

FACULDADE DE ENGENHARIA DA UNIVERSIDADE DO PORTO

Numerical Studies for the design of a Micro-Propulsion System: The effect of Material Properties

David Mendonça Dias

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Dissertation submitted in Fulfilment of the Requirements for:

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(Specialization in Energy & Fluids)

Supervisor: Professor Alexandre Miguel Prior Afonso (PhD)

Second Supervisor: Professor Pedro Miguel Rebelo Resende (PhD)

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Abstract

Numerical Studies for the design of a Micro-Propulsion System: The effect of Material Properties

Keywords: numerical study, microcombustion, micropropulsion, heat loss, laminar flow dynamics, pulsatory flame burst, stable flame, fabrication materials, hydrogen, complex geometry, wavy microchannel, MEMS

The increasing demand on combustion based micro-power generation systems, mainly due to the high energy density of hydrocarbon fuels, created a great opportunity to develop portable power devices, which can be applied on micro unmanned aerial vehicles, micro-satellite thrusters, or micro chemical reactors and sensors. Also, the need for better and cheaper communications networks and control systems has led space companies to invest in micro and meso satellites, such as CubeSat. This master's thesis will study numerically micro-combustion to design micro-propulsion, which can be applied on micro unmanned aerial vehicles or CubeSat.

For these numerical studies, the open source code OpenFOAM (Open Field Operation and Manipulation) was chosen because it is an open source package that is widely accepted by the computational fluid dynamics community, both in academia and industry. In this thesis, we will use a numerical framework for the numerical modeling of laminar flows with homogeneous reactions, *CHTlaminarSMOKE*, that allows for the solution of Navier-Stokes equations for complex and general geometries. This code uses very detailed kinetics to model the reactions, and will be used to estimate the detailed propulsion effects in the micro-chamber geometries.

In this master's thesis, we conduct a numerical study of flame dynamics in complex geometries, exploring the impact of various materials commonly used in aerospace applications on propulsion. By adjusting input parameters and observing operational conditions, we aim to understand how different materials affect the design and performance of novel propulsion systems. We examine five material groups, including adiabatic materials, ceramics (LTCC and HTCC), metals (two stainless steels), amorphous materials (two high-temperature glasses), and high thermal conductivity materials (silicon, aluminum, and copper-tungsten alloys).

In the conclusion of our simulations, we have identified three primary dynamics: stable flames, pulsatory flame burst (PFB), and extinction. In the context of PFB, it is notable that an increase in inlet velocity leads to a decrease in the heat release rate carried through vortices, causing a delay in ignition. This delay is reflected in a decrease in pulsatory burst frequency and an increase in the maximum heat release rate. Additionally, when heat conduction within the walls is introduced, higher material conductivity results in a more pronounced heat flux due to conduction in the solid, exacerbating the retrograde flow of energy and leading to increased PFB frequencies. Furthermore, owing to their enhanced heat dissipation properties, these materials exhibited lower temperature values in both the fluid and solid phases, along with reduced temperature gradients along the walls of the microchannel.

Furthermore, our research uncovered novel dynamics during the transient evolution of the system, including transitional and migrating PFB, Backward Ignition Resurgence, and Stable to Flashback. The latter discovery prompted us to reconsider the microchannel's geometry to prevent this undesirable dynamic in future research.

Regarding the propulsion performance of the microchannel, our observations indicate that both velocity and equivalence ratio are pivotal factors in enhancing specific impulse values. Notably, materials with greater thermal dissipation exhibited a reduction in specific impulse values, particularly noticeable in the maximum values, which has adverse implications for overall efficiency and performance.

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Resumo

Estudos Numéricos para o Design de um Sistema de Micropropulsão: O Efeito das Propriedades dos Materiais

Palavras-chave: estudo numérico, microcombustão, micropropulsão, perda de calor, fluxo laminar, chama estável, explosão de chama pulsatória, materiais de fabricação, hidrogênio, geometria complexa, microcanal ondulado, MEMS

A crescente procura por sistemas de microgeração de energia baseados na combustão, principalmente devido à elevada densidade energética dos combustíveis de hidrocarbonetos, criou uma grande oportunidade para o desenvolvimento de dispositivos de energia portáteis, que podem ser aplicados em micro veículos aéreos não tripulados, propulsores de microsátélites ou reatores químicos e sensores microscópicos. Além disso, a necessidade de redes de comunicação e sistemas de controle melhores e mais baratos levou as empresas espaciais a investirem em micro e meso satélites, como o CubeSat. Este trabalho estudará numericamente a microcombustão para projetar micropropulsores, que podem ser aplicados em micro veículos aéreos não tripulados ou CubeSats.

Para esses estudos numéricos, o código aberto OpenFOAM (Open Field Operation and Manipulation) foi escolhido porque é um pacote de código aberto amplamente aceito pela comunidade de dinâmica de fluidos computacional, tanto na academia quanto na indústria. Nesta tese, utilizaremos um quadro numérico para a modelagem numérica de fluxos laminares com reações homogêneas, *CHTlaminarSMOKE*, que permite a solução das equações de Navier-Stokes para geometrias complexas e gerais. Este código utiliza cinética muito detalhada para modelar as reações e será usado para estimar os efeitos detalhados de propulsão nas geometrias de microcâmaras.

Nesta tese de mestrado, realizamos um estudo numérico da dinâmica das chamas em geometrias complexas, explorando o impacto de diversos materiais comumente usados em aplicações aeroespaciais na propulsão. Ajustando parâmetros de entrada e observando condições operacionais, pretendemos compreender como diferentes materiais afetam o design e o desempenho de sistemas de propulsão inovadores. Examinamos cinco grupos de materiais, incluindo materiais adiabáticos, cerâmicos (LTCC e HTCC), metais (dois aços inoxidáveis), materiais amorfos (dois vidros de alta temperatura) e materiais de alta condutividade térmica (silício, alumínio e ligas de cobre-tungstênio).

Nos instantes finais das nossas simulações, identificamos três dinâmicas principais: chamas estáveis, explosões de chama pulsatória (PFB), e extinção. No contexto das PFB, é notável que um aumento na velocidade de entrada conduz a uma diminuição na taxa de libertação de calor transportada através de vórtices, causando um atraso na ignição. Este atraso reflete-se numa redução na frequência das explosões pulsatórias e num aumento na taxa máxima de libertação de calor. Além disso, quando é introduzida a condução de calor nas paredes, uma maior condutividade do material resulta num fluxo de calor mais pronunciado devido à condução no sólido, exacerbando o retrocesso do fluxo de energia e levando a um aumento das frequências das PFB. Além disso, devido às suas propriedades aprimoradas de dissipação de calor, esses materiais apresentaram valores de temperatura mais baixos tanto na fase líquida como sólida, juntamente com gradientes de temperatura reduzidos ao longo das paredes do microcanal.

Além disso, nesta dissertação descobrimos novas dinâmicas durante a evolução transitória do sistema, incluindo PFB de transição e migração, Ressurgimento de Ignição Reversa e Regime Estável para Flashback. Esta última descoberta levou-nos a reconsiderar a geometria do microcanal para prevenir esta dinâmica indesejável em futuras pesquisas.

No que diz respeito ao desempenho de propulsão do microcanal, as nossas observações indicam que tanto a velocidade como a razão de equivalência são fatores cruciais para aumentar os valores de impulso específico. Notavelmente, os materiais com maior dissipação térmica apresentaram uma redução nos valores de impulso específico, especialmente nos valores máximos, o que tem implicações adversas para a eficiência e o desempenho globais.

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Résumé

Études Numériques pour la Conception d'un Système de Micropropulsion : L'effet des Propriétés des Matériaux

Mots-clés: étude numérique, microcombustion, micropropulsion, perte de chaleur, écoulement laminaire, éclatement pulsatoire de flamme, flamme stable, matériaux de fabrication, hydrogène, géométrie complexe, microcanal ondulé

L'augmentation de la demande en systèmes de microgénération d'énergie basés sur la combustion, principalement en raison de la haute densité énergétique des carburants hydrocarbonés, a créé une excellente opportunité pour développer des dispositifs d'alimentation portables, pouvant être appliqués sur des micro-drones, des propulseurs de microsattelites, ou des réacteurs chimiques et des capteurs microscopiques. De plus, le besoin de réseaux de communication et de systèmes de contrôle meilleurs et moins chers a incité les entreprises spatiales à investir dans des microsattelites et des nanosattelites, tels que le CubeSat. Cette thèse de master étudiera numériquement la microcombustion afin de concevoir une micropropulsion, qui pourra être appliquée sur des micro-drones ou des CubeSats.

Pour ces études numériques, le code source ouvert OpenFOAM (Open Field Operation and Manipulation) a été choisi car il s'agit d'un package open source largement accepté par la communauté de la dynamique des fluides numérique, tant dans le milieu académique que dans l'industrie. Dans cette thèse, nous utiliserons un cadre numérique pour la modélisation numérique des écoulements laminaires avec des réactions homogènes, appelé *CHTlaminarSMOKE*, qui permet la résolution des équations de Navier-Stokes pour des géométries complexes et générales. Ce code utilise une cinétique très détaillée pour modéliser les réactions et sera utilisé pour estimer les effets détaillés de la propulsion dans les géométries de microchambre.

Dans cette thèse de master, nous menons une étude numérique de la dynamique des flammes dans des géométries complexes, explorant l'impact de divers matériaux couramment utilisés dans les applications aérospatiales sur la propulsion. En ajustant les paramètres d'entrée et en observant les conditions opérationnelles, nous visons à comprendre comment différents matériaux affectent la conception et les performances de systèmes de propulsion novateurs. Nous examinons cinq groupes de matériaux, notamment les matériaux adiabatiques, les céramiques (LTCC et HTCC), les métaux (deux aciers inoxydables), les matériaux amorphes (deux verres haute température) et les matériaux à haute conductivité thermique (silicium, aluminium, et alliages de cuivre-tungstène).

Dans la conclusion de nos simulations, nous avons identifié trois dynamiques principales : des flammes stables, des explosions de flammes pulsées (PFB) et l'extinction. Dans le contexte des PFB, il est remarquable qu'une augmentation de la vitesse d'entrée entraîne une diminution du débit de chaleur transporté par des tourbillons, provoquant un retard à l'allumage. Ce retard se traduit par une réduction de la fréquence des explosions pulsées et une augmentation du débit de chaleur maximal. De plus, lorsque la conduction de chaleur à travers les parois est introduite, une conductivité thermique plus élevée du matériau entraîne un flux de chaleur plus prononcé par conduction dans le solide, exacerbant le reflux d'énergie et conduisant à une augmentation des fréquences de PFB. De plus, en raison de leurs propriétés améliorées de dissipation de chaleur, ces matériaux présentaient des températures plus basses à la fois dans la phase liquide et solide, ainsi que des gradients de température réduits le long des parois du micro-canal.

De plus, nos recherches ont révélé de nouvelles dynamiques lors de l'évolution transitoire du système, notamment des PFB de transition et de migration, une résurgence d'allumage inverse et une stabilité jusqu'à un flashback. Cette dernière découverte nous a amenés à reconsidérer la géométrie du micro-canal pour prévenir cette dynamique indésirable dans les futures recherches.

