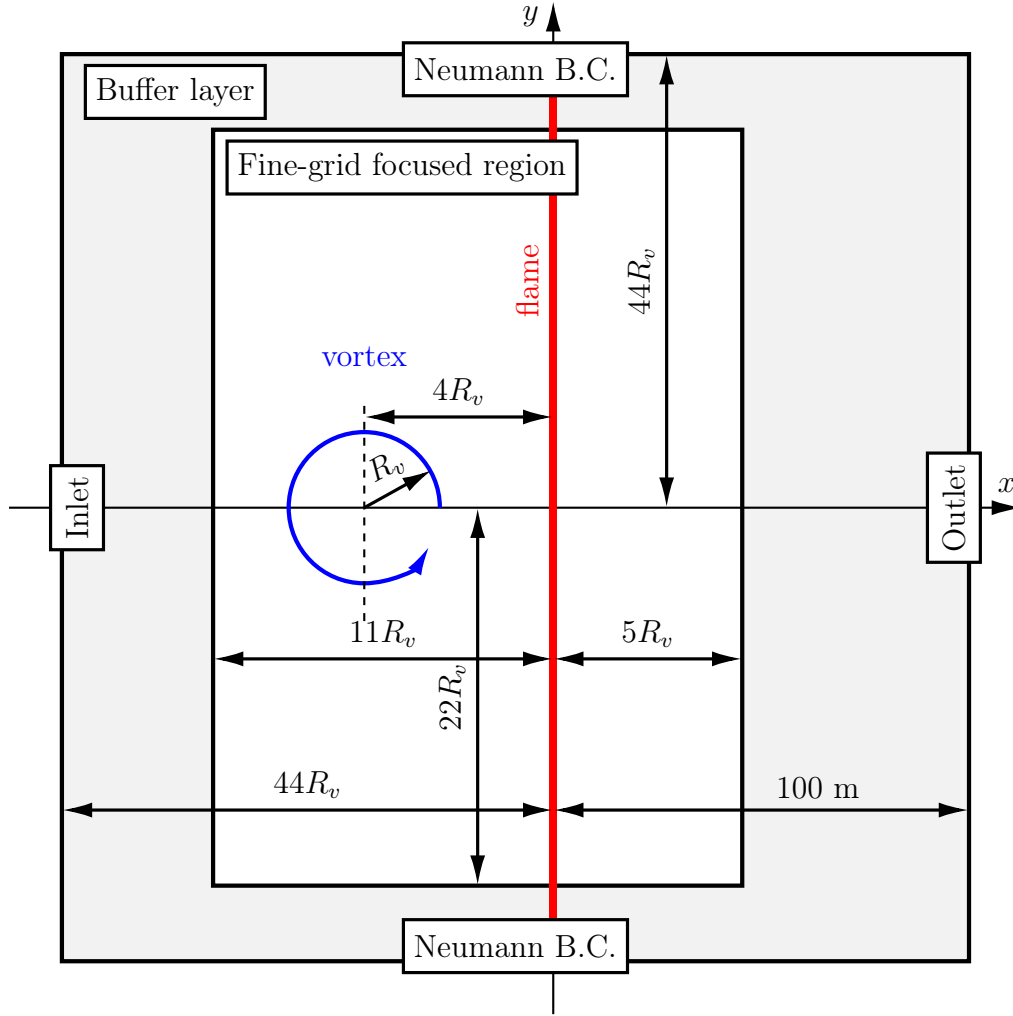


Figure 4.1: Schematic of a flame-vortex interaction.

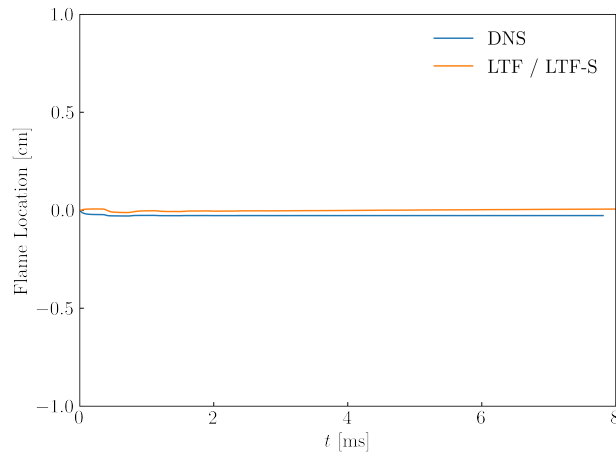


Figure 4.2: The converged steady flame locations for grids of DNS, LTF, and LTF-S.

4.1.2 Introduction of a Single Euler Vortex

After generating the stationary flame, an Euler vortex was imposed upstream to interact with both the flow field and the flame front.

The velocity and pressure fields associated with the imposed vortex are given by

$$u = U_\infty - \frac{C_R (y - y_c)}{R_v^2} \exp\left(-\frac{r^2}{2}\right), \quad (4.1)$$

$$v = \frac{C_R (x - x_c)}{R_v^2} \exp\left(-\frac{r^2}{2}\right), \quad (4.2)$$

$$p = p_\infty - \frac{\rho C_R^2}{2R_v^2} \exp(-r^2), \quad (4.3)$$

$$C_R = u_{cv} R_v \sqrt{e}, \quad (4.4)$$

where u and v denote the velocity components in the x and y directions, respectively, and u_{cv} is the maximum circumferential velocity. The variable p represents the static pressure, and e is Napier's constant. The parameter R_v is the characteristic vortex radius, and r^2 is defined as

$$r^2 = \frac{(x - x_c)^2 + (y - y_c)^2}{R_v^2}. \quad (4.5)$$

Quantities indexed with ∞ correspond to free-stream properties, whereas x_c and y_c specify the coordinates of the vortex center.

In this validation study, an Euler vortex with radius $R_v = 5\delta^0$ is considered, and three values of the maximum circumferential velocity are examined: $u_{cv} = 0.1, 1$, and $10 s_u^0$. Interpreting the vortex diameter and the circumferential velocity as representative of the integral length scale and the characteristic fluctuation (turbulent) velocity, respectively, the corresponding turbulent Reynolds number

$$Re = \frac{2R_v u_{cv}}{s_u^0 \delta^0} \quad (4.6)$$

takes the values 1, 10, and 100 for $u_{cv} = 0.1, 1$, and $10 s_u^0$, respectively. For $u_{cv} = 0.1 s_u^0$, the interaction is expected to produce a mildly wrinkled flame, whereas $u_{cv} = 1 s_u^0$ is anticipated to yield a corrugated flame front. For the highest intensity case, $u_{cv} = 10 s_u^0$, the strong vortex is expected to generate pockets of unburned and/or burned gases associated with highly wrinkled or corrugated flame structures.

In Fig. 4.3, the vortex conditions are positioned on a turbulent combustion regime diagram adapted from Peters (2000) [16]. The vortex integral length scale l_o is taken as $2R_v$. For $u_{cv} = 0.1 s_u^0$, the interaction is expected to cause only a slight deformation of the flame, since $Re_o \leq 1$ and a *laminar* vortex stretching mechanism is anticipated. When $u_{cv} = 1 s_u^0$, the vortex size corresponds to the characteristic scale separating *wrinkled* from *corrugated* flame behavior. This characteristic vortex size is known as the Gibson scale, and the resulting flame distortion is expected to be on the same order as the vortex size. For the highest intensity case, $u_{cv} = 10 s_u^0$, the condition falls within the *reaction sheet* regime. In this turbulent combustion region, the preheat zone of the flame's inner structure can be influenced by small

eddies, which may disturb the preheat zone and enhance both mass and heat transfer. Under such a strong *single* vortex, pockets of unburned and/or burned gases are expected to form, associated with strongly corrugated flame fronts.

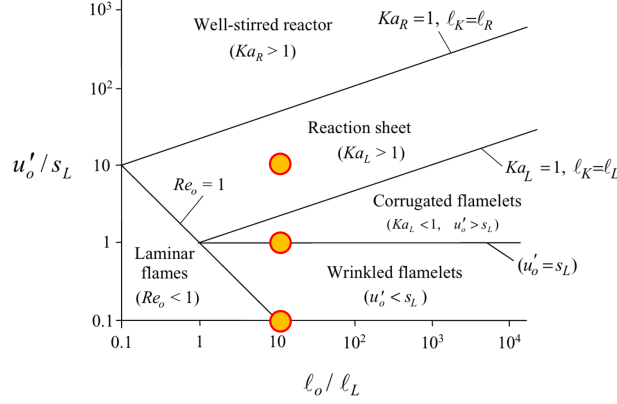


Figure 4.3: Mapping of the vortex conditions onto the turbulent combustion diagram (adapted from [16])

4.1.3 Numerical Configuration

Two computational grids are constructed for the simulations. In the fine-grid region, the spatial resolution for the DNS is set to $\Delta x = \Delta y = 20 \mu\text{m}$, whereas for the LTF [36] and LTF-S models a coarser resolution of $\Delta x = \Delta y = 100 \mu\text{m}$ is employed. The grid spacing for the LTF and LTF-S simulations is chosen as large as possible while still adequately resolving the Euler vortex and preserving the initial velocity and pressure fields.

It is important to note that, in the absence of TF models (i.e. for an under-resolved DNS) with $\Delta x = \Delta y = 100 \mu\text{m}$, nonphysical flame wrinkling and numerical instabilities develop, preventing the establishment of even a nominally stationary flame.

At the inlet boundary, a stoichiometric mixture at 300 K is prescribed with the laminar flame speed, while the pressure is determined by extrapolation. At the outlet, as well as at the upper and lower boundaries, all flow variables are extrapolated. Furthermore, the Markstein length ratio appearing in Eq. (3.81), originally introduced for the cylindrical flame configuration, is employed here without modification.

4.1.4 Grid Convergence

Resolution Confirmation of the Single Vortex

To verify the grid convergence for the three vortex conditions described above, five grid resolutions were employed. These are summarized in Table 4.1, where $R_v/\Delta x$ represents the number of grid points used to resolve the characteristic vortex radius. Figure 4.4 presents the initial vorticity fields for the three vortex cases computed on the finest grid ($\Delta x = 40 \mu\text{m}$).

	Grid 1	Grid 2	Grid 3	Grid 4	Grid 5
R_v [cm]	$R_v = 5\delta^0 = 0.18$				
Δx [cm]	0.032	0.016	0.008	0.004	0.010
$R_v/\Delta x$ [-]	5.625	11.25	22.5	45	18

Table 4.1: Verification of grid convergence for resolving the vortex.

For this two-dimensional vortex, the vorticity is given by

$$\boldsymbol{\omega} = \nabla \times \mathbf{u} = \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right) \mathbf{i}_z, \quad (4.7)$$

where the unit vector $\mathbf{i}_z$ is normal to the x - y plane. As shown in Fig. 4.4, the magnitude of $\boldsymbol{\omega}$ reaches its maximum at the vortex core and decreases to zero at $r = \sqrt{x^2 + y^2} = R_v$. The magnitude of $\boldsymbol{\omega}$ is positive because the vortex rotates counterclockwise. For $r > R_v$, a region with negative vorticity where $\frac{\partial v}{\partial x} < \frac{\partial u}{\partial y}$, which appears like a counter-rotating vortex. This arises because the vortex is embedded in an otherwise quiescent flow field: the reduction of the velocity from the vortex edge toward the ambient flow produces a strain rate, and the standard definition of the vorticity could not distinguish pure rotational motion from this shear-induced contribution.

Figure 4.5 shows the decay of the volume-averaged vorticity magnitude $\bar{\omega}$ as a function of the non-dimensional time $t^* = t s_u^0 / R_v$. The quantity $\bar{\omega}$ is defined as

$$\bar{\omega} = \int_{V_{\text{total}}} |\boldsymbol{\omega}| dV, \quad (4.8)$$

where V_{total} denotes the entire volume of the computational domain.

For grid spacings Δx smaller than $100 \mu\text{m}$, the evolution of $\bar{\omega}$ collapses onto a single curve, reaching 97.5% of the initial vorticity $\bar{\omega}_0$ at $t^* = 4$. The relative discrepancy among these converged grid sizes remains below 0.2%. With a grid size of $\Delta x = 100 \mu\text{m}$, the vortex radius is resolved by 18 grid points, which is consistent with the finding of Hanada (2021) [89], who reported that at least 16 points are required to adequately resolve the vortex radius.

Resolution Confirmation of the Premixed Flame

Since the computational domain for the flame-vortex interaction is much smaller than that used for the cylindrical, outwardly propagating flame, we were able to perform a simulation with a finer grid spacing of $\Delta x = 10 \mu\text{m}$ to verify grid convergence for the flame resolution. Figure 4.6 compares the flame shapes at various non-dimensional times t^* for $\Delta x = 10$ and $20 \mu\text{m}$. The $T = 1200 \text{ K}$ isotherms nearly coincide, further confirming that a grid spacing of $\Delta x = 20 \mu\text{m}$ is sufficient to accurately resolve the flame.

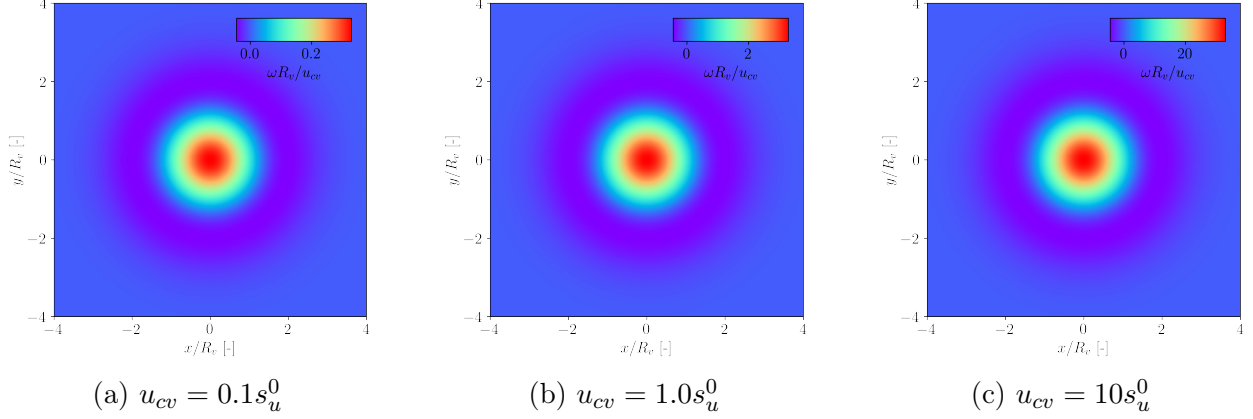


Figure 4.4: Initial vorticity distribution for the vortex conditions of $u_{cv}=0.1$, 1.0 , and $10s_u^0$. ($\Delta x = 40 \mu\text{m}$)

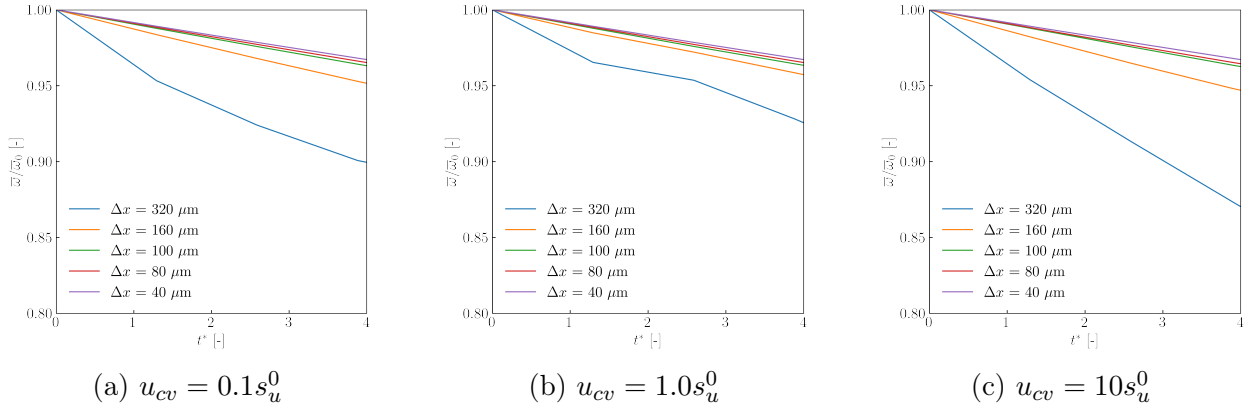


Figure 4.5: Grid resolution confirmation for the vortex conditions of $u_{cv}=0.1$, 1.0 , and $10s_u^0$.

4.2 Result and Discussion

4.2.1 Flame Deformation during Flame-Vortex Interaction

Figures 4.7, 4.8, and 4.9 present the evolution of flame deformation induced by a vortex convected downstream at various non-dimensional times. The non-dimensional time is defined as $t^* = ts_u^0/R_v$, such that $t^* = 1, 2, 3, 4$ correspond to the vortex having been displaced by $1, 2, 3$, and $4R_v$ from its initial position, respectively. As shown in Figs. 4.7–4.9, the outer edge of the vortex reaches the initially planar flame at approximately $t^* = 1.5$.

With increasing circumferential velocity of the vortex, the resulting flame deformation becomes more pronounced and occurs earlier in time, even when the vortical structures arrive at the same spatial location. The vortex with $u_{cv} = 0.1s_u^0$ possesses the lowest kinetic energy and is only capable of inducing small-amplitude perturbations (*wrinkles*) on the flame front. For the intermediate case, $u_{cv} = 1s_u^0$, the vortex entrains high-temperature burned products into the unburned mixture, leading to the formation of a semicircular flame front by $t^* = 4.0$.

In the strongest-vortex case, $u_{cv} = 10s_u^0$, the structure not only entrains a substantial fraction of the burned gases but also folds the distorted flame front such that it merges with

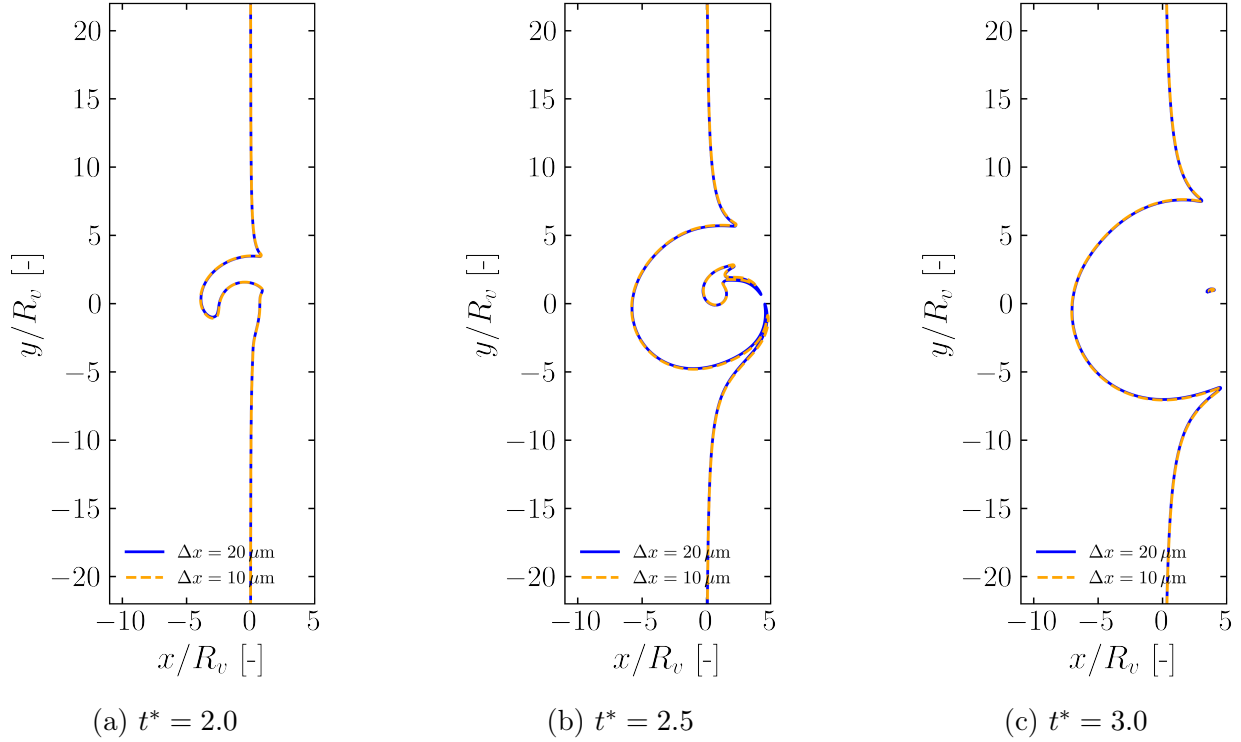


Figure 4.6: Grid resolution confirmation for the premixed stoichiometric H_2/Air . ($u_{cv} = 10s_u^0$).

pre-existing flame surfaces. As a consequence, a portion of the unburned mixture becomes encapsulated within the burned region, a configuration characteristic of the corrugated flamelet regime. After this unburned gas “pocket” is fully consumed, at approximately $t^* = 3.0$, a larger semicircular flame front establishes and subsequently propagates outward in a quasi-steady manner.

Moreover, the vortex-induced circular flame configuration leads to local gas expansion and the formation of diverging streamlines. These diverging streamlines are advected by the oncoming flow toward the flame and impose additional stretching on the flame fronts at the upper and lower boundaries of the domain. The resulting positive curvature reduces the local burning velocity, causing the flame to lag relative to the incoming flow. This behavior is consistent with Fig. 3.3, which demonstrates that positive stretch suppresses the burning velocity of stoichiometric premixed H_2/air flames.

4.2.2 Result of $u_{cv} = 0.1$, and $1s_u^0$

Figures 4.10 and 4.11 present a comparison of the instantaneous flame configurations at each nondimensional time t^* . Both the LTF and LTF-S models reproduce the global flame dynamics induced by the impinging vortex in qualitative agreement with the DNS results. Nonetheless, the LTF model systematically underpredicts the stretched flame speed as a consequence of excessive flame thickening, which in turn yields a delayed propagation of the semicircular flame front.

By contrast, the flame topology obtained with the LTF-S model exhibits excellent agree-

ment with DNS, featuring an almost identical semicircular flame shape and spatial location. In addition, the LTF-S model reliably captures the small-scale flame wrinkling observed in the region immediately below the semicircular flame at $t^* = 4.0$ for $u_{cv} = 0.1$ and $1s_u^0$. These results demonstrate that the LTF-S model can accurately predict flame propagation under combined curvature and strain effects even on a comparatively coarse computational grid.

The temporal evolution of the global fuel consumption rate is presented in Fig. 4.13 and Fig. 4.14 to enable a quantitative comparison among the DNS, LTF, and LTF-S models. The global consumption rate is defined as the volume integral of the fuel reaction rate over the entire domain and is evaluated as

$$\Omega_{\text{fuel}} = -\frac{1}{\rho_u (Y_{\text{fuel},u} - Y_{\text{fuel},b})} \int_{V_{\text{total}}} \dot{\omega}_{\text{fuel}} dV, \quad (4.9)$$

where V_{total} denotes the total volume of the computational domain, and $Y_{\text{fuel},u}$ and $Y_{\text{fuel},b}$ are the mass fractions of fuel (here H_2) in the unburned and burned gases, respectively. The results indicate that the LTF-S model reproduces the DNS behavior with high fidelity. This agreement demonstrates that the LTF-S model quantitatively captures the enhancement of the effective flame area induced by vortex–flame interaction, even at relatively coarse grid resolutions. In contrast, the LTF model exhibits a delayed increase in the global consumption rate and ultimately predicts a lower asymptotic level, which can be attributed to excessive flame thickening that suppresses the flame dynamical response.

4.2.3 Result of $u_{cv} = 10s_u^0$

Figure 4.14 compares the temporal evolution of the flame front obtained from DNS, LTF, and LTF-S for the case $u_{cv} = 10s_u^0$. For this higher circumferential velocity of the incoming vortex, the flame front experiences pronounced swirling, forming a large semicircular structure compared with the lower-velocity case. The swirled flame subsequently folds back and reattaches to the original flame front, thereby entrapping a pocket of unburned gas within the burned-gas region. This unburned-gas pocket vanishes at approximately $t^* = 3.0$, after which the flame propagates while largely preserving its semicircular configuration. The LTF-S model reproduces the DNS flame morphology with high fidelity, including the generation and disappearance of the unburned-gas pocket, whereas the LTF model exhibits a noticeable delay in flame propagation.

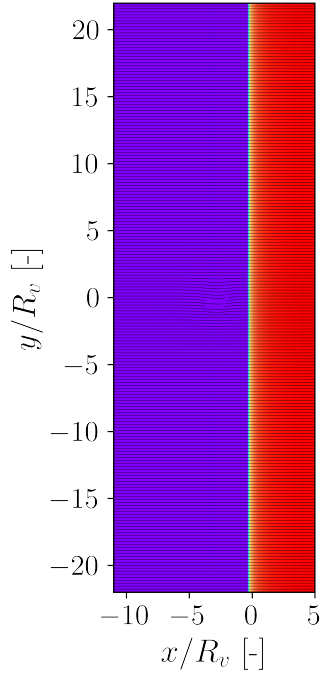
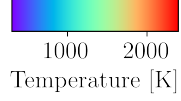
Figure 4.15 presents the time evolution of the global consumption rate. The LTF-S model accurately predicts the DNS solution, including both the timing and magnitude of the initial peak, as well as the smaller secondary peak in the global consumption rate. When the flame fronts merge, the effective flame surface area is reduced, leading to an abrupt decrease in the global consumption rate Ω at $t^* = 2.5$. The maximum value of Ω predicted by the LTF and LTF-S models was lower than the DNS results because the artificially thickened flame fails to represent flame segments with strong curvature, leading to a loss of fine flame surface detail, as reported in [47].

Moreover, for $t^* > 3.0$ (during the quasi-steady propagation phase), the global consumption rate predicted by the LTF-S model remains in close agreement with the DNS result, indicating that the flame geometry is captured with good accuracy. Overall, these results demonstrate

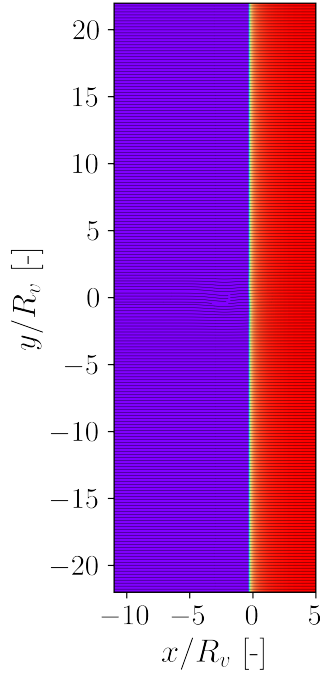
that the LTF-S model reproduces both the quantitative and qualitative features of the flame dynamics observed in DNS, even when using comparatively coarse grid resolutions.

Figure 4.16 demonstrates the snapshots of the total stretch rate along with its two distinct contributions: the curvature-driven and strain-driven stretch rates. The peak stretch rate exceeds $K = 2500 \text{ s}^{-1}$, which is higher than that observed in cylindrical flames (yet still below the extinction stretch rate). This vortex-induced stretch configuration also confirms the prediction accuracy of the LTF-S model under negatively stretched conditions. In the “comma-shaped” pocket of the unburned gas, the curvature is negative, whereas vortex-induced straining dominates and results in a positive overall stretch rate. Equation (3.49) remains valid in this strongly stretched region.

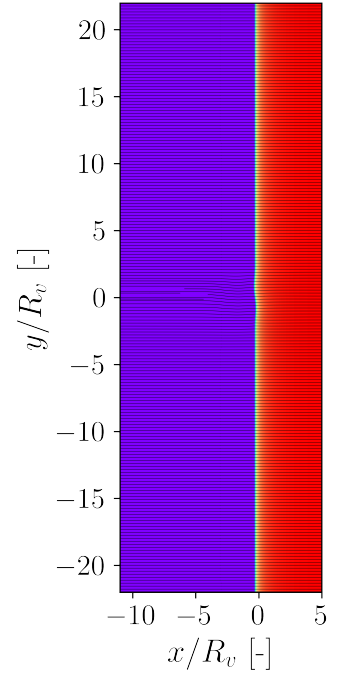
Figure 4.17 presents snapshots of the LTF-S model parameters, χ and ψ . These parameters correctly identify the flame region, with χ controlling flame thickening and ψ adjusting the flame speed. The thickening factor $1 + \chi$ has an average value of about 2.0. However, in the region where the flame fronts merge and the temperature gradient steepens as two approaching flames compress each other. A local value of $1 + \chi$ close to 4.0 is used for this area requiring higher resolution. Since $1 + \chi$ remains greater than 1, the spatial distribution of ψ closely follows that of the total stretch rate shown in Fig. 4.16.



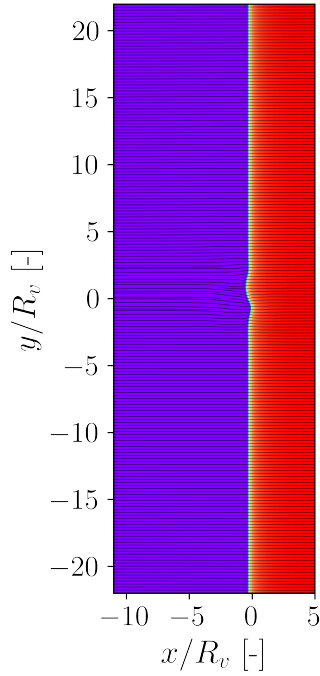
(a) $t^* = 1.5$



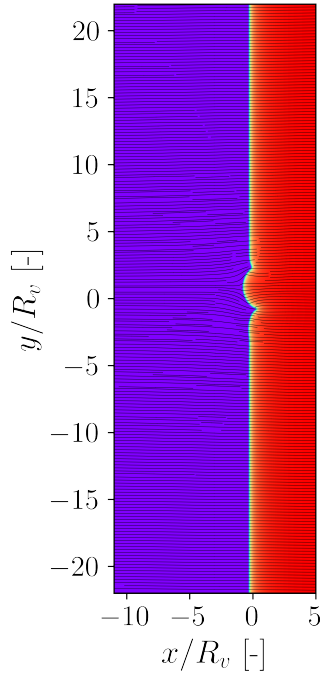
(b) $t^* = 2.0$



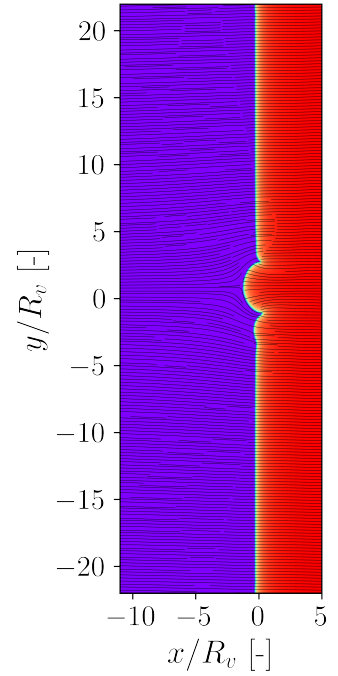
(c) $t^* = 2.5$



(d) $t^* = 3.0$

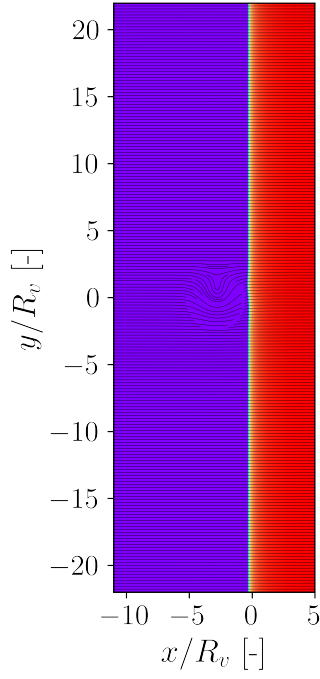
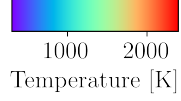


(e) $t^* = 3.5$

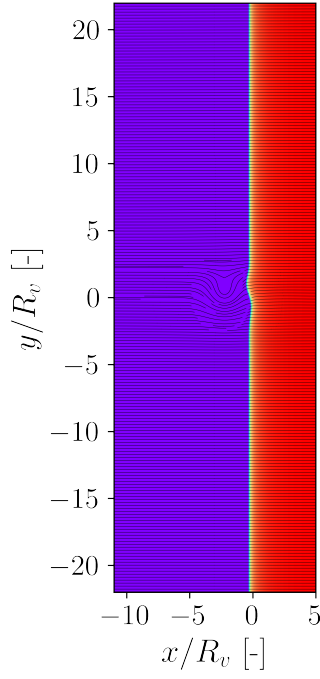


(f) $t^* = 4.0$

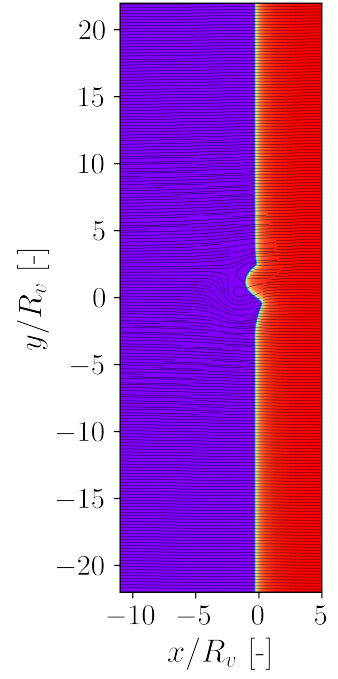
Figure 4.7: Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 0.1s_u^0$. The thin lines represent the streamlines.