En ce qui concerne les performances de propulsion du micro-canal, nos observations indiquent que la vitesse et le rapport d'équivalence sont des facteurs essentiels pour améliorer les valeurs de l'impulsion spécifique. Notamment, les matériaux présentant une meilleure dissipation thermique ont montré une réduction des valeurs de l'impulsion spécifique, en particulier des valeurs maximales, ce qui a des implications défavorables pour l'efficacité globale et les performances.

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Zusammenfassung

Numerische Studien für die Gestaltung eines Mikroantriebssystems: Die Auswirkung von Materialeigenschaften

Schlüsselwörter: numerische Studie, Mikroverbrennung, Mikroantrieb, Wärmeverlust, pulsativer Flammenstoß, stabile Flamme, Herstellungsmaterialien, Wasserstoff, komplexe Geometrie, wellenförmiger Mikrokanal, laminare Strömung

Die steigende Nachfrage nach Verbrennungsbasierten Mikroenergieerzeugungssystemen, hauptsächlich aufgrund der hohen Energiedichte von Kohlenwasserstoffbrennstoffen, hat eine großartige Gelegenheit zur Entwicklung tragbarer Stromgeräte geschaffen, die auf Mikrodrohnen, Mikrosatellitenantrieben oder Mikrochemiereaktoren und Sensoren angewendet werden können. Auch der Bedarf an besseren und kostengünstigeren Kommunikationsnetzen und Steuersystemen hat Raumfahrtunternehmen dazu veranlasst, in Mikro- und Mesosatelliten wie CubeSat zu investieren. Diese Masterarbeit wird die Mikroverbrennung numerisch untersuchen, um Mikroantriebe zu entwerfen, die auf Mikrodrohnen oder CubeSat angewendet werden können.

Für diese numerischen Studien wurde der Open-Source-Code OpenFOAM (Open Field Operation and Manipulation) ausgewählt, da er ein Open-Source-Paket ist, das von der Gemeinschaft der Computational-Fluid-Dynamics sowohl in der Akademie als auch in der Industrie weitgehend akzeptiert wird. In dieser Arbeit verwenden wir einen numerischen Rahmen zur numerischen Modellierung laminarer Strömungen mit homogenen Reaktionen, *CHTlaminarSMOKE*, der die Lösung der Navier-Stokes-Gleichungen für komplexe und allgemeine Geometrien ermöglicht. Dieser Code verwendet sehr detaillierte Kinetik zur Modellierung der Reaktionen und wird verwendet, um die detaillierten Propulsionseffekte in den Mikrokanalgeometrien abzuschätzen.

In dieser Masterarbeit führen wir eine numerische Studie zur Flammendynamik in komplexen Geometrien durch und erforschen die Auswirkungen verschiedener Materialien, die in der Luft- und Raumfahrtindustrie häufig verwendet werden, auf die Propulsion. Durch Anpassung der Eingabeparameter und Beobachtung der Betriebsbedingungen möchten wir verstehen, wie verschiedene Materialien das Design und die Leistung neuartiger Antriebssysteme beeinflussen. Wir untersuchen fünf Materialgruppen, darunter adiabatische Materialien, Keramiken (LTCC und HTCC), Metalle (zwei Edelmetalle), amorphe Materialien (zwei Hochtemperaturgläser) und Materialien mit hoher thermischer Leitfähigkeit (Silizium, Aluminium und Kupfer-Wolfram-Legierungen).

Im Abschluss unserer Simulationen haben wir drei Hauptdynamiken identifiziert: stabile Flammen, pulsierende Flammenausbrüche (PFB) und Auslöschung. Im Kontext von PFB ist bemerkenswert, dass eine Erhöhung der Einlassgeschwindigkeit zu einer Verringerung der durch Wirbel getragenen Wärmeabgaberate führt, was zu einer Verzögerung der Zündung führt. Diese Verzögerung spiegelt sich in einer Verringerung der Pulsationsfrequenz und einer Erhöhung der maximalen Wärmeabgaberate wider. Darüber hinaus führt die Einführung der Wärmeleitung in den Wänden bei höherer Materialleitfähigkeit zu einem ausgeprägteren Wärmefluss durch Leitung im Feststoff, was den Rückfluss von Energie verschlimmert und zu erhöhten PFB-Frequenzen führt. Zusätzlich wiesen diese Materialien aufgrund ihrer verbesserten Wärmeabfuhr-Eigenschaften niedrigere Temperaturen in der Flüssig- und Feststoffphase auf, zusammen mit reduzierten Temperaturgradienten entlang der Wände des Mikrokanals.

Des Weiteren haben unsere Forschungen während der transienten Entwicklung des Systems neue Dynamiken aufgedeckt, darunter Übergangs- und wandernde PFB, Rückwärtszündwiederkehr und Stabil-zu-Flashback. Diese letzte Entdeckung veranlasste uns, die Geometrie des Mikrokanals neu zu überdenken, um diese unerwünschte Dynamik in zukünftigen Forschungen zu verhindern.

Hinsichtlich der Antriebsleistung des Mikrokanals deuten unsere Beobachtungen darauf hin, dass sowohl Geschwindigkeit als auch Äquivalenzverhältnis entscheidende Faktoren zur Steigerung des spezifischen Impulses sind. Bemerkenswerterweise zeigten Materialien mit höherer thermischer Ableitung eine Verringerung der spezifischen Impulswerte, insbesondere bei den maximalen Werten, was nachteilige Auswirkungen auf die Gesamteffizienz und Leistung hat.

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Dedico esta dissertação aos meus maravilhosos **avôs** e **avós**.

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“A amizade é o maior sentimento que não morre.”

Florbela Espanca

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[Sunday regards a picture of Carl's late father]

[Billy Sunday]: “*What the hell did he (your father)
ever say to make you try so hard?*”

[Carl Brashear]: “*Be the best.*”

[Billy Sunday]: “*Well, you are.*”

Dialogue in the movie “*Men of Honor*”

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Contents

Abstract	i
Resumo	iii
Résumé	v
Zusammenfassung	vii
Agradecimentos / Acknowledgments	xi

I *Initia Nova* **1**

1 Introduction	3
1.1 Framework and Motivation	3
1.2 Computational Framework	5
1.3 Objectives	6
1.4 Dissertation outline	6

II *Fundamenta Theorica* **9**

2 Literature Review	11
2.1 A Review on Combustion	11
2.1.1 Introduction	11
2.1.2 Combustion in stoichiometric conditions	11
2.1.3 Air-fuel ratio and equivalence ratio	12
2.1.4 Mass and molar fractions	13
2.1.5 Autoignition temperatures and flammability limits	14
2.1.6 First law of thermodynamics	15
2.1.7 Absolute enthalpies and enthalpy of formation	16
2.1.8 Enthalpy of combustion and heating values	17
2.1.9 Adiabatic flame temperature	17
2.1.10 Flame burning speed	19
2.2 A Review on Heat Transfer	19
2.2.1 Understanding heat transfer in combustion	19
2.2.2 Delving into Conduction	20
2.2.3 Delving into Convection	22
2.2.4 Delving into Radiation	22

2.3	A Review on Microcombustion	23
2.3.1	Definition of micro-scale Combustion	24
2.3.2	Challenges on microcombustion	24
2.3.2.1	Short resistance time	25
2.3.2.2	High heat loss ratio	25
2.3.2.3	Weak flame stability	26
2.3.3	Typical length and time scales and phenomena	26
2.3.4	Flammability limits in micro-combustion and quenching diameter	27
2.3.5	Classification of flame types	29
2.3.6	Classification of micro-flame behaviours	30
2.3.6.1	Flashback and blow-off	30
2.3.6.2	Steady <i>versus</i> non-steady flames	30
2.3.6.3	Mild combustion	31
2.3.6.4	Stable flames	32
2.3.6.5	FREI: Flames with repetitive extinction and ignition	33
2.3.6.6	PFB: pulsatory flame burst	35
2.3.7	Investigations in microcombustion	37
2.3.7.1	Investigations in wavy wall geometries	40
2.4	A Review on Micropropulsion	41
2.4.1	Overview on micropropulsion systems	41
2.4.2	Micropropulsion systems performance	42
2.4.2.1	Thrust and specific impulse	42
2.4.2.2	Thrust key indicators	43
2.4.3	Conventionally manufactured micropropulsion systems	44
2.4.3.1	Pulsed plasma thruster	44
2.4.3.2	Field emission electric propulsion	45
2.4.3.3	Other relevant micropropulsion system technologies	45
2.4.4	Micro-Electro-Mechanical Systems	47
2.4.4.1	MEMS Manufacturing	47
3	Governing Equations and Numerical Modelling	49
3.1	Computational Fluid Dynamics	50
3.1.1	Perspective	50
3.1.2	Main concept	50
3.2	Governing Equations	52
3.2.1	Gas phase equations	52
3.2.2	Gas-solid phases equations	53
3.3	Numerical Model	54
3.3.1	Gas phase computational approach and modeling	54
3.3.2	Gas-solid phases computational approach	56
3.3.3	Gas-solid phases numerical modeling	58
3.4	Kinetic mechanism	59
3.5	Additional Remarks	59
4	Software Framework and Methodology	61
4.1	Introduction	61
4.2	Structure	62
4.2.1	File Structure for CHT	63
4.3	Pre-Processing	65

4.3.1	Mesh Generation	65
4.3.1.1	<i>blockMesh</i>	65
4.3.1.2	<i>snappyHexMesh</i>	66
4.3.2	Boundary Conditions	67
4.3.3	Discretisation and solution of equations	69
4.3.4	Simulation control	69
4.3.5	Flame ignition	69
4.4	Simulation	70
4.5	Post-Processing	71
4.5.1	ParaView Overview	71
4.6	Computational Resources	72
4.7	Model Configuration	73
4.7.1	Used Meshes	73

III *Investigatio de Materia* 75

5	Characterizing the Thermal Behavior of Different Materials using a Spark	77
5.1	Case Introduction	77
5.2	Simulation settings	80
5.3	Dynamics of adiabatic materials	81
5.3.1	Stability map	81
5.3.2	Flame behaviour in adiabatic materials	81
5.3.2.1	Stable flame dynamics	82
5.3.2.2	Pulsatory flame burst dynamics	88
5.4	Dynamics of amorphous materials	100
5.4.1	Stability map	101
5.4.2	Stable flame and transitional Pulsatory Flame Burst (tPFB) dynamics	101
5.4.3	Stable to Flashback Dynamics	108
5.4.4	Pulsatory flame burst dynamics	110
5.4.5	Migrating Pulsatory Flame Burst (mPFB)	118
5.4.6	Overview of Fused Silica	121
5.5	Dynamics of ceramics materials	125
5.5.1	Stability map for ceramic materials	125
5.5.2	Blow-off due to heat loss to the wall	128
5.5.3	Overview of ceramics materials	131
5.6	Dynamics of steels materials	135
5.6.1	Stability map for steels materials	136
5.6.2	Backward Ignition Resurgence	138
5.6.3	Overview of steels materials	141
5.7	Dynamics of conductor materials	142
5.7.1	Stability map for thermal conductor materials	143
5.7.2	Exploring the behavior of conductive materials with initial imposed temperature profiles	144
5.8	Materials overview	146
5.9	Micropropulsion performance analysis	149

IV	<i>Conclusio Perpetua</i>	153
6	Summary and Outlook	155
6.1	Key findings	155
6.1.1	Improvements on fundamental dynamics understanding	155
6.1.2	Understanding material impact on the microchannel dynamics	155
6.1.2.1	Novel dynamics discovered	156
6.1.2.2	Comparison between materials	157
6.2	Limitations and weaknesses	158
6.3	Future Research	158
	References	161
V	<i>Appendices</i>	179
A	<i>chtlaminarSMOKE</i> solver files	181
A.1	chtlaminarSMOKE policy file	181
A.2	<i>system Files</i>	185
A.3	<i>constant Files</i>	188
B	Kinetic Mechanism of the Combustion Reaction	191
C	OpenFOAM Standard Boundary Conditions	197
D	Setting up a simulation	201
E	Data analysis programs	203
E.1	Fast Fourier Transform	203
E.2	Cumulative integral	204

List of Figures

1.1	History and forecast of the number of accumulated (a) micro- and (b) nano- and pico- satellites using a logistic growth model [3].	4
1.2	Logotypes of: (a) Creck Modelling Group; (b) OpenSMOKE++ Framework; (c) GridFEUP.	5
2.1	(a) Schematic of fixed-mass system with moving boundary above piston. (b) Control volume with fixed boundaries and steady flow. [15]	16
2.2	Evolution of T_{af} by varying ϕ , for various fuels [31].	18
2.3	Laminar flame speed of H_2 /air at Normal Temperature and Pressure (NTP) as a function of equivalence ratio (a) and normalized equivalence ratio (b), where the symbols denote experimental results [34].	19
2.4	Schematics of [38] (a) Combined convection and radiation conditions; (b) Combined convection, radiation and heat flux.	20
2.5	Differential control volumes [37] (a) $dx dy dz$, for conduction analysis in Cartesian coordinates (x, y, z) . (b) $dr \cdot r d\phi \cdot dz$, for conduction analysis in Cylindrical coordinates (r, ϕ, z)	21
2.6	Two types of convection [38]: (a) Forced convection; (b) Free convection.	22
2.7	(a) The three kinds of radiation flux: emissive power, irradiation, and radiosity [38]; (b) The absorption, reflection, and transmission of incident radiation by a semitransparent material [38].	23
2.8	(a) The dependence of the normalized burning velocity on the normalized radiative heat loss of a one-dimensional planar flame [40]; (b) Burning rate, solid line, and normalized flame propagation speed U_B , dash-dotted line, plotted against the ratio of flame thickness to channel width, d , for selected values of reduced heat transfer coefficient, k , with in a quiescent, two dimensional channel flow [71].	28
2.9	Differences in Premixed and Diffusion flames: (a) Laminar premixed flame. (b) Turbulent premixed flame. (c) Laminar diffusion flame. (d) Turbulent diffusion flame [74].	29
2.10	Flashback and Blow-off for flames with fixed swirl: a) flashback; b) before flashback; c) stable flame; d) after blow-off [77].	30
2.11	Time-spectrum (up) and Power Series (down) for different Non-steady combustion modes in ducted premixed flames: a) Periodic; b) Quasi-periodic; c) Chaotic [79].	31
2.12	Schematic representation of a stable micro-flame [91].	32
2.13	Direct photographs of [86]: (a) stable flame; (b) FREI.	33
2.14	Repetitive extinction-ignition dynamics using hydroxide mass fraction (Y_{OH}) [99].	34
2.15	Streamlines of the flow field and heat release rate distribution for the pulsatory flame burst dynamics with $U_{in} = 6$ [m/s], with 10 ms intervals [113].	36

2.16	Streamlines of the flow field and temperature distribution for the pulsatory flame burst dynamics with $U_{in} = 6$ [m/s], with 10 ms intervals [113].	36
2.17	Example of a Backward-Facing Step Insertion in a Microcombustor, used in Li et al. [125].	38
2.18	Schematics of the microburner used in Yang et al. [129].	38
2.19	Microcombustor with Cavity Schematic [132]: (a) Longitudinal Plane; (b) Transverse Plan.	39
2.20	Flame dynamics diagrams [107]: Effect of U_{in} and ϕ for a channel width of: a) 0.6 mm; b) 0.8 mm.	39
2.21	Classification of micropropulsion concepts (based on [9]): the systems highlighted with (†) are manufactured with conventional methods whereas the ones without made using MEMS and silicon technologies.	41
2.22	Diagram of a MPS showing the variables and their indexes (adapted from [9]). . .	42
2.23	Pulsed Plasma Thruster: (a) Working principle [148]; (b) Prototype by AIS [149].	44
2.24	Field emission electric propulsion: (a) Working principle [157]; (b) Prototype by TU Dresden [158].	45
2.25	Working principle of: (a) Colloid thruster [165]; (b) Ion thruster [166]; (c) Hall thruster [165]; (d) Solar sail [167].	46
2.26	Metal MEMS fabrication process [170].	47
3.1	Movement of a Fluid Element in Fluid Flow ([171])	51
3.2	Numerical algorithm adopted in the <i>laminarSMOKE</i> code [177].	56
3.3	FFTB Algorithm [178]	57
3.4	TFFB Algorithm [178]	57
3.5	hFTB Algorithm [178]	57
3.6	hFFB Algorithm [178]	57
3.7	Numerical algorithm adopted in the <i>chtlaminarSMOKE</i> code [13].	58
4.1	OpenFOAM® Logo.	61
4.2	Case directory structure.	62
4.3	Case directory structure adapted for CHT.	63
4.4	A <i>blockMesh</i> base block with vertice and edge naming convention [184].	66
4.5	Application examples of <i>snappyHexMesh</i> : (a) creation of the background mesh; (b) cell splitting by surface; (c) cell splitting by region and cell removal; (d) final surface snapping [183].	67
4.6	The subdivision of the surface for the purpose of the boundary condition application [177].	68
4.7	ParaView® Logo.	71
4.8	The paraFOAM window [186].	71
4.9	Toolbars in ParaView [186].	72
4.10	Schematic illustration of the computational domain.	73
4.11	Used meshes with resolution: (a) Gas phase modelling (only <i>fluidRegion</i>). (b) Gas-solid phase modelling (<i>fluidRegion</i> mesh in blue, <i>solidRegion1</i> mesh in red and <i>solidRegion2</i> in yellow).	74
5.1	Graphical representation of the spark imposed within the microchannel with walls.	77
5.2	Stability map for the various simulations conducted with the adiabatic microchannel ($\phi = 0.7, 1.1, 1.3$ from [112]).	81

5.3	Streamlines of the flow field and distribution of heat release rate for stables cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).	82
5.4	Streamlines of the flow field and distribution of temperature for stables cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).	83
5.5	Heat release rate and temperature profiles along the x axis (centerline) for the adiabatic stable cases.	84
5.6	Temporal evolution of T_{avg} , T_{max} and q'''_{avg} for the the adiabatic stable cases.	85
5.7	Streamlines of the flow field and distribution of OH mass fraction for stables cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).	86
5.8	Temperature profiles at the end of spark ($t = 0.5$ [m/s] for: a) Ad4Sp; b)Ad8Sp.	87
5.9	Comparison between the cases Ad4Sp (light blue lines), Ad6Sp (dark blue lines) and Ad8Sp (black lines) of the main species mass fractions in axial direction along the centerline.	87
5.10	Streamlines of the flow field and distribution of heat release rate for Ad10Sp, in 15 [μ s] intervals.	88
5.11	Streamlines of the flow field and distribution of heat release rate for Ad12Sp, in 15 [μ s] intervals.	89
5.12	Five stages of Pulsatory Flame Burst.	90
5.13	Heat release rate profiles along the x axis (centerline) for Ad10Sp (left) and Ad12Sp (right).	91
5.14	Temperature profiles along the x axis (centerline) for Ad10Sp (left) and Ad12Sp (right).	92
5.15	Streamlines of the flow field and distribution of Temperature for Ad10Sp, in 15 [μ s] intervals.	95
5.16	Streamlines of the flow field and distribution of Temperature for Ad12Sp, in 15 [μ s] intervals.	96
5.17	Evolution of the maximum values of the heat release rate and temperature along time, inside of the burner, for <u>Ad10Sp</u> (left) and <u>Ad12Sp</u> (right), zoomed in for $t = [2.000, 2.400]$ ms.	97
5.18	Evolution of the average values of the heat release rate and temperature along time, inside of the burner, for <u>Ad10Sp</u> (left) and <u>Ad12Sp</u> (right), zoomed in for $t = [2.000, 2.400]$ ms.	97
5.19	Evolution of the maximum and average values of the heat release rate and temperature along time, inside of the burner, for <u>Ad10Sp</u> (solid lines) and <u>Ad12Sp</u> (dashed lines).	97
5.20	Power Spectrum (q''') versus frequency (f) for <u>Ad10Sp</u> and <u>Ad12Sp</u>	99
5.21	A Single PFB Cycle Illustrated in 5 Stages: (a) q''' ; (b) T	100
5.22	Stability map for the various simulations using a spark conducted with amorphous materials.	101
5.23	Streamlines of the flow field and distribution of temperature for <u>FS4Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	101
5.24	Streamlines of the flow field and distribution of heat release rate for <i>fluidRegion</i> and the heat flux due to conduction for <i>solidRegion</i> 's for <u>FS4Sp</u>	101
5.25	Temporal evolution of maximum and average values of heat release rate and temperature for <u>FS4Sp</u> and <u>Ad4Sp</u> (for comparison).	102
5.26	Temporal evolution of maximum values of heat release rate and temperature for <u>FS4Sp</u> (zoomed into tPFB).	103