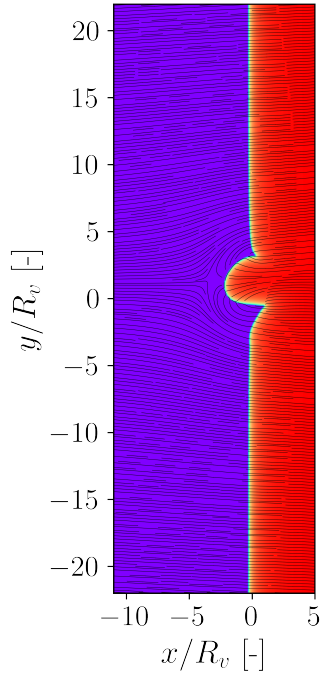
(a) $t^* = 1.5$



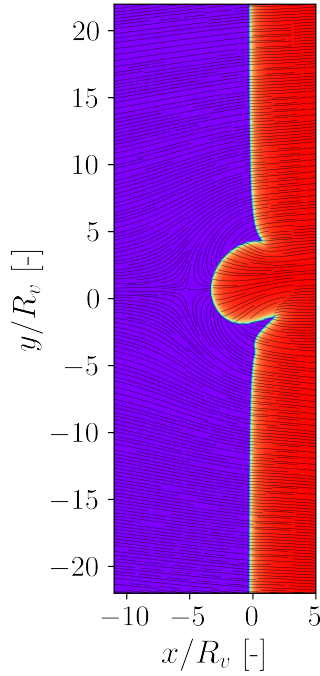
(b) $t^* = 2.0$



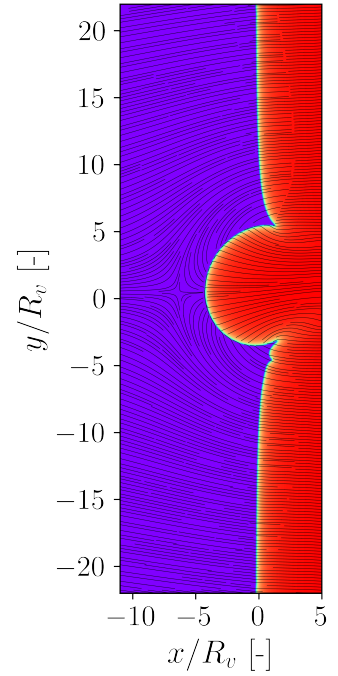
(c) $t^* = 2.5$



(d) $t^* = 3.0$



(e) $t^* = 3.5$



(f) $t^* = 4.0$

Figure 4.8: Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 1s_u^0$. The thin lines represent the streamlines.

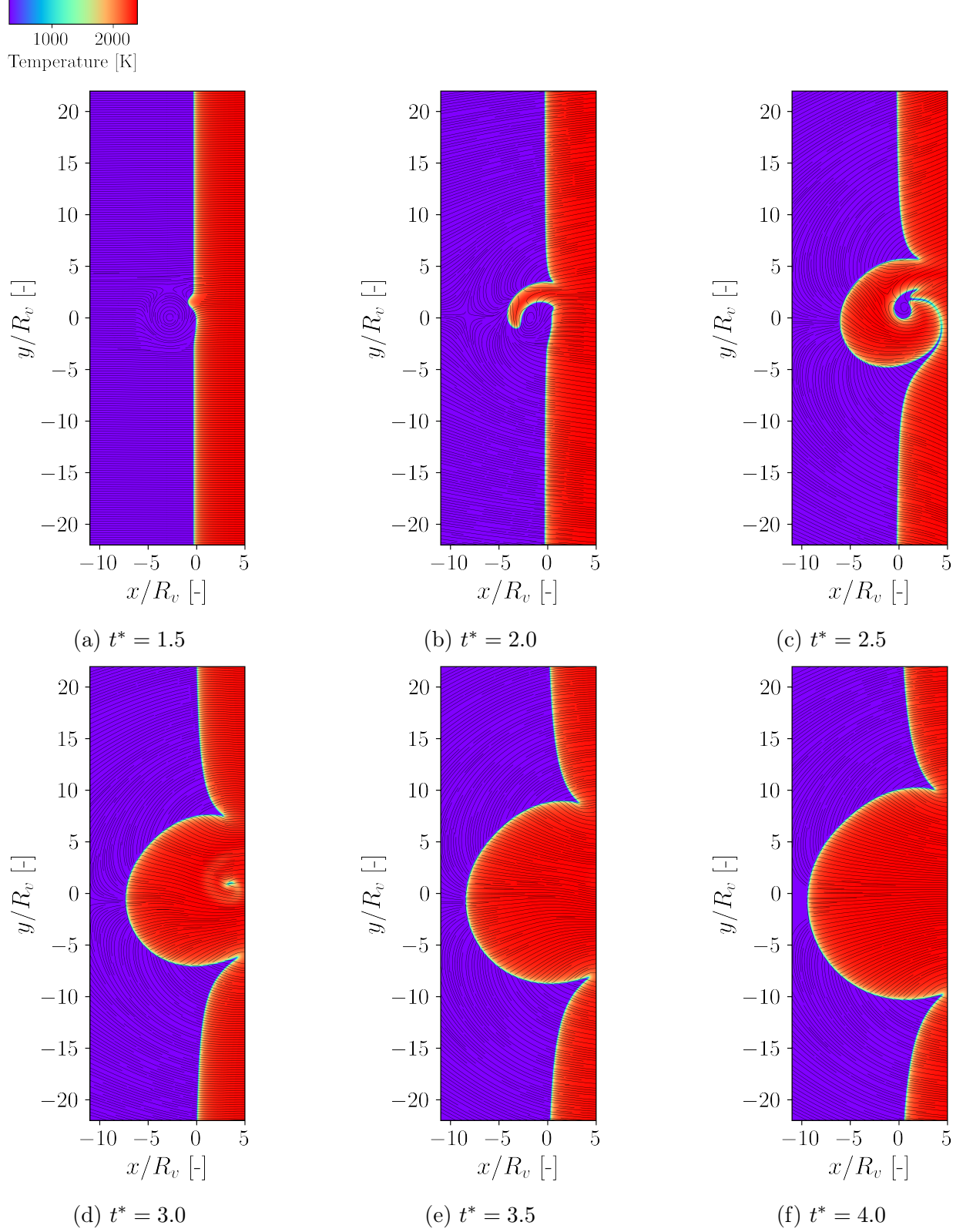


Figure 4.9: Sequential temperature snap shots of DNS during the flame-vortex interaction for the case of $u_{cv} = 10s_u^0$. The thin lines represent the streamlines.

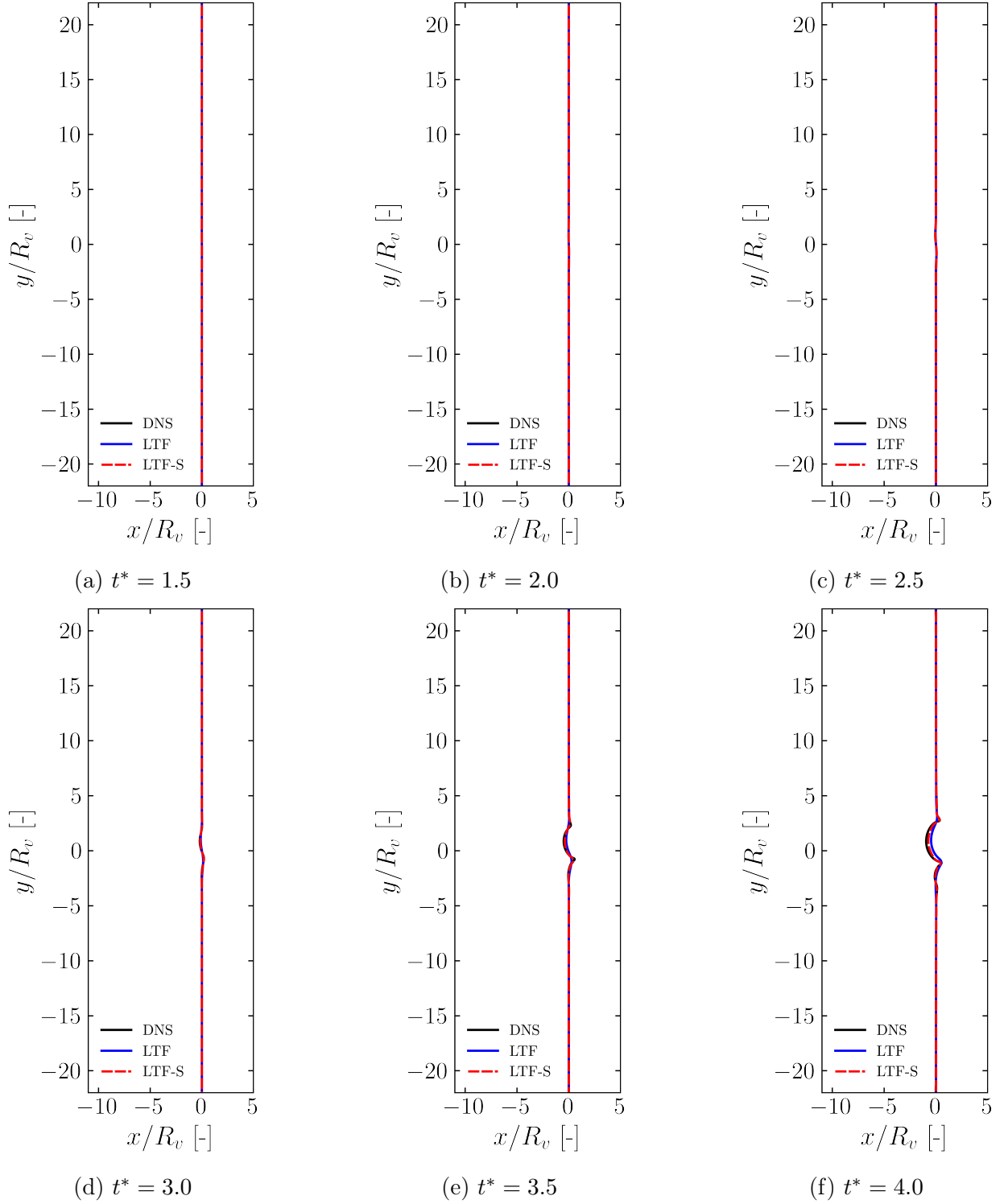


Figure 4.10: Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 0.1s_u^0$.

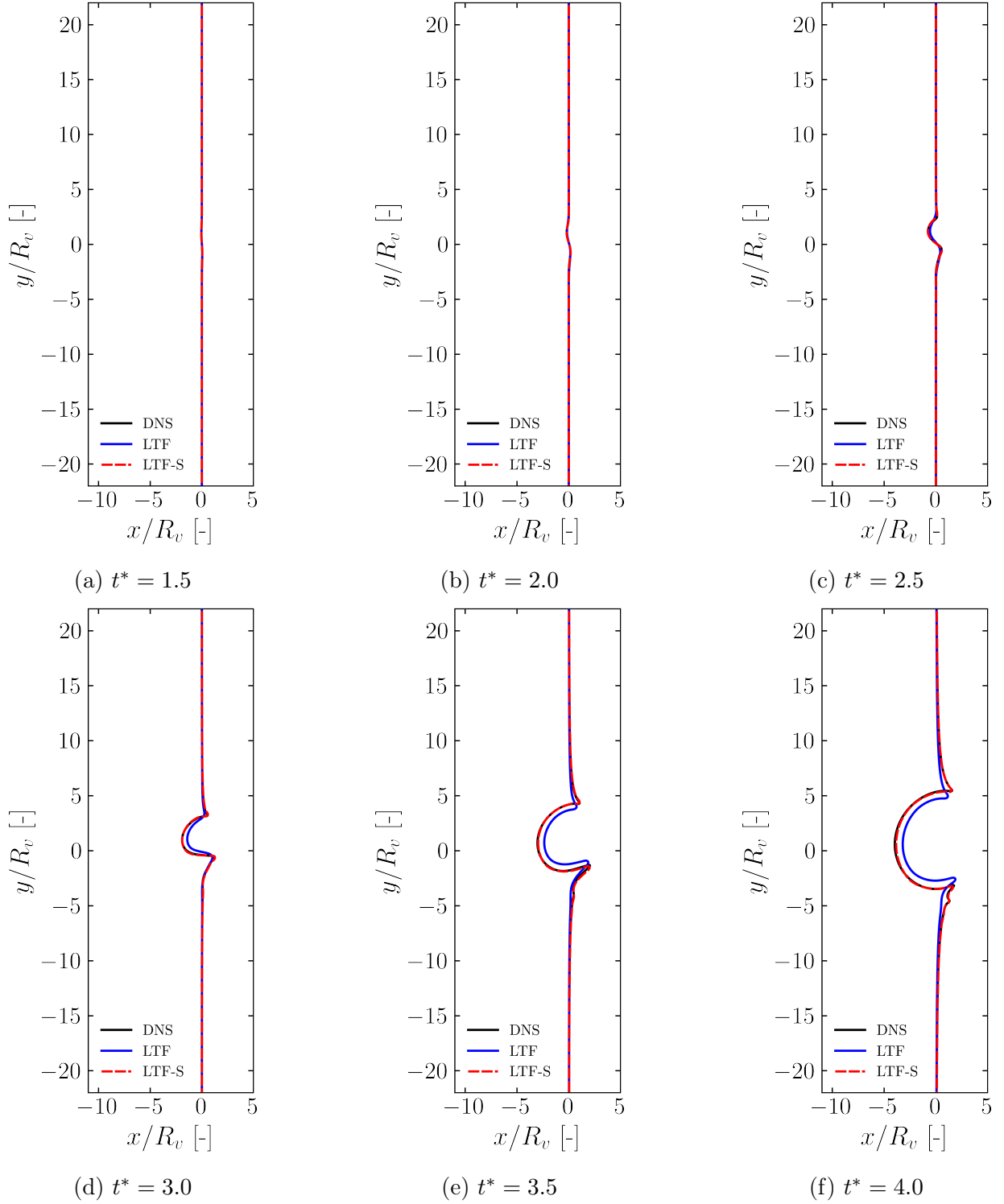


Figure 4.11: Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 1s_u^0$.