5.27	Temporal evolution of average values of heat release rate and temperature for <u>FS4Sp</u> (zoomed into tPFB).	103
5.28	Streamlines of the flow field and distribution of heat release rate for <u>FS4Sp</u> , in 20 $[\mu\text{s}]$ intervals, over 1 cycle tPFB.	104
5.29	Distribution of wall heat flux for <u>FS4Sp</u> , in 20 $[\mu\text{s}]$ intervals, over 1 cycle tPFB.	104
5.30	Heat release rate (left) and Temperature (right) profiles along the x axis (centerline) for <u>FS4Sp</u> .	105
5.31	Evolution of temperature and heat release rate profiles along the x axis (centerline) for the <u>FS4Sp</u> and comparison with <u>Ad4Sp</u> .	106
5.32	Variation of average and maximum heat flux in the solid (conduction) along the x and y directions.	107
5.33	Variation of the heat flux to the outside, q'_{out} , at the outer wall of <i>solidRegion2</i> (just one cell in z direction).	107
5.34	Changes in Total, Convection, and Radiation Heat Fluxes to the surrounding environment throughout the simulation, alongside fluctuations in average and maximum Temperature of the solid wall.	107
5.35	Streamlines of the flow field and distribution of heat release rate for <u>FS6Sp</u> , in 20 $[\mu\text{s}]$ intervals.	109
5.36	The existing microchannel geometry and the suggested modification to mitigate flashback within the 1 st convex zone.	110
5.37	Streamlines of the flow field and distribution of heat release rate for <i>fluidRegion</i> and the heat flux due to conduction for <i>solidRegion</i> 's for <u>FS10Sp</u> .	111
5.38	Evolution of the maximum (top) and average (bottom) values of the heat release rate and temperature along time, inside of the microchannel, for <u>FS10Sp</u> , zoomed in at $t = [3.000, 3.800]$ ms.	111
5.39	Streamlines of the flow field and distribution of temperature for <u>FS10Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	112
5.40	Temporal evolution of heat flux in solid wall (in the x and y directions (q''_x and q''_y), total heat flux lost to the surroundings (q_{out}), and average solid wall temperature (T_s) throughout the time interval $t = [3.000, 3.800]$ ms in the <u>FS10Sp</u> scenario.	114
5.41	Temporal evolution of temperature profiles: average values of T_{wall} (outer surface), T_s (solid), and T_{int} (solid-fluid interface), along with peak temperatures across the entire wall during the time interval $t = [3.000, 3.800]$ ms for the <u>FS10Sp</u> scenario.	114
5.42	Heat release rate (left) and heat flux in the x (top right for each column) and y directions (bottom right) profiles along the x axis (centerline) for <u>FS10Sp</u> during one PFB cycle.	117
5.43	Evolution of maximum and average values of heat release rate and temperature in the fluid for <u>FS12Sp</u> , over time $t = [0.800, 4.000]$ [ms].	118
5.44	Evolution of various characteristics over time, specifically at the center of the convex zone (bottom: H_2 mass fraction and fluid temperature) and at the center of the solid wall (top: heat flux in the y direction and solid temperature), located approximately at $x \approx 6.5$ [mm] for the <u>FS12Sp</u> scenario, within the time range $t = [2.000, 3.000]$ [ms].	119
5.45	Visualizing the culmination of mPFB: streamlines of the flow field and temperature distribution in the microchannel for <u>FS12Sp</u> , captured at 20 $[\mu\text{s}]$ intervals.	120
5.46	A single PFB cycle with heat loss present in the microchannel illustrated in 5 stages: (a) Heat Release Rate; (b) Temperature.	121
5.47	Power Spectrum (q''') versus frequency (f) for <u>Ad10Sp</u> and <u>FS10Sp</u> .	121

5.48	Temperature profiles in <i>solidRegion1</i> along the microchannel length in the fluid-solid interface, T_{int} , for <u>FS10Sp</u> (left) and <u>FS12Sp</u> (right).	124
5.49	Stability map for the various simulations using a spark conducted with ceramic materials.	125
5.50	Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for <u>LT8Sp</u> , <u>LT10Sp</u> and <u>LT12Sp</u> , from top to bottom respectively.	126
5.51	Streamlines of the flow field and distribution of the H_2 mass fraction for <u>LT8Sp</u> , <u>LT10Sp</u> and <u>LT12Sp</u> , from top to bottom respectively.	126
5.52	Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for <u>HT4Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	127
5.53	Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for <u>HT6Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	127
5.54	Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for <u>HT8Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	127
5.55	Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for <u>HT10Sp</u> and <u>LT12Sp</u>	128
5.56	Streamlines of the flow field and distribution of temperature (<i>FluidRegion</i> and <i>SolidRegion</i> 's), in $50 [\mu\text{s}]$ starting from $t = 0.90 [\text{ms}]$ for: (a) <u>FS4Sp</u> ; (b) <u>LT4Sp</u> ; (c) <u>HT4Sp</u>	129
5.57	Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for <u>FS4Sp</u> (top), <u>LT4Sp</u> (middle) and <u>HT4Sp</u> (bottom).	130
5.58	Stability map for the various simulations using a spark conducted for the stainless steels.	136
5.59	Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for <u>SS6Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	136
5.60	Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for <u>SS8Sp</u> (<i>FluidRegion</i> and <i>SolidRegion</i> 's).	137
5.61	Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for <u>SS10Sp</u> (top), <u>SS12Sp</u> (middle) and <u>CS12Sp</u> (bottom).	137
5.62	Streamlines of the flow field and distribution of the H_2 mass fraction for <u>SS10Sp</u> (top), <u>SS12Sp</u> (middle) and <u>CS12Sp</u> (bottom).	138
5.63	Temporal evolution of the average values of heat release rate and temperature for <u>CS8Sp</u> during $t = [0; 4.500] [\text{s}]$	138
5.64	Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for <u>CS8Sp</u> , during Backward Ignition Resurgence, in $10 [\mu\text{s}]$ intervals.	139
5.65	Temporal evolution of the average values of heat release rate and temperature for <u>CS8Sp</u> , in the solid-fluid interface on the first convex zone at $x \approx 3.0 [\text{mm}]$, during $t = [0; 4.500] [\text{s}]$	140
5.66	Stability map for the various simulations using a spark conducted with conductor materials.	143
5.67	Visual representation of the initial temperature imposition on microchannel walls alongside the spark inside the microchannel.	145
5.68	Stability map for the various simulations using a spark and imposed initial temperatures conducted with conductor materials.	145

5.69	Stability map for the various simulations using a spark in function of the thermal conductivity of the materials.	146
5.70	Stability map for the various simulations using a spark in function of the thermal diffusivity of the materials.	147
5.71	Temperatures in the solid and fluid domain for the different materials and simulations.	148
5.72	Maximum and average heat release rate for the different materials and simulations.	148
5.73	Specific thrust <i>versus</i> the inlet velocity for different materials.	150
5.74	Average and maximum values of the specific thrust for different materials and simulations.	151
5.75	Average and maximum values of the specific thrust for adiabatic materials using different equivalency ratios.	152

List of Tables

1.1	Classification for Smallsats and Launch vehicles [3].	3
2.1	Molecular Weight of some chemical elements	13
2.2	Autoignition Temperatures (AIT) for Various Fuels with air and pure O ₂	14
2.3	Flammability Limits for various fuels [25]	15
2.4	Adiabatic flame temperature and Maximum flame burning speed of common re-actants in a combustion reaction [33]	18
2.5	Typical length and time scales in micro-scale combustion, adapted from Ju et al. [40]	26
2.6	Non-dimensional parameters vs. micro-scale combustion phenomena, from Ju et al. [40]	27
3.1	Overview of the coupling algorithms based on Nettis [178]	57
4.1	List of cell selection shapes [184]	66
4.2	Employed mesh specifications for the computational regions	74
5.1	Chosen materials for this study and their key heat transfer properties	78
5.2	Series of simulations done utilizing the spark initial condition	79
5.3	T boundaryField of the for both <i>fluidRegion</i> and <i>solidRegion1</i> and <i>solidRegion2</i> for the initial timestep	80
5.4	Maximum and average values for temperature and heat release rate for the adiabatic stable cases	85
5.5	Maximum and average heat release rate values for the adiabatic PFB cases	90
5.6	Maximum and average temperature values for the adiabatic PFB cases	90
5.7	Signal spectral analysis results for frequency, f and maximum amplitude values, A^{var} , for the simulations <u>Ad10Sp</u> and <u>Ad12Sp</u>	99
5.8	Maximum and average values for temperature and heat release rate for <u>FS4Sp</u> and <u>Ad4Sp</u> (for comparison)	102
5.9	Cumulative E_{out} for <u>FS4Sp</u> (Part 1)	108
5.10	Cumulative E_{out} for <u>FS4Sp</u> (Part 2)	108
5.11	Maximum and average temperature values for the fluid domain for <u>FS10Sp</u> and comparison with <u>Ad10Sp</u>	113
5.12	Maximum and average heat release rate values for the fluid domain for <u>FS10Sp</u> and comparison with <u>Ad10Sp</u>	113
5.13	Maximum and average temperature values for the solid domain for <u>FS10Sp</u>	115
5.14	Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for <u>FS10Sp</u>	115

5.15	Signal spectral analysis results for frequency, f , and maximum amplitude values, A^{var} , for the simulations <u>FS10Sp</u> and <u>Ad10Sp</u>	116
5.16	Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the simulations <u>FS10Sp</u> and <u>Ad10Sp</u>	116
5.17	Maximum and average temperature values for the fluid domain for the Fused Silica simulations	122
5.18	Maximum and average heat release rate values for the fluid domain for the Fused Silica simulations	122
5.19	Maximum and average temperature values for the solid domain for the Fused Silica simulations	123
5.20	Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for the Fused Silica simulations	123
5.21	Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the Fused Silica that resulted in PFB	123
5.22	Maximum and average temperature values for the fluid domain for the LTCC and HTCC simulations	131
5.23	Maximum and average heat release rate values for the fluid domain for the LTCC and HTCC simulations	131
5.24	Signal spectral analysis results for amplitude values, A^{var} , for HTCC and LTCC that resulted in PFB	133
5.25	Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for HTCC and LTCC that resulted in PFB	133
5.26	Maximum and average temperature values for the solid domain for LTCC and HTCC simulations	134
5.27	Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for LTCC and HTCC simulations	134
5.28	Chemical composition of two stainless steels: AISI 310 [196] and AISI 430 [197]	135
5.29	Maximum and average temperature values for the fluid domain for the Stainless Steels simulations	141
5.30	Maximum and average heat release rate values for the fluid domain for the Stainless Steels simulations	141
5.31	Maximum and average temperature values for the solid domain for the Stainless Steels simulations	141
5.32	Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for the Stainless Steels simulations	142
5.33	Signal spectral analysis results for amplitude values, A^{var} , for the Stainless Steels simulations that resulted in PFB	142
5.34	Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the Stainless Steels simulations that resulted in PFB	142
C.1	Basic boundary conditions [183]	197
C.2	Constraint boundary conditions [183]	198
C.3	Generic boundary conditions [183]	198
C.3	Continuation of previous Table [183]	199
C.4	Wall boundary conditions [183]	200

List of Code Listings

5.1	Imposed Spark Function in C++	78
5.2	Snippet from the <i>funkySetFields</i> FoamFile for imposing wall temperatures in a microchannel during the first time-step using C++	144
5.3	Snippet of the Initialization .sh Bash shell script (Unix) used to change the temperature field of the walls during the first time-step.	145
A.1	<i>chtlaminarSMOKE</i> policy file in C++.	184
A.2	<i>fvSchemes</i> file in C++.	185
A.3	<i>fvSolution</i> file in C++.	186
A.4	<i>controlDict</i> file in C++.	187
A.5	<i>transportProperties</i> file for <i>solidRegion1</i> in C++.	188
A.6	<i>solverOptions</i> file for <i>fluidRegion</i> in C++.	190
D.1	Initialization .sh Bash shell script (Unix) file, to start a job in HPC.	201
D.2	Snippet of the Mesh generation and refinement Bash shell script (Unix).	202
E.1	Fast Fourier Transform script file in MATLAB.	203
E.2	Cumulative integral script file in MATLAB.	204

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Nomenclature

Glossary

e. g.	stands for the Latin <i>exempli gratia</i> , or “for example”
et al.	stands for the Latin <i>et al.</i> , or “and others”
etc.	stands for the Latin <i>et caetera</i> , or “and other similar things”
i.e.	stands for the Latin <i>id est</i> , or “that is”

Acronyms

1D	One dimension
2D	Two dimensions
3D	Three dimensions
Ad	Adiabatic
AIS	Applied Ion Systems
AIT	Autoignition Temperature
Al	Aluminium
BC	Boundary Condition
BG	Borosilicate Glass
BIR	Backward Ignition Resurgence
C++	Programming language C++
CFD	Computational Fluid Mechanics
CHT	Conjugate heat transfer
CPU	Central Processing Unit
CRECK	Chemical Reaction Engineering and Chemical Kinetics Lab
CS	Stainless Steel High Carbon
CT	Copper-Tungsten
CV	Control volume
DFT	Discrete Fourier Transform
EGR	Exhaust gas recirculation
EPR	Engine pressure ratio
ETR	Engine temperature ratio

FD	Fully-developed
FEED	Field emission electric propulsion
FFT	Fast Fourier Transform
FFTB	Flux Forward Temperature Back
FREI	Flame with Repetitive Extinction and Ignition
FS	Fused Silica
FVM	Finite Volume Method
GUI	Graphical User Interface
hFTB	Heat Transfer Coefficient Forward Temperature Back
hFFB	Heat Transfer Coefficient Forward Flux Back
HHV	Higher heating value
HPC	High Performance Computing
HTCC	High Temperature Co-fired Ceramic
Im	Simulations with Spark and initial imposed temperature
LHV	Lower heating value
LTCC	Low Temperature Co-fired Ceramic
LV	Satellite Launch vehicle
MEMS	Micro-Electro-Mechanical System
MOL	Method of Lines
mPFB	Migrating Pulsatory Flame Burst
MPS	Micropropulsion system
NTP	Normal Temperature and Pressure
OpenFOAM	Open source Field Operation And Manipulation
PFB	Pulsatory Flame Burst
PISO	Pressure Implicit Based Algorithm
PPT	Pulsed plasma thruster
PSD	Power Series
RAM	Random-access memory
Si	Silicon
SmallSat	Small satellites with mass lower than 500 [kg]
Sp	Simulations with Spark
SS	Stainless Steel Low Carbon
SSSF	Steady-state, Steady-flow
TFFB	Temperature Forward Flux Back
tPFB	Transitional Pulsatory Flame Burst

Operators

avg	Average of a set of elements
max	Maximum of a set of elements
min	Minimum of a set of elements
d	Derivative
$\frac{d}{dx}$	Derivative with respect to the x -coordinate
δ	Infinitesimal change or differential
$\frac{\partial}{\partial t}$	Partial derivative with respect to time
$\frac{\partial}{\partial x}$	Partial derivative with respect to the x -coordinate
$\frac{\partial}{\partial y}$	Partial derivative with respect to the y -coordinate
$\frac{\partial}{\partial z}$	Partial derivative with respect to the z -coordinate
Δ	Absolute / relative difference
$\int$	Integral over variable
$\oint$	Closed line integral operator, used to represent integration around a closed path
∇	Three-dimensional del operator (vector of partial derivatives)
Σ	Sum of a series of terms

Roman Symbols

a_p	Planck mean absorption coefficient	$[\text{m}^{-1}]$
$a_{p,k}$	Extinction coefficient for species k	$[\text{m}^{-1}]$
A	Area	$[\text{m}^2]$
A/F	Air-Fuel ratio	$[-]$
A_{sur}	Heat transfer surface area	$[\text{m}^2]$
$A_{\sim}^{\text{var}}$	Scaled amplitude value of signal of certain variable	$[-]$
Bi	Biot dimensionless number	$[-]$
$\mathbf{C}$	Vector representing convective transport rates of ψ	$[-]$
Co	Courant dimensionless number	$[-]$
C_p	Specific heat capacity at constant pressure	$[\text{J}/(\text{kg} \cdot \text{K})]$
d	Characteristic size of combustor inner diamete (combustor scales)	$[\text{mm}]$
d_0	Quenching diameter (limiting tube diameter)	$[\text{mm}]$
d_h	Interior wall heat dissipation rate	$[\text{W}]$
d_s	Characteristic length scale of the structure (solid phase)	$[\text{mm}]$
$\mathbf{D}$	Vector representing diffusive transport rates of ψ	$[\text{mm}]$
Da	Damköhler dimensionless number	$[-]$

D_k	Individual-species mixture-averaged diffusion coefficient	[m ² /s]
e	Specific system's stored energy (per unit mass)	[J/kg]
E	System's stored energy (includes the internal, kinetic, and potential energy)	[J]
E'	Mixture combustion heat release rate	[W]
E''	Heat dissipation rate of the inner wall	[W]
E_{out}	Cumulative heat loss to the surroundings	[J]
E_{rad}	Emissive Power	[W/m ²]
ℓ_{fl}	Flame length (visible extent of combustion along a flame front)	[mm]
f	Frequency	[Hz]
F	Force	[N]
F/A	Fuel-Air ratio	[–]
Fo	Fourier dimensionless number	[–]
g	Acceleration due to gravity (gravitational forces)	[m/s ²]
$\mathbf{g}$	Acceleration vector due to gravity	[m/s ²]
G	Irradiation	[W/m ²]
G_{abs}	Absorbed irradiation	[W/m ²]
G_{rfl}	Reflected irradiation	[W/m ²]
G_{tr}	Transmitted irradiation	[W/m ²]
h	Enthalpy	[J/kg]
$\bar{h}$	Absolute enthalpy	[J/kg]
$\bar{h}_f^0$	Enthalpy of formation	[J/kg]
$\bar{h}_s$	Sensible enthalpy	[J/kg]
I_{sp}	Specific impulse	[N/s]
J	Radiosity	[W/m ²]
k	Convective heat loss (microcombustion)	[–]
Kn	Knudsen dimensionless number	[–]
L	Length	[m]
L/h	Length-to-height ration	[–]
Le	Lewis dimensionless number	[–]
m	Mass of a system / substance	[kg]
$\dot{m}$	Mass flowrate	[kg/s]
MW	Molecular weight	[mol/kg]

n	Number of moles	[mol]
Nu	Nusselt dimensionless number	[—]
NC	Number of species in the mixture	[—]
p_k	Partial pressure of species k	[Pa]
P	Pressure	[Pa]
$q''_{x,y,z}$	Heat transfer rate per unit area perpendicular to the direction of transfer	[W/m ²]
$q'''_{x,y,z}$	Heat transfer rate per unit area perpendicular to the direction of transfer	[W/m ³]
q'''	Heat Release Rate	[W/m ³]
q'''_{avg}	Average Heat Release Rate	[W/m ³]
q'''_{max}	Maximum Heat Release Rate	[W/m ³]
$\mathbf{q}''$	Heat flux vector (considering heat transfer rate in different directions)	[W/m ²]
$q\&$	Heat loss density	[W/m ²]
$\overline{q\&''}$	Average heat loss density	[W/m ²]
$\dot{q}$	Heat generation rate per unit volume	[W/m ³]
q_{tot}	Cumulative integrated heat release rates	[W]
Q	Energy transfer or heat exchanged	[J]
$\hat{Q}$	Energy transfer or heat exchanged (per unit mass)	[J/kg]
$\dot{Q}$	Rate of heat transfer	[W]
$\mathbf{R}$	Vector of rates of change of ψ due to chemical reactions	[—]
S_0	Time step modifier for faster convergence in solid energy simulations.	[—]
S	Surface	[m ²]
S/V	Surface-to-volume ratio	[m ⁻¹]
t	Time	[s]
T	Temperature	[K]
T_{af}	Adiabatic flame temperature	[K]
T_{amb}	Ambient temperature	[K]
T_f	Temperature of the fluid	[K]
T_∞	Temperature of the fluid far from the surface	[K]
T_{int}	Temperature of the solid-fluid interface	[K]
T_s	Temperature of the solid	[K]
T_{sur}	Temperature of body surface	[K]
T_{wall}	Temperature of the surroundings	[K]

u	Internal energy of a system/state	[J]
U	Absolute velocity	[m/s]
U_{fl}	Flame speed	[m/s]
U_{in}	Absolute inlet velocity	[m/s]
U_{out}	Absolute outlet velocity	[m/s]
v	Velocity	[m/s]
$\mathbf{v}$	Velocity vector	[m/s]
V	Volume	[m ³]
$\mathbf{V}_C$	Constant correction factor for mass conservation (species independent)	[m/s]
$\mathbf{V}_k$	Diffusion velocity vector of species k	[m/s]
$\mathbf{V}_k^C$	Corrective diffusion velocity for species k	[m/s]
w	Work done (per unit mass)	[J/kg]
$\dot{W}$	Rate of work done	[W]
W	Work done	[J]
x_f	Point along the centerline of the chamber where flame becomes observable	[mm]
x_i	Initial anchoring point of the flame (location where combustion initiates)	[mm]
Y	Mass fraction	[–]
z	Vertical height above a reference point	[m]

Greek symbols

α_{rad}	Absorptivity (radiation)	[–]
α_T	Thermal diffusivity of the material	[m ² /s]
βH	Normalized heat loss	[–]
χ	Molar fraction	[–]
d_0	Quenching diameter	[–]
δ_α	Thermal diffusion length	[–]
δ_D	Mass diffusion length	[–]
δ_f	Flame thickness	[–]
$\delta \hat{Q}$	Specific energy transfer or heat exchanged during a thermodynamic cycle	[J/kg]
δt	Ratio between the time step	[s]
$\delta \hat{W}$	Specific net work done during a thermodynamic cycle	[J/kg]
δx	Cell size in the direction of the velocity	[m]
Δh_c	Heat of combustion / heating value	[J/kg]
Δh_R	Enthalpy of combustion (per mass of mixture)	[J/kg]

ε_{rad}	Emissivity (radiation)	[—]
Γ_{jk}	Binary diffusion coefficient between species j and k	[m ² /s]
λ	Thermal conductivity	[W/(m · K)]
λ_{fp}	Mean free path	[—]
∇T	Gradient of temperature	[K/m]
∇Y_k	Gradient of mole fraction of species k	[m ⁻¹]
Ω	Burning rate	[—]
$\dot{\Omega}_k$	Formation rate of species k	[kg/s]
ϕ	Equivalency Ratio	[—]
ψ	Primary variables vector (mass fractions and temperature)	[—]
ρ	Density	[kg/m ³]
σ	Stefan-Boltzmann constant	[W/(m ² · K ⁴)]
τ_c	Characteristic combustion time	[—]
τ_{res}	Flow residence time	[—]
τ_{rad}	Transmissivity (radiation)	[—]
τ_a	Time scale of acoustic wave	[—]
τ_α	Diffusion time scale of gas-phase	[—]
τ_c	Characteristic combustion time	[—]
τ_f	Characteristic flow time	[—]
τ_h	Time scale of heat loss	[—]
τ_{ig}	Ignition time scale	[—]
τ_{res}	Flow residence time	[—]
τ_s	Diffusion time scale of solid-phase	[—]
τ_{st}	Fluid stress tensor	[Pa]
Θ_k	Thermal diffusion ratio of species k	[—]