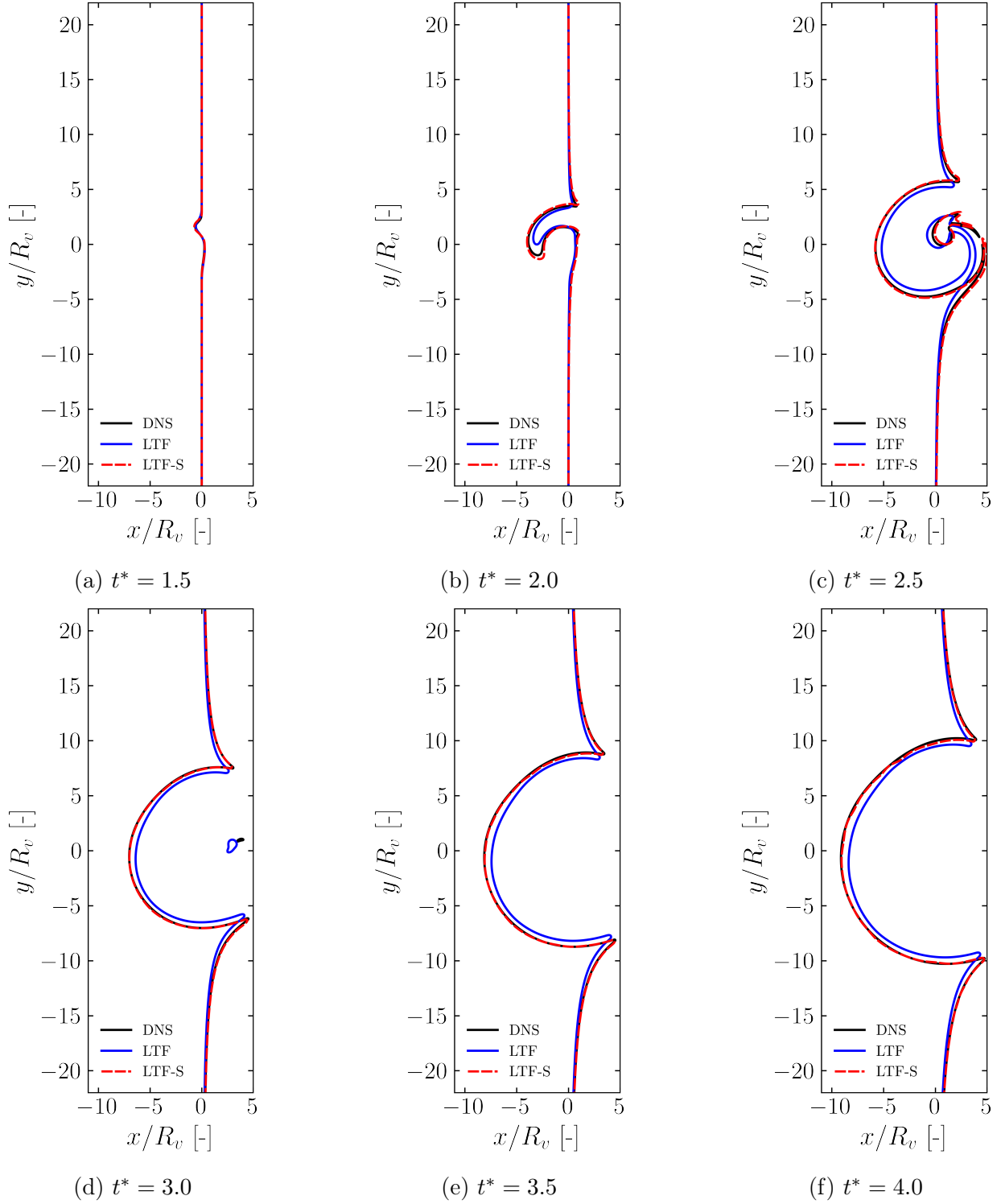


Figure 4.12: Comparisons of the sequential flame shapes in the flame-vortex interaction problem for the case of $u_{cv} = 10s_u^0$.

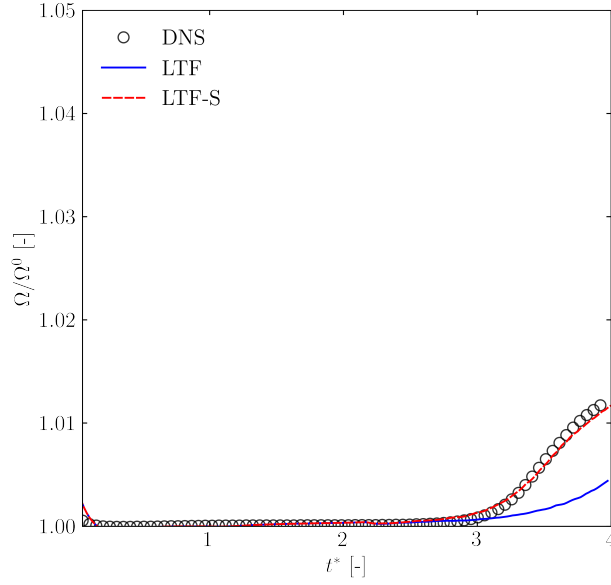


Figure 4.13: Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 0.1s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.

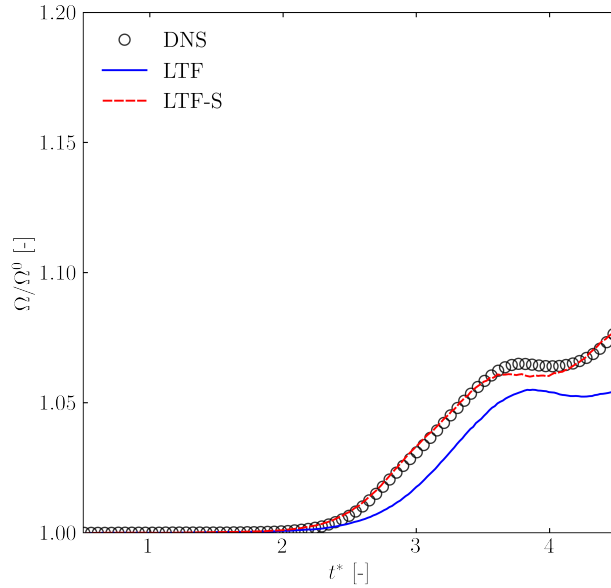


Figure 4.14: Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 1s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.

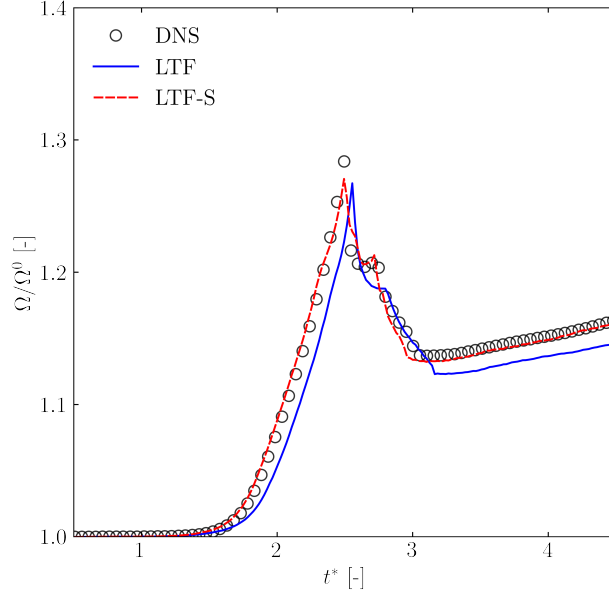


Figure 4.15: Time histories of global consumption rate in a flame-vortex interaction problem for the case of $u_{cv} = 10s_u^0$. Ω_0 is the initial value, which represents the consumption rate of the steady flame before interacting with the vortex.

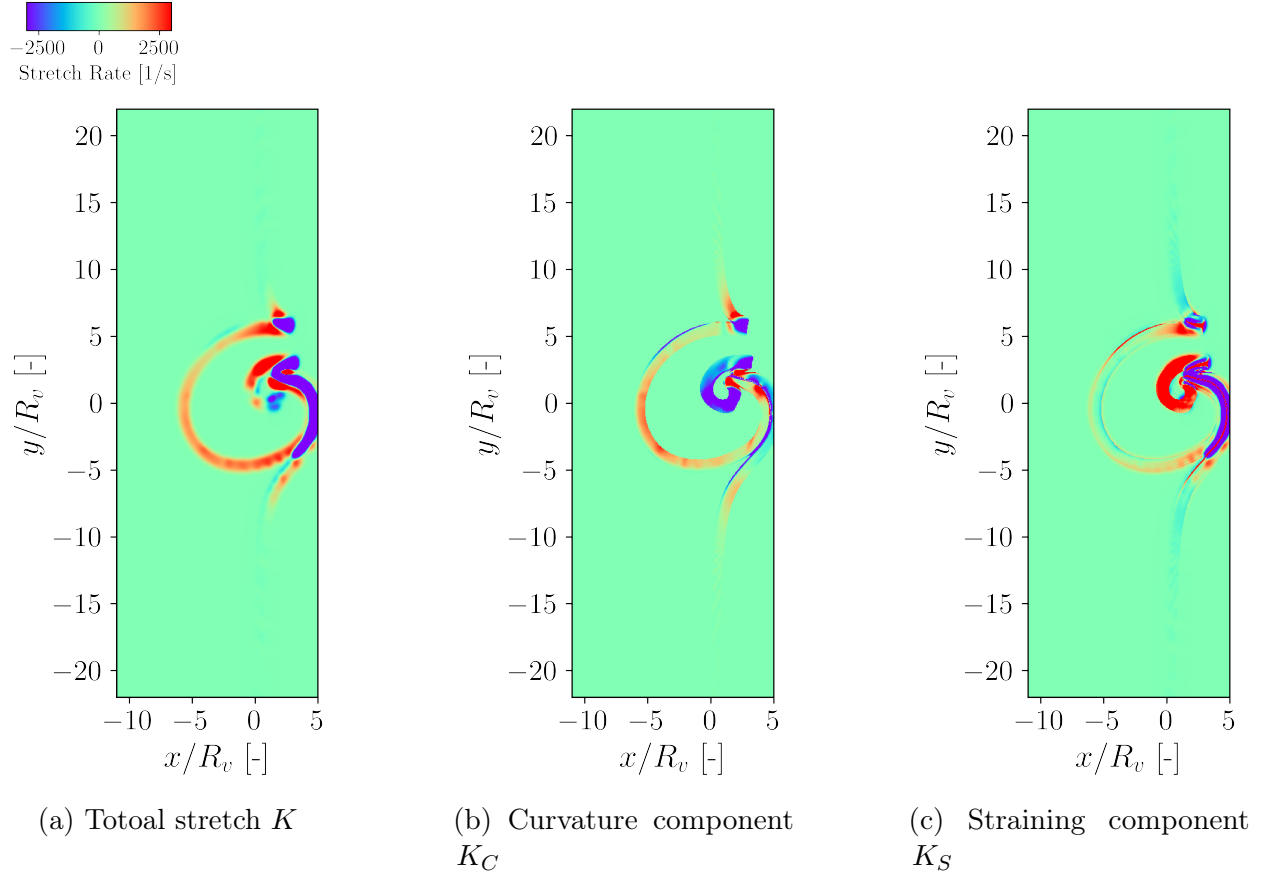


Figure 4.16: Stretch components distributions of LTF-S model at $t^* = 2.5$ for $u_{cv} = 10s_u^0$.

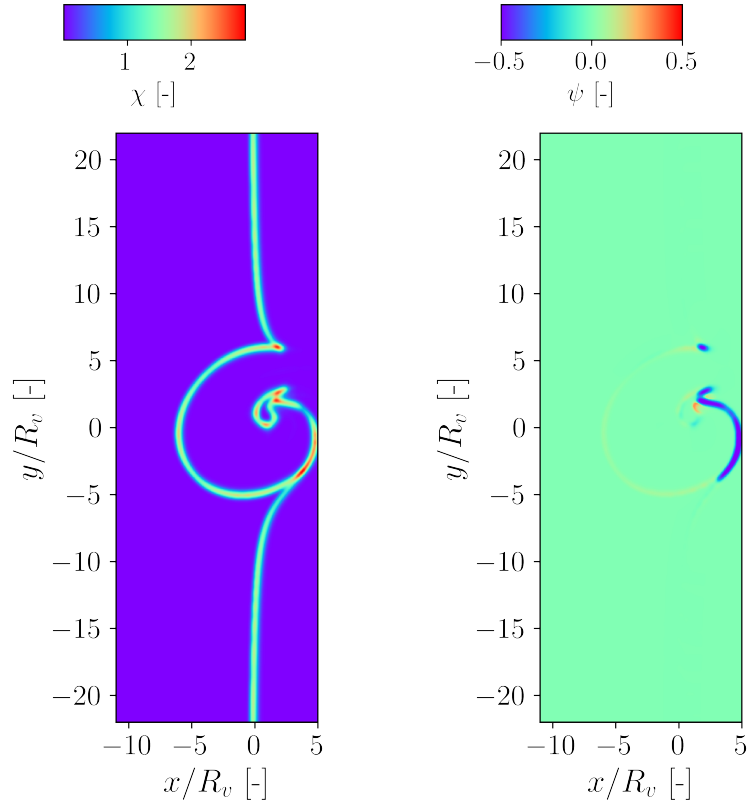


Figure 4.17: Distributions of the LTF-S model parameters χ and ψ at $t^* = 2.5$ for $u_{cv} = 10s_u^0$.

Chapter 5

Extension of LTF-S Model to Hydrocarbon Fuel

Among the parameters to decide the ψ , the laminar burning velocity and the Markstein length are the unique values that can be easily acquired by canonical one-dimensional simulations. As for the linear relationship between the Markstein length ratio and the effective thickening factor, the proportional coefficient A for the other fuels must be decided. This study further examined the Markstein length ratio for hydrocarbon fuels, specifically methane (CH_4) and propane (C_3H_8), and determined that $A = 0.5$ can be regarded as a universal value when using the LTF-S model to predict premixed flames of H_2 , CH_4 , and C_3H_8 . Following this validation, we applied the LTF-S model to a realistic premixed combustion scenario: a perforated-plate burner. The LTF-S model was used to predict both the global fuel consumption rate and the local stretched burning velocity. In this configuration, the planar flame between the flame base and flame tip is subjected only to stretch effects caused by aerodynamic straining of the flow. (A canonical one-dimensional configuration for such pure stretch is the counter-flow premixed flame, but this case is difficult to reproduce with a multidimensional flame solver.) The high-fidelity predictions obtained with the LTF-S model confirm that the Markstein length determined from a curved flame propagation configuration—namely, a two-dimensional, outwardly propagating cylindrical flame—is also valid for purely strain-induced conditions. This, in turn, extends the general applicability of the LTF-S model.

5.1 Validation of LTF-S by Premixed CH_4 and C_3H_8 Flame

5.1.1 Numerical Configuration

Following chapter 3, the two-dimensional cylindrically propagating premixed flame configuration is used in this validation as well. The computations are conducted on a rectangular Cartesian domain of length 1000 cm. A locally refined region is employed to resolve the premixed flame front with high fidelity. The fine-grid-focused region used a larger side length 20 cm ($l = 12$ cm for H_2), as the premixed flames of CH_4 and C_3H_8 take more time to get rid of the effect of the initial ignition to achieve the steady propagating stage. In this region, grid

Fuel	ϕ [-]	s_u^0 [cm/s]	$\mathcal{L}_{u,DNS}$ [cm]	δ^0 [cm]	T_{ad} [K]	Le_{eff} [-]	C_χ [-]
CH ₄	0.6	10.8284	0.01869	0.1012	1670.283	0.9906	400
	0.8	25.1957	0.01511	0.0565	2003.418	1.0028	
	1.0	34.1210	0.01701	0.0480	2230.640	1.0409	
	1.2	31.1554	0.01367	0.0496	2137.695	1.0491	
	1.4	16.5148	0.02168	0.0849	1980.442	1.0509	
	1.6	8.27071	0.06618	0.1581	1832.942	1.0510	
C ₃ H ₈	0.6	17.6012	0.03431	0.0634	1701.339	1.8832	400
	0.8	36.7913	0.01741	0.0391	2042.588	1.8643	
	1.0	49.1082	0.01557	0.0331	2266.555	1.8613	
	1.2	49.1153	0.00916	0.0318	2200.613	1.3458	
	1.4	32.5796	-0.00569	0.0443	2047.903	1.1484	
	1.6	14.3534	-0.00793	0.0875	1901.388	1.1158	

Table 5.1: Summary of the parameters. The laminar burning velocity s_u^0 , the flame thickness δ^0 , and the adiabatic flame temperature T_{ad} are calculated by Cantera. The Markstein length is calculated using Ember. The C_χ shown here is used for the simulation of LTF-S model.

points are uniformly distributed, and the coordinate system’s origin is centered there.

Outside the fine-grid-focused region, the mesh spacing is gradually increased toward the outer boundaries in order to reduce the influence of the Neumann boundary conditions imposed at those boundaries. Within the refined region, two uniform grid resolutions, $\Delta x = 0.032$ cm and $\Delta x = 0.064$ cm, are employed for simulations using the LTF model.

To establish the initial flame, a high-temperature burned-gas region at chemical equilibrium is prescribed within a circular domain ($r \leq 0.5$ cm) centered in the fine-grid-focused region. This burned-gas zone is surrounded by unburned premixed reactants at an initial temperature $T_u = 300$ K. Across the interface between the unburned and burned gases, the temperature and species mass fraction profiles are smoothly connected using an error-function distribution. The equilibrium composition and temperature of the burned gas are obtained from Cantera. The CH₄/Air flames simulated using the *FFCM-1* detailed chemical kinetic mechanism (38 species / 291 reactions), and the C₃H₈/Air flames adopted the *GRI-Mech 3.0* mechanism (53 species / 325 reactions). The equivalence ratio is varied from 0.6 to 1.6, and the corresponding fundamental flame parameters are summarized in Table 5.1. Note that the flame thicknesses of CH₄ flames are larger than those of H₂ and C₃H₈ (which are nearly comparable), resulting in the use of a relatively small thickening factor for the simulations using LTF model. Consequently, a coarser grid resolution $\Delta x = 0.064$ cm is employed to vary the effective thickening factor $\delta_{LTF}/\delta_{DNS}$.