Superscripts

$(-)^0$	Reference state
$(-)^{\text{var}}$	Relative to variable VAR

Subscripts

$(-)_{1-2}$	State 1 to 2
$(-)_{\text{abs}}$	Absorbed
$(-)_{\text{air}}$	Air component
$(-)_{\text{amb}}$	Ambient

$(-)_\text{avg}$	Average
$(-)_\text{b}$	Blackbody
$(-)_\text{ch}$	Microcombustor chamber
$(-)_\text{conv}$	Convection
$(-)_\text{cv}$	Control volume
$(-)_\text{f}$	Fluid
$(-)_\text{fl}$	Flame
$(-)_\text{fuel}$	Fuel component
$(-)_i$	Species i
$(-)_{i,j,k}$	Unit vectors in Cartesian coordinate systems
$(-)_\text{in}$	Inlet
$(-)_\text{max}$	Maximum
$(-)_\text{mix}$	Mixture
$(-)_\text{out}$	Outlet
$(-)_\text{prod}$	Products
$(-)_\text{rad}$	Radiation
$(-)_\text{reac}$	Reactants
$(-)_\text{ref}$	Reference
$(-)_\text{rfl}$	Reflected
$(-)_{r,\phi,z}$	Cylindrical coordinate directions
$(-)_\text{s}$	Solid
$(-)_\text{tot}$	Total
$(-)_\text{tr}$	Transmitted
$(-)_\text{wall}$	Wall
$(-)_{x,y,z}$	Cartesian coordinate directions

Accents

$\overline{(-)}$	Average value of a quantity (-)
$\hat{(-)}$	Normalize a quantity (-) by the mass (quantity per unit mass)
$ (-) $	Magnitude of quantity (-)

Elements

Ar	Argon
C	Carbon

He	Helium
H	Hydrogen
N	Nitrogen
O	Oxygen

Chemical Species

Ar	Argon
CO	Carbon monoxide
CO ₂	Carbon dioxide
H	Hydrogen
H ₂	Hydrogen
H ₂ NO	Nitroxyl
H ₂ O	Water
H ₂ O ₂	Hydrogen peroxide
HCO	Formyl radical
He	Helium
HNNO	Nitrosyl hydrazine
HNO	Nitrosyl hydride
HNO ₂	Nitric acid
HO ₂	Hydroperoxyl radical
HONO	Nitrous acid
HONO ₂	Nitric acid anhydride
N	Nitrogen
N ₂	Nitrogen gas
N ₂ H ₂	Dinitrogen hydride
N ₂ H ₃	Diazene
N ₂ H ₄	Hydrazine hydrate
N ₂ O	Nitrous oxide
NH	Amine or ammonia
NH ₂	Amino radical
NH ₃	Ammonia
NNH	Hydrazine
NO	Nitric oxide
NO ₂	Nitrogen dioxide
NO ₃	Nitrate
O	Atomic oxygen
O ₂	Oxygen gas
OH	Hydroxyl radical

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Part I

Initia Nova

INITIA:: (noun) *the point of time or space
at which anything begins*

NOVA:: (adj.) *recently created or having
started to exist recently*

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Chapter 1

Introduction

*“If a man will begin with certainties, he shall end in doubts;
but if he will be content to begin with doubts he shall end in certainties.”*

Sir Francis Bacon

1.1 Framework and Motivation

Today, the space sector differs greatly from the landscape of just a few decades ago. We have officially entered what is often referred to as the “*New Space Age*” [1]. This era is characterized by a remarkable reduction in launch costs and a continual rise in the number of entities launching satellites into orbit [2]. As a result, we are currently observing a shift within the space industry towards miniaturization. The driving forces behind this transformation are primarily centered on the goals of cost reduction and the hastening of development timelines for space missions.

According to findings by Wekerle et al. [3], approximately one-third of the 2,500 satellites launched from 1997 to 2017 had a wet mass^(a) below 500 kg, commonly referred to as *Smallsats*. They are launched into orbit as secondary payloads and are deployed into orbit by satellite launch vehicles (LV). Typically, *Smallsats* are categorized based on their mass and Table 1.1 presents a classification system, based on the system’s mass, for both *Smallsats* and LV’s.

Table 1.1: Classification for Smallsats and Launch vehicles [3].

Smallsats	Wet Mass
Pico-Satellite	≤ 1 kg
Nano-Satellite	1 – 10 kg
Micro-Satellite	11 – 100 kg
Mini-Satellite	101 – 500 kg
Launch Vehicles	Payload Capacity
Micro-LV	≤ 500 kg
Small-LV	501 – 2,000 kg
Medium-LV	2,001 – 20,000 kg
Heavy-LV	$> 20,000$ kg

^(a)The term “wet mass” for a satellite refers to its total mass, encompassing all components and systems, when it is fully fueled with propellants

In addition to *Smallsats*, other commonly used definitions include *CubeSats*^(b) and *PocketQubes*^(c), both of which consist of one or more cubic units. In low Earth orbits, they typically generate approximately 2 [W] and 0.5 [W] of power, respectively [6].

The *Smallsat* market has already experienced significant growth and is anticipated to expand even further in the coming decade [2]. Notably, the number of *Smallsats* launched between 2012 and 2017 nearly matches the total accumulated (launched into to space and in orbit) in the preceding 15 years [3], and this translate to a increasing trend in the number of accumulated satellites in space (Figure 1.1 for context), with a more pronounced change on nano- and pico-satellites.

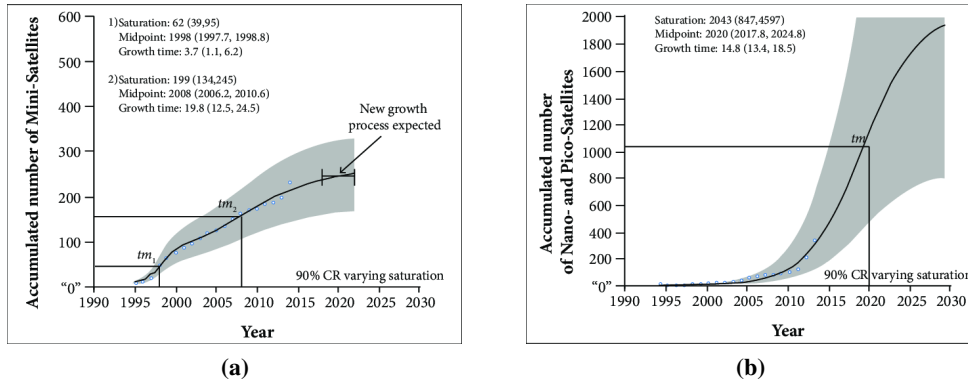


Figure 1.1: History and forecast of the number of accumulated (a) micro- and (b) nano- and pico- satellites using a logistic growth model [3].

This transition aligns with the broader technological industry. We have witnessed a significant technological evolution in the development of micro and nano devices. In other words, progress is moving towards minimizing conventional mechanics, exemplified by the increasing utilization of microchips, small-scale sensors and actuators, drones, microsatellites, and more. Consequently, it has become an imperative to seek efficient energy sources capable of supplying the required power to increasingly smaller and compact mechanisms.

As a result of these advancements, micro-fabrication technology has enabled the integration of electrical and mechanical components into a single system known as MEMS (Micro Electro-Mechanical Systems) [7]. Typically, the external power supply in this sort of device is provided by batteries, however due to their limits, alternative efforts have been made to leverage the high energy density of hydrocarbon fuels by building micro-combustion chambers. Among these developments, MEMS devices stand out as promising candidates for miniaturization, particularly in the realm of small spacecraft.

Our research is centered on MEMS microthrusters, specifically designed for nano- and pico-satellites. In this context, propulsion systems are of paramount importance as they greatly enhance the scope of applications for these small satellites. These micropropulsion systems have the capability to generate thrust at the micro- to milli-Newton level [8], and have the potential to bring about a significant transformation in satellite capabilities. They empower these satellites to perform attitude maneuvers, including tasks such as reaction wheel desaturation, attitude control, and the correction of minor disturbances. Additionally, the propulsion system could facilitate adjustments to the satellite's orbital insertion [9], further enhancing their versatility and functionality.

^(b)Defined as having a volume of $10 \times 10 \times 10$ [cm³] and a wet mass (per unit) ≤ 1.3 [kg] [4]

^(c)Defined as having a volume of $5 \times 5 \times 5$ [cm³] and a wet mass (per unit) ≤ 180 [g] [5]

1.2 Computational Framework

The utilization of micropropulsion is gaining increasing significance within the scientific community due to the growing demand for smaller devices, prompting the progressive investigation of phenomena at the micrometer scale. However, micropropulsion employing microchannels with reactive gas flow is inherently linked to the phenomenon of microcombustion, which currently faces several practical limitations concerning design and thermal efficiency. Consequently, numerous studies have been conducted to explore this promising field, encompassing both energy-related aspects and gas acceleration.

Most researchers have historically leaned on ANSYS Fluent® and similar ANSYS products, known for their robust capabilities in computational fluid dynamics (CFD). Nevertheless, the substantial expense associated with annual licensing, ranging from 15,000 to 30,000 euros, coupled with an extra 3,000 to 6,000 euros for updates, renders these software solutions less economically feasible for a broader audience encompassing both the scientific and commercial sectors.

As an alternative, a group of researchers from Politecnico di Milano, from the the CRECK Modeling Group Lab (Figure 1.2a), has developed an application named OpenSMOKE++ (Figure 1.2b) for the open-source platform OpenFOAM [10]. OpenSMOKE++ serves as a versatile framework designed for numerical simulations of reactive systems featuring intricate kinetic mechanisms, encompassing numerous chemical species and reactions. Its functionalities span kinetic preprocessor solvers, ideal reactor solvers, laminar flames and flamelets solvers, as well as a graphical post-processor.

In OpenSMOKE++, the framework was integrated with OpenFOAM, enabling the creation of three solvers: *laminarSMOKE*, *flameletSMOKE*, and *edcSMOKE*. These solvers model reacting flows in complex 2D/3D geometries with detailed kinetics, both in steady-state and unsteady conditions. In this work we used *laminarSMOKE* [11, 12], which serves as a solver capable of modeling multidimensional laminar flames for both stable and unstable flows, with or without structured meshes.

This application has been made freely available as open-source code for the entire scientific community. Notably, Cova [13] validated the usage of this solver in the study of diffusive and premixed flames involving hydrogen and methane as fuels in 2016. Consequently, for the simulations conducted in this dissertation, the *laminarSMOKE* solver and an adapted *CHTlaminarSMOKE* (to include the gas-solid phase modeling as will be explained in Chapter 3) was employed as the preferred tool. For conducting all the simulations in this dissertation, we were granted access to the High Performance Computing Grid at FEUP (Figure 1.2c).