In addition to the two-dimensional configuration, an open-source one-dimensional transient flame solver, Ember, is employed to efficiently evaluated the Markstein length. Our previous investigation demonstrated that Ember [81] yields Markstein lengths in good agreement with those obtained from two-dimensional DNS studies of premixed H₂/Air flames.

5.1.2 Markstein Length Ratio for CH_4 and C_3H_8

The Markstein lengths for premixed CH_4/Air and $\text{C}_3\text{H}_8/\text{Air}$ flames are listed in Table 5.1. For premixed $\text{C}_3\text{H}_8/\text{Air}$ flames, the Markstein length becomes negative under fuel-rich conditions, which contrasts with the behavior of H_2/Air flames. This trend is driven by the effect of preferential diffusion: as the mixture becomes richer in fuel, the lighter oxidizer O_2 diffuses toward the reaction zone more quickly than the heavier fuel C_3H_8 . This observation aligns with the decrease in effective Lewis number, Le_{eff} , reported in [76]. In comparison, the Markstein lengths for premixed CH_4/Air remain positive over the entire equivalence ratio range considered. Since the effective Lewis number for premixed CH_4/Air is close to unity, the variation of Markstein length follows a pattern similar to that of the flame thickness.

Figure 5.1 shows that the Markstein length ratio, $\mathcal{L}_{u,\text{LTF}}/\mathcal{L}_{u,\text{DNS}}$, varies linearly with the effective flame-thickening factor of the LTF model, $\delta_{\text{LTF}}^0/\delta_{\text{DNS}}^0$, for both CH_4/Air and $\text{C}_3\text{H}_8/\text{Air}$ flames. Similar to the hydrogen case, distinct proportionality factors are obtained: $A = 0.588$ for premixed CH_4/Air and $A = 0.446$ for premixed $\text{C}_3\text{H}_8/\text{Air}$. These findings confirm that the LTF-S framework can also be applied to these hydrocarbon fuels. When combined with the previously determined value $A = 0.579$ for H_2/Air , the proportionality coefficient A is seen to lie within the interval 0.4–0.6. In addition, Figure 5.2 explores the effect of the initial temperature on the proportionality coefficient for H_2/Air flames, and verifies that it likewise remains confined to this range.

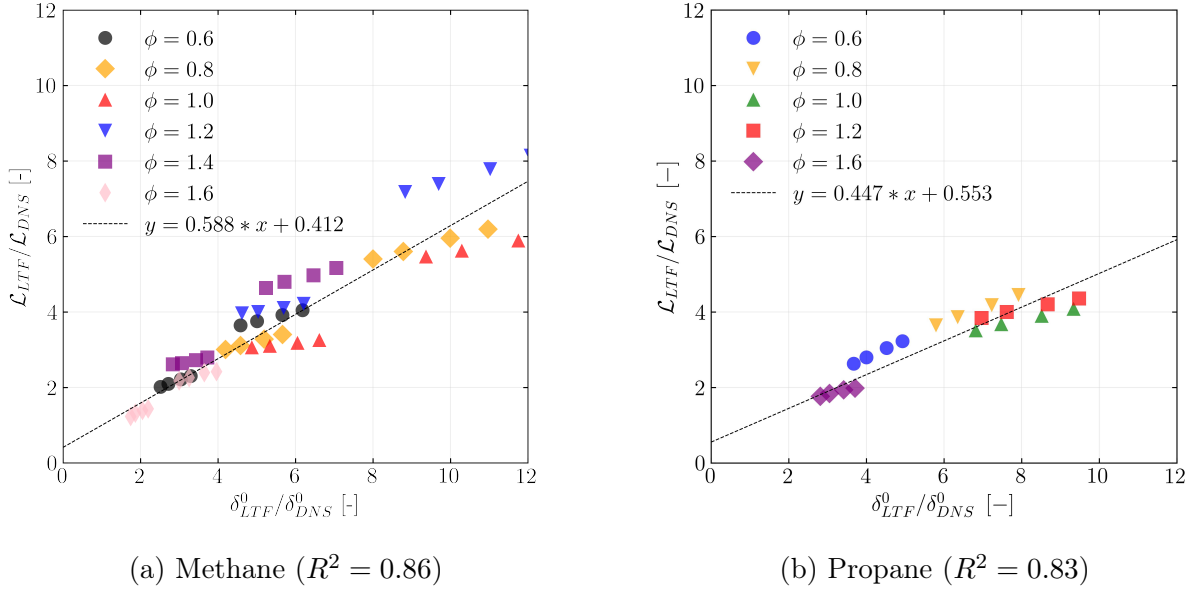
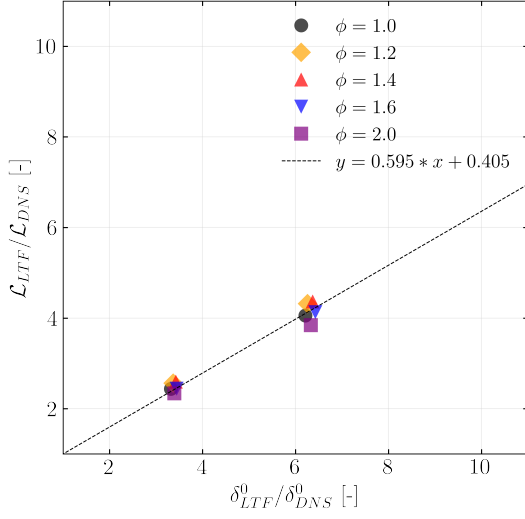
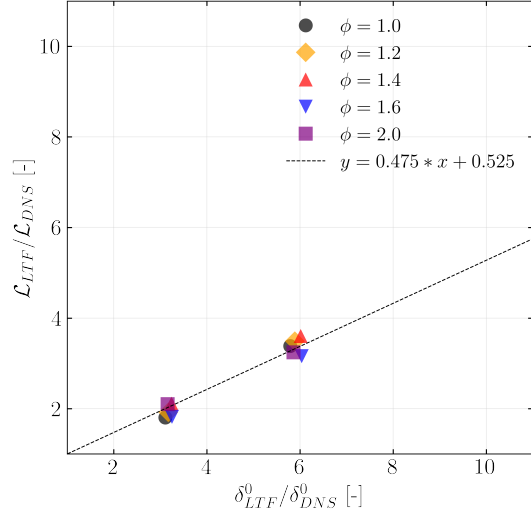


Figure 5.1: Relationship between the Markstein length and flame thickness ratios in a cylindrical flame propagation problem.

As discussed in 3.3, for a constant thickening factor, the Markstein length ratio $\mathcal{L}_{u,\text{LTF}}/\mathcal{L}_u$ scales linearly with the flame thickening factor $1 + \chi$. Since the TF model preserves the non-dimensional flame parameters, this linear proportionality implies that the Markstein length of the thickened flame, $\mathcal{L}_{u,\text{TF}}$, depends solely on the thickened flame thickness δ_{TF} . In



(a) $T_u = 400 \text{ K}$ ($R^2 = 0.97$)



(b) $T_u = 500 \text{ K}$ ($R^2 = 0.95$)

Figure 5.2: Relationship between the Markstein length and flame thickness ratios in a cylindrical flame propagation problem for the premixed hydrogen and air flames. These results acquired by using two sizes, $\Delta x = 0.016$, and 0.032 cm , with $C_\chi = 400$.

the LTF model, however, the spatially varying thickening factor produces a linear relationship (Eq. (3.85)) between the Markstein length ratio and the thickening factor. Because the LTF and LTF-S models also conserve the non-dimensional parameters, the proportionality coefficient primarily arises from the distributed nature of the thickening factor. The different proportionality constants A found for H_2 , CH_4 , and C_3H_8 are likely attributable to variations in flame structure. In particular, differences in the temperature field within the flame affect how the thickening factor is applied, thereby producing the observed variations in A .

5.1.3 Sensitivity of A

Here, we conducted a sensitivity analysis of A on the prediction of stretched burning velocities. From Eqs. (43), (51), the stretched burning velocity predicted by the LTF-S model is given as:

$$s_{u,\text{LTF-S}} = \left(1 + \frac{(\mathcal{L}_{u,\text{LTF}} - \mathcal{L}_u) K}{s^0 - \mathcal{L}_{u,\text{LTF}} K} \right) s_{u,\text{LTF}},$$

Substituting Eq. (55) into Eq. (A.1) yields

$$s_{u,\text{LTF-S}} = \left\{ 1 + \frac{A(F-1)\mathcal{L}_u K}{s_u^0 - [A(F-1) + 1]\mathcal{L}_u K} \right\} s_{u,\text{LTF}} \quad (5.1)$$

Fuel	ϕ [-]	T_u [K]	s_u^0 [cm/s]	$\mathcal{L}_{u,DNS}$ [cm]	δ^0 [cm]	T_{ad} [K]	C_χ [-]
H ₂	1.0	400	361.758	0.01123	0.0428	2435.935	400
		500	528.360	0.01462	0.0465	2483.484	
	1.2	400	416.487	0.01162	0.0420	2427.927	
		500	595.307	0.01488	0.0455	2484.465	
	1.4	400	448.519	0.01250	0.0409	2354.591	
		500	635.431	0.01545	0.0442	2419.046	
	1.6	400	462.047	0.01409	0.0405	2278.666	
		500	654.303	0.01715	0.0438	2347.741	
	2.0	400	454.762	0.01727	0.0410	2137.800	
		500	648.931	0.02116	0.0448	2213.023	

Table 5.2: Summary of the parameters of H₂/air for different initial temperatures ($T_u = 400$ and 500 K).

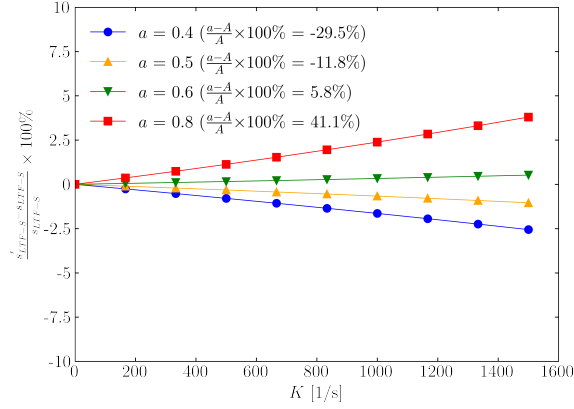


Figure 5.3: Sensitivity of the proportional constant in Eq. (3.84) on the prediction of the stretched burning velocity.

where $F = \delta_{LTF}/\delta_{DNS}$ is a thickening factor. If a different proportional constant a is used in Eq. (55), the stretched burning velocity is obtained as:

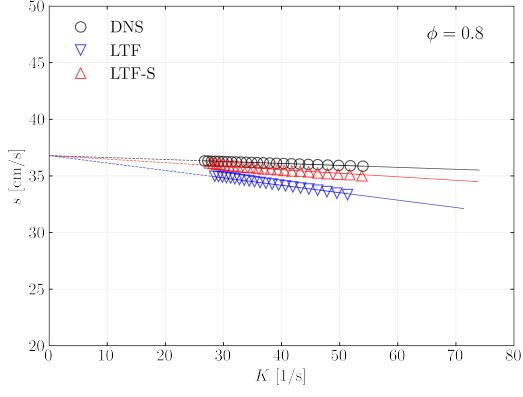
$$s'_{u,LTF-S} = \left\{ 1 + \frac{a(F-1)\mathcal{L}_u K}{s_u^0 - [a(F-1) + 1]\mathcal{L}_u K} \right\} s_{u,LTF-S} \quad (5.2)$$

Therefore, the difference $s'_{u,LTF-S} - s_{u,LTF-S}$ represents the error introduced when a proportional constant a is used instead of the correct constant A , as determined from the simulation. Figure 5.3 presents the resulting error in predicting stretched burning velocities caused by adopting various proportional constants. The case considered is a stoichiometric H₂/air flame with $s_u^0 = 228.504$ cm/s and $\mathcal{L}_u = 0.00667$ cm. A thickening factor of $F = 1 + \chi = 3.975$, obtained from the simulation with $\Delta x = 0.016$ cm, is employed. The figure illustrates how different selections of a lead to discrepancies in the predicted stretched burning velocities relative to the reference value ($A = 0.579$ for H₂). (This analysis can also help assess how

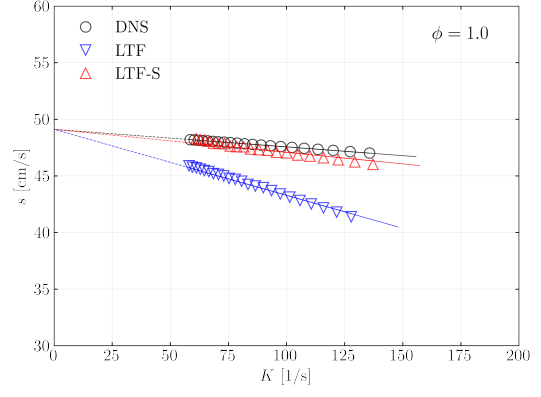
chosen target Markstein lengths affect the accuracy of stretched burning velocity predictions.) Based on these results, selecting A within the range 0.4–0.6 leads to an error of only about 5%. Consequently, we infer that $A = 0.5$ can be adopted as a universal value for LTF-S simulations. Since the laminar burning velocity s_u^0 and the Markstein length $\mathcal{L}$ can be easily obtained via one-dimensional simulations, this universal choice of A enhances the practicality and ease of applying the LTF-S model.

5.1.4 Validation of the LTF-S Model for Premixed C₃H₈/Air Flames

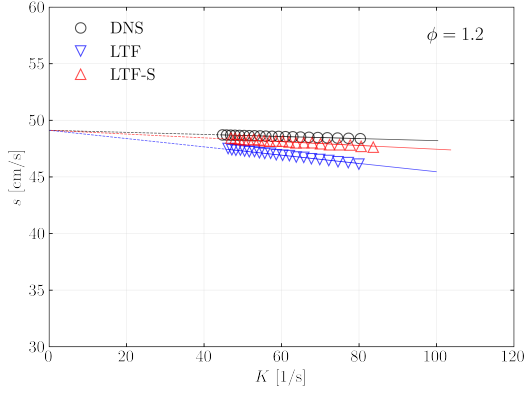
Based on the above discussion, simulations employing the LTF-S model are carried out for C₃H₈/air with a proportional coefficient of $A = 0.5$. Figure 5.4 presents a comparison of the propagation speeds predicted by the LTF-S model over a range of equivalence ratios. The reference DNS data are obtained from the simulations using Ember. The parameters adopted in the LTF-S model are summarized in Table 5.1. The LTF-S model accurately reproduces both positive and negative responses to flame stretch, with predicted propagation speeds closely matching the actual flame results from Ember.



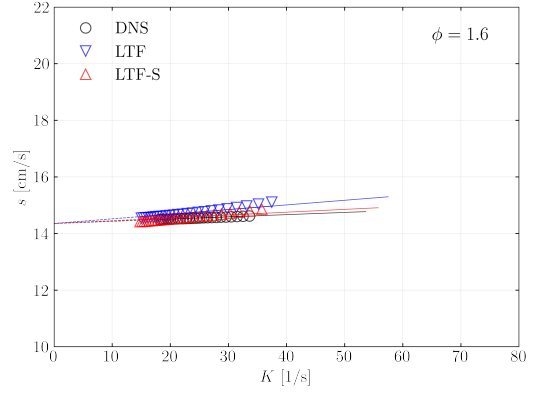
(a) $\phi = 0.8$



(b) $\phi = 1.0$



(c) $\phi = 1.2$



(d) $\phi = 1.6$

Figure 5.4: Comparison of the burning velocity s against stretch rate for various equivalence conditions in a cylindrical flame propagation problem. In the figures, the lines drawn using a linear least-squares fit represent the linear relationship between burning velocity and stretch rate. The results of DNS is simulated by a open-source flame solver, Ember. The two-dimensional simulations of the LTF and LTF-S models use the grid size $\Delta x = 0.032$ cm.

5.2 Perforated-plate Burner Flame

This study further assessed the LTF-S model using a practical burner setup, namely a perforated-plate burner. Such burners are widely used in the water heaters and the gas stoves. As premixed mixtures flow through the slots or holes, their velocity increases, which helps prevent flash-back of the premixed flame. Due to its simple geometry, many researchers have adopted this burner configuration to validate the combustion model and to study combustion phenomena, including flame-acoustic interactions [90] and premixed flame flash-back [91].

5.2.1 Numerical Configuration

This study adopts the burner geometry from a previously established benchmark configuration (Kornilov 2009 [90]). Figure 5.5 shows one of the fine-grid-refined regions among the four sectors of the burner. (Although only one flame section is shown in Fig. 5.5 and in the simulation results, the actual computation includes four flame sections. Through trial-and-error tests, we found that pressure waves in the horizontal direction can become significant and cause oscillations that destabilize the flame. Increasing the domain width in the horizontal direction can suppress these oscillations.) For the DNS, a uniform grid spacing of $\Delta x = \Delta y = 0.0025$ cm is used, whereas for the simulations with the LTF-S model, a coarser grid spacing of $\Delta x = \Delta y = 0.01$ cm is employed. Premixed $\text{C}_3\text{H}_8/\text{air}$ flames with equivalence ratios $\phi = 1.0$ and $\phi = 1.2$ are investigated, as their thin flame thicknesses require a larger number of grid points for adequate flame resolution.

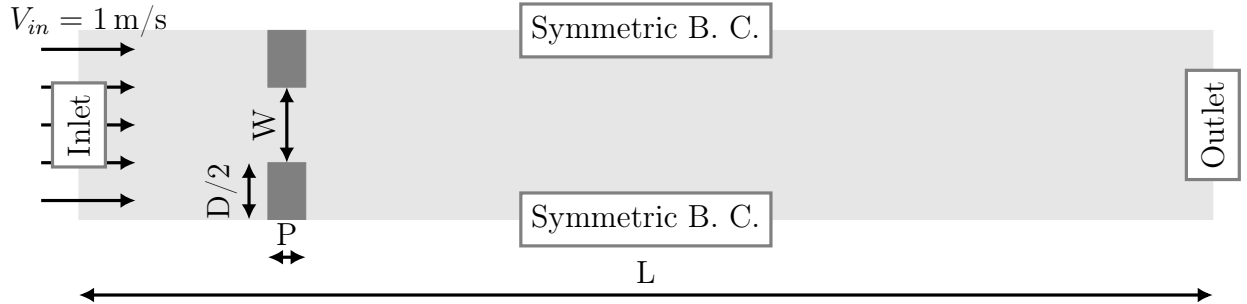


Figure 5.5: Schematic of the two-dimensional perforated burner adapted from Kornilov 2009 [90]. ($L = 30$ mm, $D = 3$ mm, $W = 2$ mm, and $P = 1$ mm)

At the inlet, a premixed $\text{C}_3\text{H}_8/\text{air}$ reactant stream at $T = 300$ K is imposed with a uniform axial velocity of $u_{\text{in}} = 100$ cm/s, while the pressure is obtained via extrapolation from the interior domain. At the outlet, all flow and thermochemical variables (u , v , p , T , ρ , Y_i) are extrapolated. Symmetric boundary conditions are enforced at the top and bottom boundaries of the domain. These symmetric conditions are implemented by introducing an additional row of grid points (indexed as $J + 1$) along the L direction in Fig. 5.5. The variables on this extra row are set equal to the same values as those on one skipped row (indexed as $J - 1$), with the exception that the v -velocity component is given the opposite sign ($v_{i,J+1} = -v_{i,J-1}$). Thus, the solution points on the row with index J satisfy the symmetric boundary conditions.

To create the burner slots, isothermal solid walls are introduced into the computational domain and held at a constant temperature of $T_{\text{wall}} = 300$ K. The initial flame is specified as

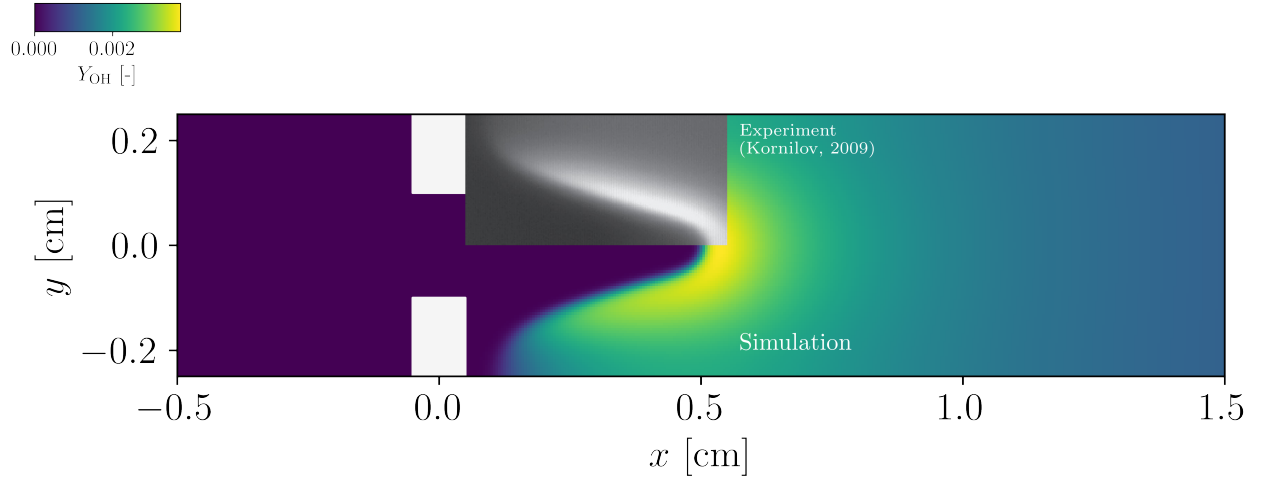
a planar, one-dimensional flame front located at $x = 0.2$ cm downstream of the wall, aligned parallel to the inlet boundary. On both the burned and unburned sides of this initial front, the streamwise velocity is set to $u = u_{\text{in}}$. The parameters employed in the LTF-S model simulations are given in Table 5.1.

5.2.2 Result and Discussion

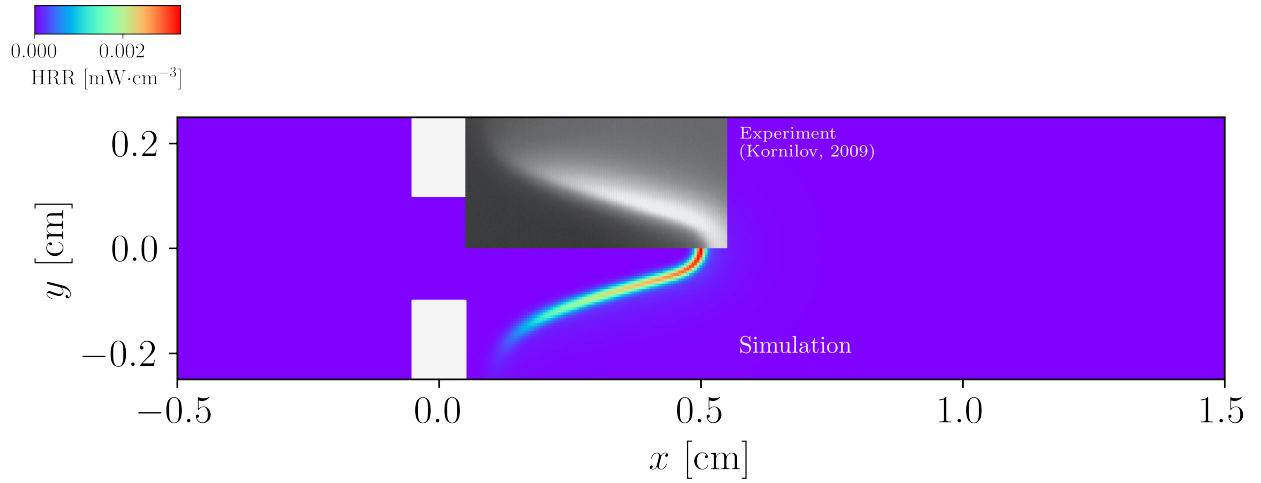
Firstly, we compare the simulation results with the experimental OH chemiluminescence image pictured by Kornilov [90]. The simulation is based on DNS data with a grid spacing of $\Delta x = 25$ cm. The premixed mixture is CH_4/air under the equivalence ratio $\phi = 0.8$. Following the configurations used by Kornilov [90] and Vance (2023) [92], the inlet velocity is set to $V_{\text{in}} = 40$ cm/s and the wall temperature to $T_{\text{wall}} = 423$ K. All other settings are the same as in the previous section.

Figure 5.6 presents the steady-state flame structure. The colored region depicts the DNS-predicted OH mass-fraction field, while the grayscale region shows the experimentally observed luminescence. Near the flame root, Y_{OH} is close to zero because the low-temperature isothermal wall quenches the flame, resulting in weak local heat release. Moving toward the flame tip, the heat release rate gradually intensifies, and the corresponding Y_{OH} accordingly increases. Note that in Fig. 5.6, the chemiluminescence region appears slightly downstream of the peak heat release rate. This may result from convection transporting the reaction-produced OH^* , which then relaxes to ground-state OH further downstream. Consequently, the experimentally observed luminescence coincides well with the simulated Y_{OH} field. The simulation results exhibit good agreement with the experimentally measured distribution.

Figures 5.7 and 5.8 show the steady-state flame shapes obtained from DNS, LTF, and LTF-S. For the simulation using a grid spacing of $\Delta x = 100$ cm, the DNS flame becomes unstable and ultimately diverges. In contrast, the LTF and LTF-S models artificially broaden the flame, which enables adequate resolution of the flame structure on this relatively coarse grid. However, the total flame lengths predicted by both LTF and LTF-S are slightly overpredicted. One contributing factor is that the thickening factor is activated in the vicinity of the isothermal wall, which results in an artificially thickened thermal boundary layer. Another factor is the negative curvature at the flame tip. In this configuration, the local flame curvature is proportional to the flame thickness; thus, the artificially thickened flame cannot accurately reproduce the smaller-radius curvature observed in the DNS.



(a) Y_{OH}



(b) Heat Release Rate

Figure 5.6: Comparison of the experimental and simulated distributions of Y_{OH} . The gray-colored portion is the experimental chemiluminescence picture by Konilov et al.[90].

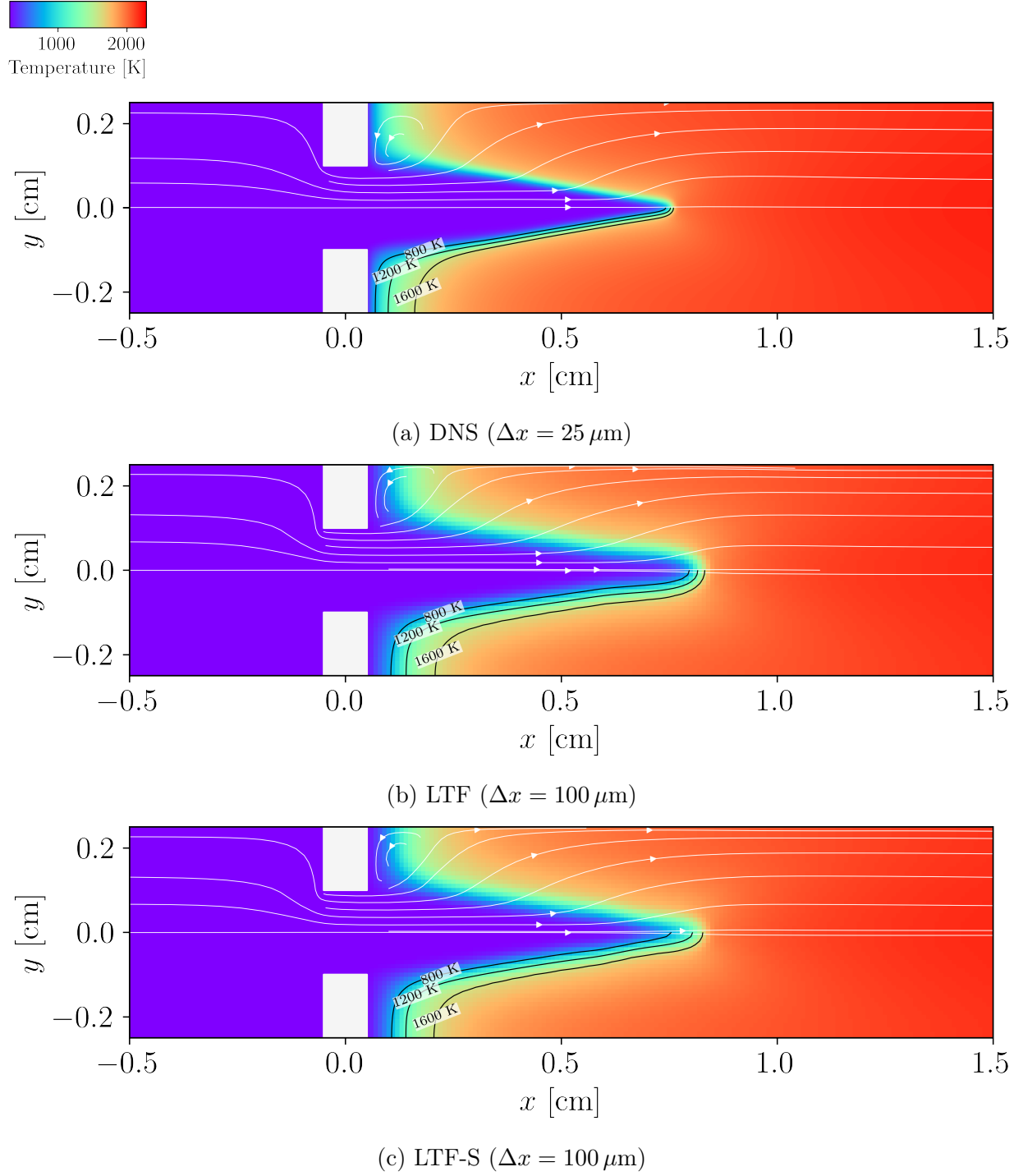


Figure 5.7: The temperature distributions of the stable perforated-plate flames of DNS, LTF, and LTF-S for $\text{C}_3\text{H}_8/\text{Air}$ under $\phi = 1.0$. (The white streamlines are presented in the upper half, and the black temperature iso-contours are displayed in the lower half.)

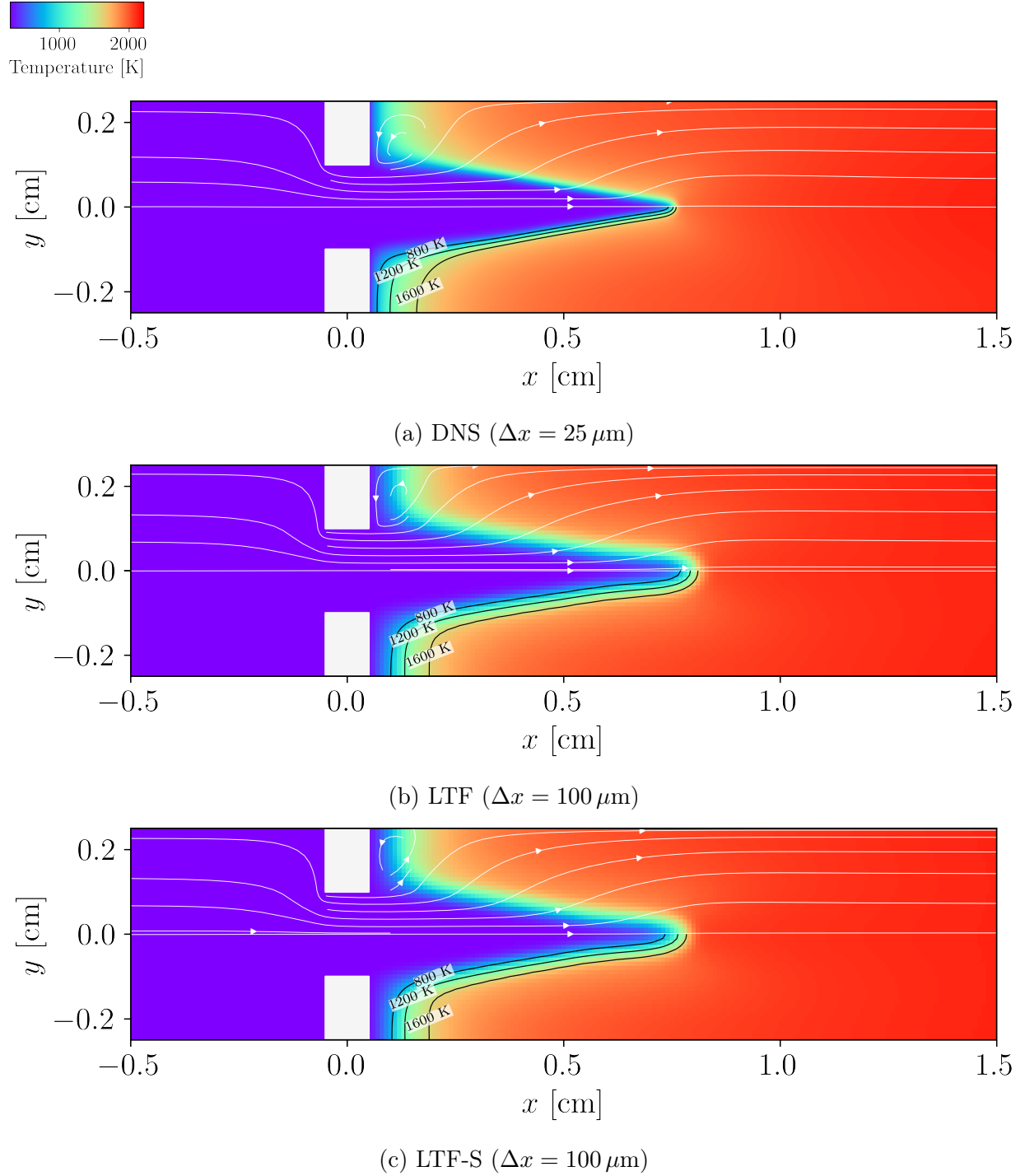


Figure 5.8: The temperature distributions of the stable perforated-plate flames of DNS, LTF, and LTF-S for $\text{C}_3\text{H}_8/\text{Air}$ under $\phi = 1.2$. (The white streamlines are presented in the upper half, and the black temperature iso-contours are displayed in the lower half.)