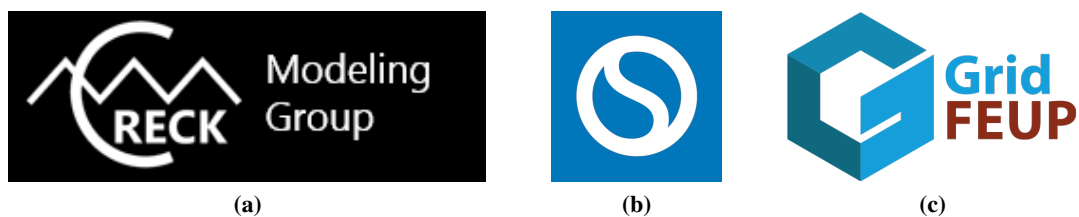


Figure 1.2: Logotypes of: (a) Creck Modelling Group; (b) OpenSMOKE++ Framework; (c) GridFEUP.

1.3 Objectives

In simple terms, we can shortly describe the objective of this dissertation as:

“Numerically explore the dynamics of combustion flames within a complex geometry, utilizing various materials commonly employed in space applications, with the aim to gain insights into their influence on propulsion and enhance our understanding of how different materials can affect the design of novel propulsion systems.”

To accomplish this goal, our efforts involved the following steps:

- Conducting an extensive review of the current state of micropropulsion and microcombustion, comprehending the underlying mechanisms and dynamics at play, and identifying the challenges, with a particular emphasis on wavy channels and intricate geometries;
- Modify the *laminarSMOKE* solver to incorporate Conjugate Heat Transfer (CHT), enabling the modeling of the solid-fluid interface. This adaptation involves defining and elucidating the numerical method employed for CHT simulations;
- Create multiple simulations, encompassing aspects like boundary conditions, initial conditions, and various simulation parameters. The aim is to generate a substantial amount of analyzable and intriguing data for further investigation;
- Conduct microcombustion simulations employing a range of diverse materials and velocities to gain a deeper comprehension of the inherent flame dynamics within intricate geometries. Explore how these various materials influence microcombustion dynamics, and analyze the fluctuations in data, particularly focusing on variables such as heat release rate, temperatures, and heat conduction.

1.4 Dissertation outline

The dissertation is divided into five **parts**, six **chapters** and five **appendices**, that approach different parts of the work:

PART I: INITIA NOVA

CHAPTER 1: INTRODUCTION

Here, in the current chapter, we explored the current landscape of microsatellites, underlining their prospective significance and relevance in the field of aerospace. Moreover, we underscored the pivotal role of micropropulsion thrusters within these systems. Additionally, we articulated our primary objective: attain a deeper understanding of how material thruster heat transfer impacts combustion and flow dynamics.

PART II: FUNDAMENTA THEORICA

CHAPTER 2: LITERATURE REVIEW

Presents a comprehensive literature review of microcombustion and micropropulsion, including their basic principles, characteristics, and previous research. The chapter also covers the current state of the art in these fields and the various materials and methods used for micro thruster fabrication.

CHAPTER 3: GOVERNING EQUATIONS AND NUMERICAL MODELLING

Describes the governing equations of the microcombustion phenomenon and the numerical modeling used to solve them. This chapter presents the numerical methods and algorithms used to simulate the microcombustion and micropropulsion systems, including their strengths and limitations.

CHAPTER 4: SOFTWARE FRAMEWORK AND METHODOLOGY

Presents the software used for case study pre-processing, post-processing of results, and how simulations were carried out. The chapter provides details on the software tools used to perform the numerical simulations, including their features, capabilities, and limitations.

PART III: INVESTIGATIO DE MATERIA

CHAPTER 5: CHARACTERIZING THE THERMAL BEHAVIOR OF DIFFERENT MATERIALS USING A SPARK

Here, we delve into an extensive analysis of the results derived from our case study. This study involved conducting a series of simulations using a spark at varying inlet velocities, spanning the range of 4 m/s to 12 m/s. To achieve this, we meticulously adjusted input parameters and closely observed operational conditions to discern the influence of different materials on the design and performance of innovative propulsion systems. Our study encompassed a total of five distinct material groups, comprising adiabatic materials, ceramics (both LTCC and HTCC), metals (specifically two types of stainless steel), amorphous materials (two variants of high-temperature glasses), and high thermal conductivity materials (such as silicon, aluminum, and copper-tungsten alloys).

PART IV: CONCLUSIO PERPETUA

CHAPTER 6: SUMMARY AND OUTLOOK

Here, we provide a concise overview of the primary conclusions derived from this study, encapsulating the outcomes and data presented in earlier chapters, and enhancing the comprehension of the key findings in this dissertation.

PART V: APPENDICES

APPENDIX A: *chtlaminarSMOKE* SOLVER FILES

This appendix contains the policy file for the numerical algorithm employed in this study. It is accompanied by the pertinent system files (*fvSchemes*, *fvSolution*, and *controlDict*) and constant files (*solverOptions* and *transportProperties*), which were explained in Chapter 4.

APPENDIX B: KINETIC MECHANISM OF THE COMBUSTION REACTION

Here we provide an overview of the chemical reactions within the extensive H_2 kinetic mechanism, denoted as POLIMI_H2CO_NOX_1412, that was utilized in this thesis. This mechanism comprises 32 distinct species and encompasses a total of 173 reactions.

APPENDIX C: OPENFOAM STANDARD BOUNDARY CONDITIONS

Within this appendix, we furnish an extensive overview of the standard boundary conditions at your disposal in OpenFOAM, which are accessible for user utilization.

APPENDIX D: SETTING UP A SIMULATION

In here, we will offer an all-encompassing guide that explains the procedures for executing a simulation on the remote High-Performance Computing (HPC) system.

APPENDIX E: DATA ANALYSIS PROGRAMS

Here, we will present two codes that were employed for data analysis during the thesis: one for performing FFT analysis (Fast Fourier Transform) and another for computing the cumulative integral of a specific variable over time.

End

In summary, this thesis undertakes a comprehensive exploration of the influence of materials on microcombustion and micropropulsion, with a specific emphasis on the characteristics of wavy nonlinear microchannels. It commences with an exploration of the foundational principles of thermodynamics and advances to sophisticated numerical simulations and innovative characterizations of the dynamics and mechanisms observed within the microchannel. This thesis significantly contributes to the ongoing progress in these fields and provides valuable insights and directions for future research and development.

Part II

Fundamenta Theorica

FUNDAMENTA:: (noun) *The base or underlying support on which something is built, established, or developed.*

THEORICA:: (noun) *a supposition or a system of ideas intended to explain something, especially one based on general principles independent of the thing to be explained.*

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Chapter 2

Literature Review

"If I have seen further it is by standing on the shoulders of giants."

Sir Isaac Newton

2.1 A Review on Combustion

In this section, we will delve into the fundamental concepts of combustion that are crucial for a thorough understanding of the results presented in the following sections. The theoretical knowledge presented in the works of [14] and [15] forms the basis for our discussion here.

2.1.1 Introduction

The definition of combustion as in Webster's Dictionary [16] is "rapid oxidation generating heat, or both light and heat; also, slow oxidation accompanied by relatively little heat and no light." For the purpose of this dissertation, we shall limit the definition to only the rapid oxidation portion, as most actual combustion devices fall within this category.

This definition emphasizes the inherent significance of chemical reactions in combustion. It also underlines the significance of combustion: burning converts energy held in chemical bonds to heat, which can be used in a variety of ways.

In essence, combustion occurs when there's a chemical interaction between a combustible, fuel, and an oxidizer, under appropriate circumstances.

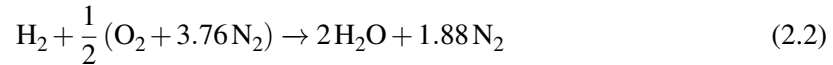
2.1.2 Combustion in stoichiometric conditions

The stoichiometric amount of oxidizer is the amount required to completely burn a given amount of fuel. When more than a stoichiometric amount of oxidizer is added, the mixture is said to be fuel lean, or just lean; when less than a stoichiometric amount of oxidizer is added, the mixture is said to be fuel rich, or rich. The stoichiometric oxidizer- (or air-) fuel ratio (mass) is calculated using simple atom balances and the assumption that the fuel interacts to generate an idle set of products.

In most situations, air is the oxidizer, and it is considered to be a mixture of 21% oxygen (O₂) and 79% nitrogen (N₂), by volume, i.e., that for each mole of O₂ in air, there are 3.76 moles of N₂:



The proportion of fuel and oxidant used determines the efficiency of the combustion process. To define this process, it is critical to understand the chemical reaction that occurs, which indicates how the reactants react with each other, resulting in combustion products. As a result, because this study will only examine the combustion processes of previously mixed combustion of premixed mixtures, and because only one type of fuel, H_2 , is used, the global chemical reaction concerns the interaction between H_2 and air ^(a):



2.1.3 Air-fuel ratio and equivalence ratio

Just like previously mentioned, air was simplified by only containing O_2 and N_2 . Knowing that, and that the fuel is H_2 , we can define the stoichiometric air-fuel ratio:

$$AF_{\text{stoich}} = \frac{m_{\text{air}}}{m_{\text{fuel}}} \quad (2.3)$$

Using Eq. (2.3) may then compute the equivalency ratio, ϕ , which is typically employed to quantify whether a fuel-oxidizer mixture is rich, lean, or stoichiometric. The equivalency ratio is calculated as

$$\phi = \frac{(A/F)_{\text{stoic}}}{(A/F)} = \frac{(F/A)}{(F/A)_{\text{stoic}}} \quad (2.4)$$

From this definition, we see that for fuel-rich mixtures, $\phi > 1$, and for fuel-lean mixtures, $\phi < 1$. For a stoichiometric mixture, ϕ equals unity. In other words:

$$0 < \phi < 1 \text{ fuel-lean}$$

$$\phi = 1 \text{ stoichiometric condition}$$

$$1 < \phi < \infty \text{ fuel-rich}$$

The equivalency ratio is the single most critical component in determining a system's performance in many combustion applications. Additional criteria used to define relative stoichiometry include percent stoichiometric air, which is related to the equivalence ratio as

$$\% \text{ stoichiometric air} = \frac{100\%}{\phi} \quad (2.5)$$

and percent excess air, as

$$\% \text{ excess air} = \frac{(1 - \phi)}{\phi} \cdot 100\% \quad (2.6)$$

^(a)It should be noted that N_2 is an inert gas that does not participate in the chemical reaction. As a result, the reaction shown in Eq. (2.2) depicts the interaction of H_2 with $\frac{1}{2} (O_2 + 3.76 N_2)$, air, yielding a single product, H_2O .