Figure 5.9 compares the temporal evolution of the global fuel consumption rate, $\Omega_{\text{C}_3\text{H}_8}$, for DNS, LTF, and LTF-S. The pronounced peak results from the interaction between the initially planar flame and the jet emerging from the slots. After this transient phase, all three simulations converge to the same asymptotic value of $\Omega_{\text{C}_3\text{H}_8}$, once the fuel consumption rate balances with the incoming fuel mass flux. For the equivalence ratio $\phi = 1.2$, in the statistically converged regime, all three results exhibit oscillations at the same frequency. This behavior likely results from pressure (or velocity) fluctuations in the upstream chamber between the inlet and the isothermal walls. (Since the thickened flame models were able to capture these oscillations, this demonstrates the potential of the LTF-S model for predicting acoustic–flame interactions.)

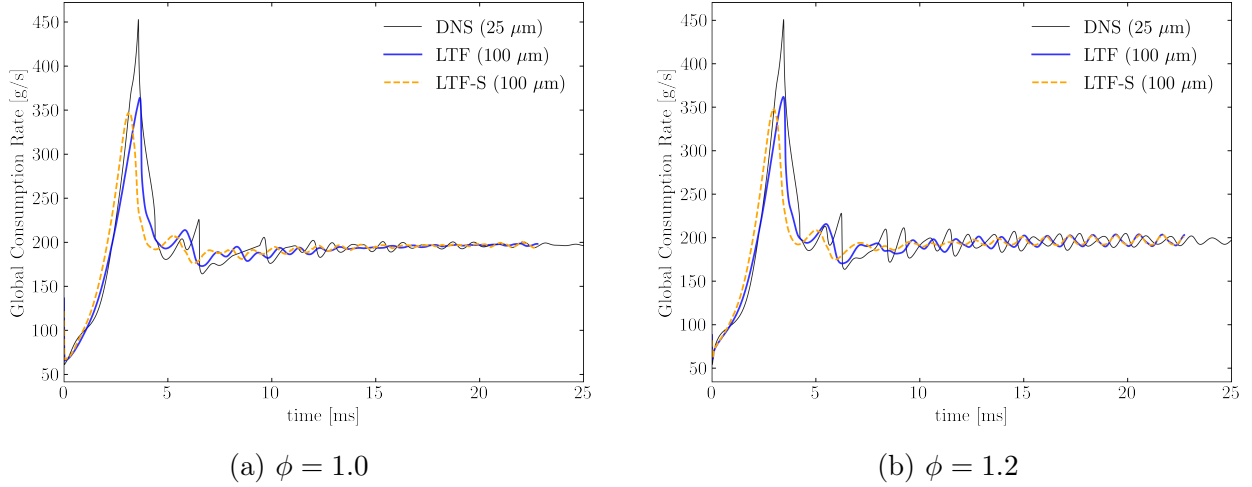


Figure 5.9: Comparison of the global consumption rate for DNS, LTF, and LTF-S.

In Fig. 5.10, the comparison of the local burning velocity as a function of the stretch rate highlights the differences between the LTF and LTF-S models. Similar to a cylindrical outwardly propagating flame, the LTF model’s predicted burning velocity shows increased sensitivity to stretch, resulting in an underestimation compared to the DNS burning velocity. These data are extracted from temperature iso-contours ($T = 800$ K, 1200 K, and 1600 K). Within this temperature range, the burning velocity displays a comparable sensitivity to stretch (similar Markstein length). For the LTF-S model, the stretched burning velocity is effectively recovered, showing good agreement with DNS results.

Although the LTF-S model accurately predicts the local burning velocity, the overall flame length (defined as the distance from the slot outlet to the flame tip) remains similar to that obtained with the original LTF model. To understand why the LTF-S model does not improve the accuracy of the flame-length prediction, we compared the flame shape, using the iso-contour $T = 1200$ K, among DNS, LTF, and LTF-S. In Fig. 5.11, for both the LTF and LTF-S thickened flames, the stand-off positions of the flame shoulders relative to the isothermal walls coincide with each other and are larger than those of the non-thickened DNS flame. This occurs because the thickening factor $1 + \chi$ is determined from the temperature gradient (Eq. (3.41)). Since a temperature gradient exists in the thermal boundary layer adjacent to the isothermal wall, χ erroneously identifies this region as part of the flame and applies the thickening there. As a result, the stand-off distance is overestimated by both

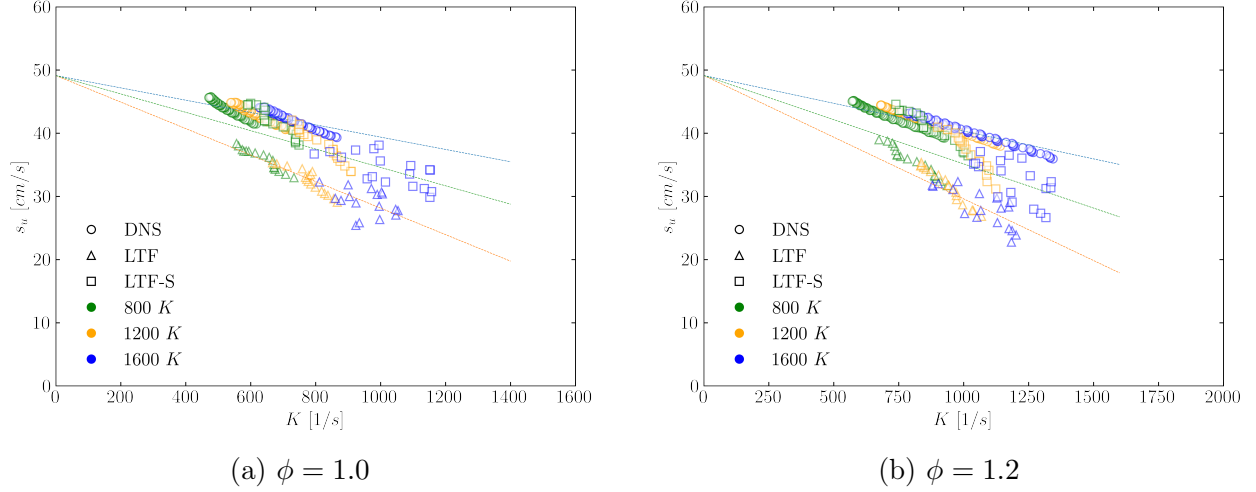


Figure 5.10: Comparison of burning velocity s_u against stretch rate K for DNS, LTF, and LTF-S. (Different colors indicate the simulation results extracted from distinct isothermal contours.)

LTF and LTF-S. If this discrepancy in stand-off distance is removed, the LTF-S flame shape closely matches that of DNS. This indicates that the flame geometry itself is essentially unchanged, despite the difference in stand-off distance between the DNS and LTF-S solutions. The flame segment in the shoulder region can freely adjust its orientation to reach a dynamic equilibrium with the freestream flow. Therefore, once the local burning velocity is correctly captured by the LTF-S model, the resulting flame shape becomes nearly identical to DNS. The accurately predicted flame shoulder then constrains the flame-tip segment, enabling a good prediction in this strongly stretched region as well.

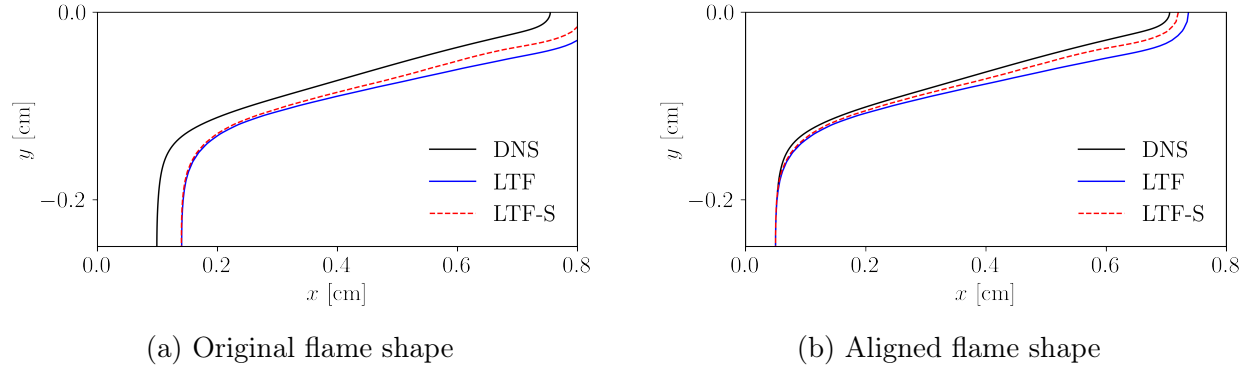


Figure 5.11: Comparison of the flame iso-contour ($T = 1200$ K) for DNS, LTF, and LTF-S. ($\phi = 1.0$)

The stand-off distance is a type of flame extinction in which excessive heat is lost to the cold wall. This flame-wall interaction is significant in practical engines. To effectively apply the LTF-S model in this situation, an additional indicator may be required to distinguish the temperature gradients arise from the flame front or from the thermal boundary layer near the wall. In this flame configuration, the heat release rate tends toward zero in the vicinity of the

wall (Fig. 5.6b). Therefore, distributions of radical or the heat release rate can be used as a reactive indicator to identify the actual flame position, which can then be combined with $1 + \chi$ to apply the flame thickening effect.

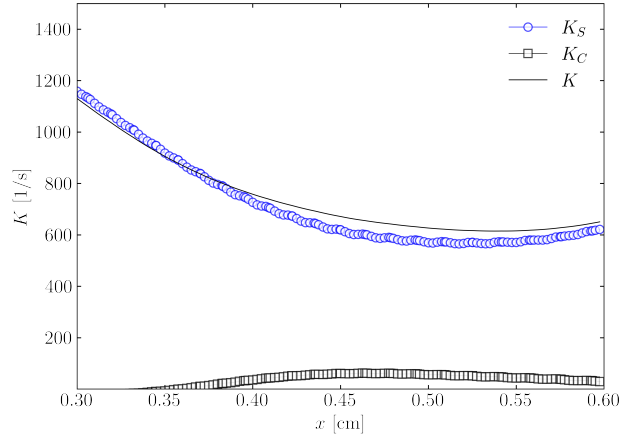


Figure 5.12: The stretch components along the iso-temperature lines ($T = 1200$ K) for C_3H_8 under $\phi = 1.2$.

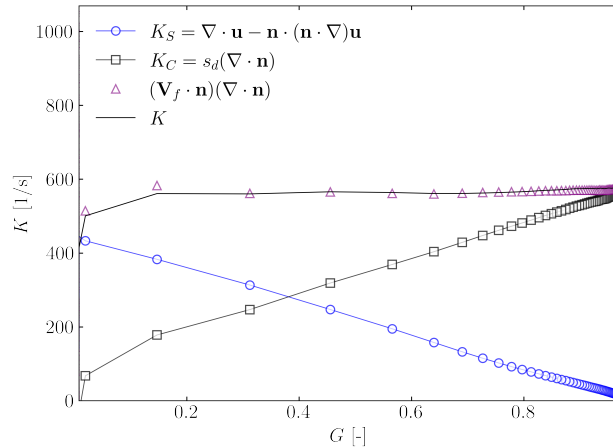


Figure 5.13: The stretch components along the flame normal direction for the cylindrical outwardly propagating flame for H_2/Air under $\phi = 1.0$. (G is the normalized temperature $G = \frac{T - T_u}{T_b - T_u}$)

5.2.3 Comment on the Distinct Stretch Components

Note that the results in Fig. 5.10 are obtained from a planar, stretched region (approximately 0.3–0.6 cm projected onto the x -axis in Fig. 5.8), where the flame front exhibits negligible curvature.

Here, we recall the formulation used to evaluate the stretch rate:

$$K = s_d \nabla \cdot \mathbf{n} + [\nabla \cdot \mathbf{u} - \mathbf{n} \cdot (\mathbf{n} \cdot \nabla) \mathbf{u}] \quad (5.3)$$

($= K_C$)
($= K_S$)

where s_d is the flame displacement speed, $\mathbf{n}$ is the unit normal vector to the flame directed toward the unburned mixture, and $\nabla \cdot \mathbf{n}$ denotes the local flame curvature. In Eq. (5.3), the first term associated with $\nabla \cdot \mathbf{n}$ represents the curvature-induced stretch contribution, K_C , whereas the second term corresponds to the strain-induced stretch contribution, K_S .

Figure 5.12 presents the distribution of these stretch contributions along each iso-temperature contour ($T = 1200$ K). The strain-induced stretch, K_S , dominates the total stretch rate in the considered region. In contrast, the stretch distribution of the cylindrical outwardly propagating flame is illustrated in Fig. 5.13, where both K_C and K_S contribute to the total stretch. As is shown in Fig. 5.13, inside the flame K_S decreases gradually toward to the burned side and the K_C acts oppositely. Their summation becomes K which values is exactly the analytical one $K = \frac{1}{R_f} \frac{dR_f}{dt}$.

Consequently, the results in Fig. 5.10 primarily reflect the influence of flow-induced straining. This supports the validity of the LTF-S model, which uses a single Markstein length from the outwardly propagating cylindrical flame to represent the combined effects of strain and curvature through a unified total stretch description.

Chapter 6

Conclusion and Future Work

6.1 Conclusion

This study proposed the LTF-S model, a novel thickened flame model designed to accurately predict stretched (and unstretched) flame propagation under flame thickening. The LTF-S model differs significantly from existing TF-based models which rely on the Lewis number correction [46–49]. The unresolved scale terms in the spatially filtered governing equations were constructed to determine the speed of unstretched and stretched flames under flame thickening, without incorporating the Lewis number correction. As a result, most of the primary non-dimensional numbers in the problem, including the Lewis number, are retained in the LTF-S model. The model utilized a linear relationship between stretched burning velocity and stretch rate with the Markstein length as the proportionality constant to construct the unresolved scale terms associated with stretching effects. The Markstein length ratio introduced in the model was found to have a linear relationship with the flame thickness ratio and the flame thickening factor. The Markstein length ratio played a crucial role in accurately predicting the flame response to stretching effects, and its estimation process was outlined. The model was validated through simulations of cylindrically propagating flame and flame-vortex interaction problems. The results of the cylindrically propagating flame problem indicated that the LTF-S model accurately predicted stretched burning velocities, even with a coarser grid resolution compared to DNS solutions. The derived Markstein length ratio was verified under various equivalence ratio conditions, including those for $Le < 1$ and $Le > 1$. Additionally, the results of the flame-vortex interaction problem demonstrated that the LTF-S model effectively captured the flame propagation behavior induced by the incoming vortex, showing its ability to accurately represent both the curvature effect and the strain effect, even on a coarse grid resolution.

The LTF-S model was further validated using the hydrocarbon fuels methane and propane. The previously proposed linear correlation between the Markstein length ratio and the flame thickening factor is confirmed for these cases, and the existence of a proportionality coefficient is demonstrated for both fuels. Although the value of this coefficient varies among different fuels, it typically lies within the range 0.4–0.6. A sensitivity analysis of the prediction error with respect to this coefficient indicates that adopting a universal value of $A = 0.5$ is appropriate for the prediction of premixed flames of hydrogen, methane, and propane.

Since the key flame characteristics—laminar burning velocity and Markstein length—can be readily obtained (for example, from one-dimensional flame simulations), the identification of a universal proportionality coefficient of $A = 0.5$ renders the LTF-S model a highly flexible and user-friendly tool for combustion simulations.

Finally, the LTF-S model is applied to a practical combustion device: a perforated-plate burner. This configuration enables for the isolated investigation of purely strain-induced flame stretch effects and the spatial variation of the local burning velocity. In this steady combustion configuration, although both the LTF and LTF-S models could predict the global consumption rate, the LTF-S model reproduced the local stretched flame speed and achieved the identical flame shape with DNS. This application indicates that the Markstein length for total stretch (under weakly stretch condition), used in the LTF-S model, could encompass both curvature-induced and strain-induced stretch effects.

6.2 Future Work

Several concerns have already been raised regarding the TF-based approach:

1. *Nonlinear Response* (between burning velocity and stretch rate): The LTF-S model proposed in this study was formulated to predict burning velocities under weakly stretched conditions, assuming a linear dependence between the stretched burning velocity and the stretch rate. Consequently, model validation was restricted to operating conditions characterized by relatively low stretch rates. Future work will aim to extend the LTF-S framework to regimes of strong stretch by adopting and generalizing the formulations employed in several existing TF-based models [48], [88].
2. *Flame Instabilities*: Analogous to the Markstein length, the characteristic size of the instability cells also represents a relevant length scale. For the thickened flame, the initial disturbances are attenuated, thereby suppressing the development of flame instabilities. In this study, the unstable branch during flame propagation is neglected, particularly for lean premixed hydrogen flames. Additional modeling efforts are required to improve the prediction of these instabilities.
3. *Turbulent Combustion Field*: The LTF-S model exhibits superior predictive accuracy for flame–vortex interaction problems, which constitute a fundamental process in turbulent combustion. However, the present work employs a relatively fine computational grid and accounts only for the resolved turbulent scales. Increasing the flame thickness effectively acts as a low-pass filter, rendering small-scale vortices inactive, even though they would interact with the physical flame in reality. The incorporation of unresolved turbulent components, and thus the extension of the model to fully turbulent flames, will be a major focus of our future research.

Appendix A

Physical Understanding on Stretched Thickened Flame

This analysis examined why the artificially thickened flame becomes more sensitive to stretch from a physical perspective. For a stretched flame, the action of stretch reveals the imbalance between the heat released in the reaction zone and the chemical energy supplied by the fresh mixture (the non-equidiffusion effect including the Lewis number effect and the preferential diffusion). When the flame thickness is increased, this imbalance is amplified, resulting in a stronger sensitivity of the flame response to stretch. (This is the conclusion of this analysis)

A.1 1D Unstretched Flame

Here we recall the one-dimensional temperature equation (Eq. (3.4)) and the progress variable equation (Eq. (3.5)). By integrating these equations throughout the flame region from $-\infty$ to ∞ , we obtain

$$\left(\rho u C_p T - \kappa \frac{dT}{dx} \right)_{-\infty}^{\infty} = -Q \int_{-\infty}^{\infty} \dot{\omega}_c dx, \quad (\text{A.1})$$

$$\rho u C_p (T_b^0 - T_u) = -Q \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx, \quad (\text{A.2})$$

and

$$\left(\rho u Y_c - \rho D_c \frac{Y_c}{dx} \right)_{-\infty}^{\infty} = \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx, \quad (\text{A.3})$$

$$\rho u (0 - Y_{c,u}) = \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx, \quad (\text{A.4})$$

where we assume the Y_c is the deficient species in the reactant mixture, and it is fully consumed by the combustion reaction. For this unstretched flame, $\rho u = \rho_u s_u^0 = \text{Const.}$ Multiply Q with

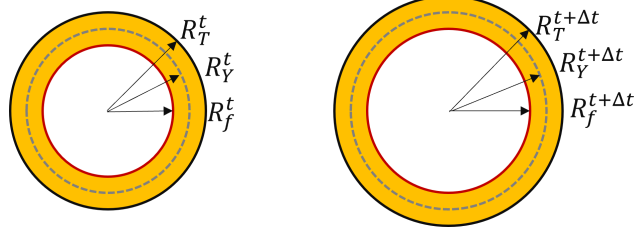


Figure A.1: Conceptual description of the flame response to stretch in the presence of the non-equiffusion effect for a two-dimensional outwardly propagating flame.

Eq. (3.5) and add to Eq. (A.2), we acquire

$$\rho u C_p (T_b^0 - T_u) = \rho u Q Y_{c,u}, \quad (\text{A.5})$$

$$C_p (T_b^0 - T_u) = Q Y_{c,u}. \quad (\text{A.6})$$

This equation indicates that the chemical energy supplied by the fresh mixture is fully reacted to generate heat, increasing the flame temperature (sensible enthalpy). This balance holds for non-unit Lewis number occasions as well.

To integrate Eq. (3.5) through the pre-heat zone, we can approximate the thickness of the deficient chemical species, similar to the derivation of Eq. (3.11).

$$\delta_Y = \frac{D_c}{u}. \quad (\text{A.7})$$

Thus, the Le number could be expressed as,

$$Le = \frac{\alpha/u}{D_c/u} = \frac{\delta_L}{\delta_Y} = \frac{\delta_T}{\delta_Y}. \quad (\text{A.8})$$

A.2 2D Cylindrical Outwardly Propagating Flame

In this unsteady flame configuration, we assume the flame at certain time t located at R_f propagates δR through Δt , as illustrated in Fig. A.1. Therefore, the chemical energy supplied by the fresh mixture is proportional to the area of an annulus,

$$\begin{aligned} \Delta A_Y &= \Delta A_Y^{t+\Delta t} - \Delta A_Y^t \\ &= \pi(R_Y + \delta R)^2 - \pi R_Y^2 \\ &= \pi(R_Y \delta R + (\delta R)^2) \\ &\approx \pi R_Y \delta R \\ &= \pi(R_f + \delta_Y) \delta R \end{aligned} \quad (\text{A.9})$$

The chemical energy supplied by ΔA_Y will increase the temperature of the gas occupied by ΔA_T ,

$$\begin{aligned}
\Delta A_T &= \Delta A_T^{t+\Delta t} - \Delta A_T^t \\
&= \pi(R_T + \delta R)^2 - \pi R_T^2 \\
&= \pi(R_T \delta R + (\delta R)^2) \\
&\approx \pi R_T \delta R \\
&= \pi(R_f + \delta_T) \delta R
\end{aligned} \tag{A.10}$$

where $R_T = R_f + \delta_T$ and $R_Y = R_f + \delta_Y$. In the same fashion with Eq. (A.6), the chemical energy supplied by the fresh mixture with area ΔA_Y increases the temperature of the gas from T_u to T_b .

$$C_p(T_b - T_u)\Delta A_T = QY_c\Delta A_Y. \tag{A.11}$$

Note that for a flame under stretch, T_b may not equal T_b^0 . For an ideal 1D non-stretched planar flame, QY_c could raise the flame temperature to the adiabatic flame temperature (Eq. (A.6)). Thus, the above equation could be written as follows,

$$C_p(T_b - T_u)\Delta A_T = C_p(T_b^0 - T_u)\Delta A_Y, \tag{A.12}$$

$$\tag{A.13}$$

$$\frac{T_b - T_u}{T_b^0 - T_u} = \frac{\Delta A_Y}{\Delta A_T} = \frac{R_f + \delta_Y}{R_f + \delta_T}. \tag{A.14}$$

Subtract 1 from both sides of the equation to obtain the correlation between stretch and flame temperature:

$$T_b - T_b^0 = \frac{T_b^0 - T_u}{R_f + \delta_T} (\delta_Y - \delta_T), \tag{A.15}$$

$$T_b^0 - T_b = \frac{T_b^0 - T_u}{R_T} \left(1 - \frac{1}{Le}\right) \delta_T. \tag{A.16}$$

For $Le > 1$ (or $Le < 1$), the heat loss is over (or less) than the chemical energy gain, resulting in a lower (or higher) flame temperature and burning intensity.

Under the same curvature $1/R_T$, when the flame thickness increases from δ_T to $F\delta_T$, the imbalance is increased by a factor of F because the flame property $(1 - 1/Le)(T_b^0 - T_u)$ stays constant. Consequently, the flame becomes more sensitive to stretch rate.

A.3 Quasi-one-dimensional Stagnation Flame

Here, we focus on a steady stagnation flame illustrated in Fig. A.2. To characterize this typically strained flame, we re-write the Eq. (3.4) and (3.5) into a quasi-one-dimensional form, with a continuity equation considering the varying stream tube area $A(x)$.

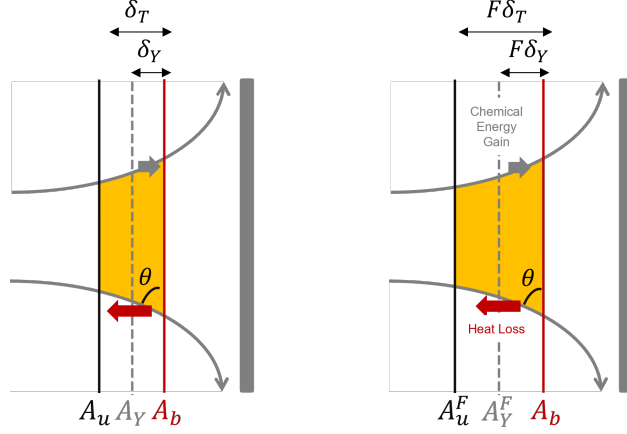


Figure A.2: Conceptual description of the flame response to stretch in the presence of the non-equi-diffusion effect for a quasi one-dimensional stagnation flame.

$$\frac{d(\rho u A)}{dx} = \frac{d\dot{m}}{dx} = 0, \quad (\text{A.17})$$

$$\frac{d}{dx} \left[A \left(\rho u C_p T - \kappa \frac{dT}{dx} \right) \right] = -A Q \dot{\omega}_c, \quad (\text{A.18})$$

$$\frac{d}{dx} \left[A \left(\rho u Y_c - \rho D_c \frac{dY_c}{dx} \right) \right] = A \dot{\omega}_c, \quad (\text{A.19})$$

where the $\dot{m} = \rho u A$ is the mass flow rate and it is conserved in x -direction. Integrating the Eq. (A.18) through the preheat zone,

$$\left[A \left(\rho u C_p T - \kappa \frac{dT}{dx} \right) \right]_{-\infty}^{x_f^-} = 0, \quad (\text{A.20})$$

$$\dot{m} C_p (T_b - T_u) - \kappa \left(\frac{dT}{dx} \right)_{x_f^-} A_u = 0. \quad (\text{A.21})$$

Note that as the convection term diverges in the stream tube and $\dot{m}$ is conserved in the selected control volume, while diffusion process is assumed to be perpendicular to the flame front, thus the heat (or chemical species) diffuses toward (or through) A_u .

By further integrating the Eq. (A.18),

$$\left(-\kappa \frac{dT}{dx} \right)_{x_f^-} = - \int_{x_f^-}^{x_f^+} Q \dot{\omega}_c dx, \quad (\text{A.22})$$

$$\kappa \left(\frac{dT}{dx} \right)_{x_f^-} = -Q \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx. \quad (\text{A.23})$$

$$(\text{A.24})$$

Multiply A_b to the above equation and add it to Eq. (A.21), the following equation could be acquire,

$$\dot{m}C_p(T_b - T_u) + \kappa \left(\frac{dT}{dx} \right)_{x_f^-} (A_b - A_u) = -A_b Q \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx. \quad (\text{A.25})$$

Note that for a one-dimensional, non-stretched flame, where $A_b = A_u$, the above expression reduces to Eq. (A.2). The diffusion term $\kappa \left(\frac{dT}{dx} \right)_{x_f^-} (A_b - A_u)$ represents the heat loss from the control volume through the diverging streamtube surface. An similar form for the equation of the chemical species (A.19) could be acquire as follows,

$$-\dot{m}Y_c + \rho D_c \left(\frac{dY_c}{dx} \right)_{x_f^-} (A_b - A_Y) = A_b \int_{x_f^-}^{x_f^+} \dot{\omega}_c dx, \quad (\text{A.26})$$

where A_Y is the area where the chemical species start to diffuse to the reaction sheet. The diffusion term here $\rho D_c \left(\frac{dY_c}{dx} \right)_{x_f^-} (A_b - A_Y)$ represents the gain of the deficient chemical species through the diverging streamtube surface. Multiply Q to Eq. (A.26) and add it to Eq. (A.25), we can acquire the following equation.

$$\dot{m} [C_p(T_b - T_u) - QY_c] + \kappa \left(\frac{dT}{dx} \right)_{x_f^-} (A_b - A_u) + \rho D_c Q \left(\frac{dY_c}{dx} \right)_{x_f^-} (A_b - A_Y) = 0. \quad (\text{A.27})$$

By substitute $QY_c = C_p(T_b^0 - T_u)$ (the Eq. (A.6)) and replacing the $\left(\frac{dT}{dx} \right)_{x_f^-}$ and $\left(\frac{dY_c}{dx} \right)_{x_f^-}$ by

$$\left(\frac{dT}{dx} \right)_{x_f^-} \approx \frac{T_b - T_u}{\delta_T}, \quad (\text{A.28})$$

$$\left(\frac{dY_c}{dx} \right)_{x_f^-} \approx -\frac{Y_{c,u}}{\delta_Y}, \quad (\text{A.29})$$

Eq. (A.27) could be written as,

$$\dot{m}C_p(T_b - T_b^0) + \kappa \frac{T_b - T_u}{\delta_T} (A_b - A_u) - \rho D_c C_p \frac{T_b^0 - T_u}{\delta_Y} (A_b - A_Y) = 0. \quad (\text{A.30})$$

This equation indicates that the combined effects of heat loss and the increase in chemical energy, induced by additional diffusion in the diverging stream, can lead to a flame temperature that becomes either super-adiabatic or sub-adiabatic under non-unity Le conditions. Here, we consider the chosen two-dimensional streamtube as a trapezoid bounded by A_u , A_b , and the diverging surface. Under this assumption, the following geometric relation can be obtained,

$$\frac{A_b - A_u}{\delta_T} = \frac{A_b - A_Y}{\delta_Y} = \frac{2}{\tan \theta}. \quad (\text{A.31})$$

Consequently, the preceding equation can be further rewritten as,

$$\dot{m}C_p (T_b - T_b^0) = - [\kappa(T_b - T_u) - \rho D_c C_p (T_b^0 - T_u)] \frac{A_b - A_u}{\delta_T}, \quad (\text{A.32})$$

$$\dot{m}C_p (T_b - T_b^0) = - \left[\kappa(T_b - T_u) - \frac{\kappa}{Le} (T_b^0 - T_u) \right] \frac{A_b - A_u}{\delta_T}, \quad (\text{A.33})$$

$$\dot{m}C_p (T_b - T_b^0) \approx -(T_b^0 - T_u) \left(1 - \frac{1}{Le} \right) \frac{A_b - A_u}{\delta_T} \kappa, \quad (\text{A.34})$$

$$\dot{m}C_p (T_b^0 - T_b) \approx (T_b^0 - T_u) \left(1 - \frac{1}{Le} \right) \frac{A_b - A_u}{\delta_T} \kappa. \quad (\text{A.35})$$

For a positive stretch (or strain) rate, $A_b - A_u > 0$, and for $Le > 1$, the term $1 - 1/Le$ in the above equation becomes positive. This indicates that the heat loss exceeds the chemical energy release, resulting in $T_b < T_b^0$.

When the flame thickness increases from δ_T to $F\delta_T$ by raising κ to $F\kappa$, and we assume that the flame experiences the same stretch (strain) rate, we have

$$\frac{A_b^F - A_u^F}{F\delta_T} \approx \frac{A_b - A_u}{\delta_T}. \quad (\text{A.36})$$

In analogy with the discussion in the previous section on the two-dimensional, outwardly propagating flame, the characteristic quantity $(1 - 1/Le)(T_b^0 - T_u)$ remains unchanged by the thickening of the flame. However, the $F\kappa$ term amplifies the imbalance by a factor of F , making the flame explicitly more sensitive to stretch.

The previous analysis basing on two canonical flame configurations collectively demonstrates that the Lewis number governs how the flame responds to stretch. For the constant TF model, which preserves the Lewis number, the flame thickening effect amplifies the stretch effect by a factor of F . This, in turn, is consistent with the results shown in 3.5, where the Markstein length ratio $\mathcal{L}_{u,\text{TF}}/\mathcal{L}_{u,\text{DNS}}$ is directly proportional to the flame-thickening factor $\delta_{\text{TF}}/\delta_{\text{DNS}}$.

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