2.1.4 Mass and molar fractions

At this juncture, it becomes pertinent to introduce the conceptualization of mass fraction denoted as Y_i . This fundamental quantity represents the ratio of the mass m_i attributed to a particular chemical species, to the overall mass of the entire mixture denoted as m_{tot} . The summation of all individual species' mass fractions within the mixture invariably yields a totality of 1, a pivotal condition signifying the conservation of mass in the system under consideration.

$$Y_i = \frac{m_i}{m_{\text{tot}}} \quad (2.7)$$

$$\sum_{i=1}^{\infty} (Y_i) = 1 \quad (2.8)$$

The species quantity can also be expressed using the mole fraction χ_i . It is defined as the ratio of the amount of a constituent n_i to the total amount of all constituents in the mixture n_{tot} . The sum of all species mole fractions is always equal to 1.

$$\chi_i = \frac{n_i}{n_{\text{tot}}} \quad (2.9)$$

$$\sum_{i=1}^{\infty} (\chi_i) = 1 \quad (2.10)$$

The conversion between mole fractions and mass fractions can be readily accomplished by employing the molecular weights of the relevant species and the overall mixture.

$$Y_i = \chi_i MW_i / MW_{\text{mix}} \quad (2.11)$$

$$\chi_i = Y_i MW_{\text{mix}} / MW_i. \quad (2.12)$$

The mixture molecular weight, MW_{mix} , is easily calculated from a knowledge of either the species mole or mass fractions:

$$MW_{\text{mix}} = \sum_i \chi_i MW_i = \frac{1}{\sum_i (Y_i / MW_i)} \quad (2.13)$$

In Table 2.1 we highlight the MW of some relevant chemical elements.

Table 2.1: Molecular Weight of some chemical elements

Element	Symbol	MW [g/kmol]
Argon	Ar	39.948
Carbon	C	12.011
Helium	He	4.003
Hydrogen	H	1.008
Nitrogen	N	14.007
Oxygen	O	15.999

2.1.5 Autoignition temperatures and flammability limits

According to Nolan, 2014 [17], the Autoignition Temperature (AIT), also known as the ignition temperature, is the minimum temperature at which a substance in air must be heated in order to commence or cause self-sustaining combustion independent of the heating source. It is an extrinsic property, which means that the value is distinct to the experimental method employed to determine it. The volume to surface ratio of the source of ignition is the most important factor influencing AIT measurement (i.e., a hot wire versus a heated cup will yield different results). For this reason, ignition temperatures should always be regarded as estimations rather than exact material properties.

The ability to calculate the auto-ignition temperature is critical in the subject of fuel safety. Several fuels are relatively volatile and can quickly combine with air to generate explosive combinations. This property is shown in Table 2.2 for various fuels. Because H_2 is the employed fuel in the work developed in this dissertation, we've highlighted the characteristics of the said chemical species.

Table 2.2: Autoignition Temperatures (AIT) for Various Fuels with air and pure O_2

Fuel		Auto Ignition Temperatures [$^{\circ}C$]		Refs.
		With Air	With Pure O_2	
Hydrogen	H_2	500-585	575-585	[18, 19]
Ammonia	NH_3	651	651	[20]
Carbon Monoxide	CO	609-703	1120-1270	[21, 22]
Methane	CH_4	537-601	1010-1090	[21, 22]
Propane	C_3H_8	490-502	940-980	[21, 22]
Ethylene	C_2H_4	425-470	920-1080	[21, 22]
Acetylene	C_2H_2	305-305	305-585	[21, 22]
n-Hexane	C_6H_{14}	238-246	431-454	[21, 22]
n-Heptane	C_7H_{16}	218-225	375-406	[21, 22]
n-Octane	C_8H_{18}	210-240	321-361	[21, 22]
Iso-Octane	C_8H_{18}	215-225	435-446	[21, 22]
Benzene	C_6H_6	560-610	875-905	[23, 24]

A small quantity of energy is required to ignite a combination. The minimum ignition energy is determined by the chemical makeup of the combination. In addition, Moreover, for flame propagation to occur, mixes must lie within two composition limitations, lower and higher flammability limits.

In Table 2.3 we show these limitations for various reactant combinations (fuel and oxidizer).

Table 2.3: Flammability Limits for various fuels [25]

Fuel		Oxidizer (% volume)			
		Air		Oxygen	
		Lower Limit	Upper Limit	Lower Limit	Upper Limit
Hydrogen	H₂	4.00	75.0	4.00	94.0
Methane	CH ₄	5.30	14.0	5.10	61.0
Propane	C ₃ H ₈	2.25	9.5	2.23	55.0
Ethyl Alcohol	C ₂ H ₅ OH	3.40	27.0	3.90	61.0
Ethyl Ether	(C ₂ H ₅) ₂ O	1.90	48.0	2.1	82.0
Methyl Chloride	CH ₂ Cl ₂	7.60	19.0	8.00	66.0
Ammonia	NH ₃	15.0	27.0	14.0	79.0

2.1.6 First law of thermodynamics

The first law of thermodynamics asserts that the cyclic integral of heat is equal to the cyclic integral of work for each cycle that a system undergoes, i.e.,

$$\oint \delta \hat{Q} = \oint \delta \hat{W} \quad (2.14)$$

where $\oint \delta \hat{Q}$ is the cyclic integral of energy transfer or net heat transferred during the cycle and $\oint \delta \hat{W}$ is the cyclic integral of work or net work done during the cycle. The first rule also entails the presence of a state function termed the system's stored energy E , and it ties the change in this function to the flow of energy from the surroundings.

Energy conservation is described for a finite change between two states, 1 and 2, for a given **fixed mass**, i.e., a system as shown in Figure 2.1a, as:

$$\underbrace{{}_1Q_2}_{\text{Heat added to system}} - \underbrace{{}_1W_2}_{\text{Work done by system on surroundings}} = \underbrace{\Delta E_{1-2}}_{\text{Change in total system energy}} \quad (2.15)$$

where the change in total energy, ΔE_{1-2} , is the sum of the internal, kinetic and potential energies, i.e.,

$$E = m \left(u + \frac{1}{2}v^2 + gz \right) \quad (2.16)$$

And Eq. (2.15) can be converted to unit mass basis and to expressed an instant in time, using instantaneous rates:

$${}_1q_2 - {}_1w_2 = \Delta e_{1-2} = e_2 - e_1 \quad (2.17)$$

and

$$\dot{Q} - \dot{W} = dE/dt \quad (2.18)$$

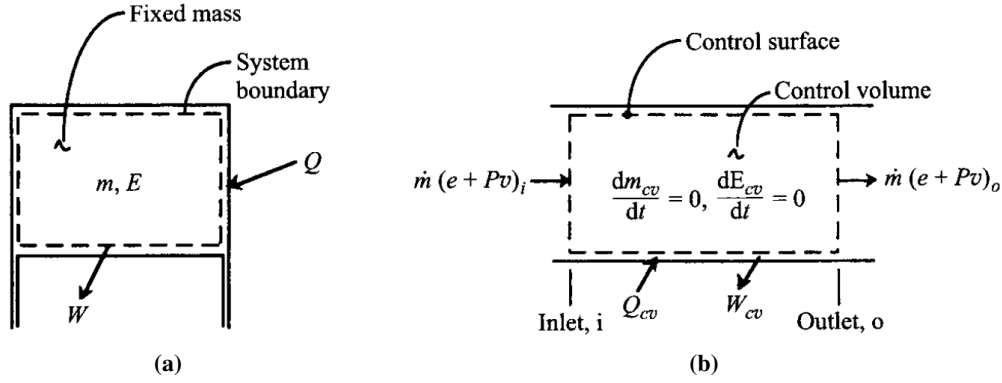


Figure 2.1: (a) Schematic of fixed-mass system with moving boundary above piston. (b) Control volume with fixed boundaries and steady flow. [15]

Then, as shown in Figure 2.1b, consider a **control volume** with fluid flowing over its borders. The steady-state, steady-flow (SSSF) variant of the first law is very relevant from past thermodynamics studies [26, 27, 28]. The SSSF first law is written as,

$$\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m}e_{out} - \dot{m}e_{in} + \dot{m}(P_{out}v_{out} - P_{in}v_{in}) \quad (2.19)$$

where $(-)_out$ and $(-)_in$ represent the outlet and inlet, respectively, and $\dot{m}$ denotes the mass flowrate. Before rewriting Eq. (2.19) in a more practical form, it is necessary to identify the key assumptions underlying this relationship:

- i) The control volume is fixed relative to the coordinate system;
- ii) The properties of the fluid at each point within the control volume, or on the control surface, do not vary with time;
- iii) Fluid properties are uniform over the inlet and outlet flow areas;
- iv) There is only one inlet and one exit stream

with that, we can rearrange Eq. (2.19) for a control volume as:

$$\dot{Q}_{cv} - \dot{W}_{cv} = \dot{m} \left[(h_{out} - h_{in}) + \frac{1}{2} (v_{out}^2 - v_{in}^2) + g(z_{out} - z_{in}) \right]. \quad (2.20)$$

and if expressing the same equation on a mass-specific basis:

$$q_{cv} - w_{cv} = h_{out} - h_{in} + \frac{1}{2} (v_{out}^2 - v_{in}^2) + g(z_{out} - z_{in}). \quad (2.21)$$

2.1.7 Absolute enthalpies and enthalpy of formation

To begin, the concept of absolute enthalpies is highly useful when working with chemically reacting systems. We can define an absolute (or standardized) enthalpy for any species as the sum of an enthalpy that includes the energy associated with chemical bonds (or lack thereof), the enthalpy of formation, h_f , and an enthalpy that is only associated with temperature, the sensible enthalpy

change, Δh_s . As a result, the molar absolute enthalpy for species i can be written as:

$$\underbrace{\bar{h}_i(T)}_{\text{Absolute enthalpy at temperature } T} = \underbrace{\bar{h}_{f,i}^0(T_{\text{ref}})}_{\text{Enthalpy of formation at standard state of reference } (T_{\text{ref}}, P^0)} + \underbrace{\Delta \bar{h}_{s,i}(T_{\text{ref}})}_{\text{Sensible enthalpy change in going from } T_{\text{ref}} \text{ to } T} \quad (2.22)$$

where, $\Delta \bar{h}_{s,i} \equiv \bar{h}_i(T) - \bar{h}_{f,i}^0(T_{\text{ref}})$.

To put Eq. (2.22) into practice, a standard reference state must be defined. We use standard-state temperature, $T_{\text{ref}} = 25 [^\circ\text{C}] = 298.15 [\text{K}]$, and pressure, $P_{\text{ref}} = P^0 = 1 [\text{atm}] = 101.325 [\text{kPa}]$, which is compatible with the Chemkin and NASA thermodynamic databases, developed in [29] and [30], respectively. Additionally, we follow the rule that enthalpies of formation are zero for elements in their naturally occurring state at the reference state temperature and pressure.

2.1.8 Enthalpy of combustion and heating values

Understanding how to describe the enthalpy for mixtures of reactants and mixtures of products allows us to define the enthalpy of reaction, or, when dealing with combustion processes, the enthalpy of combustion. Consider a steady-flow reactor in which a stoichiometric mixture of reactants enters and products leaves at standard-state conditions ($25 [^\circ\text{C}]; 1 [\text{atm}]$). The combustion process is considered to be complete, i.e., all of the fuel carbon is converted to CO_2 and all of the fuel hydrogen is transformed to H_2O . Heat must be removed from the reactor for the products to depart at the same temperature as the reactants entering. The quantity of heat lost may be linked to the absolute enthalpies of the reactant and product by using the steady-flow form of the first law Eq. (2.21):

$$q_{\text{cv}} = h_{\text{out}} - h_{\text{in}} = h_{\text{prod}} - h_{\text{reac}} \quad (2.23)$$

and the definition of the enthalpy of reaction, or the enthalpy of combustion, Δh_R (per mass of mixture), is

$$\Delta h_R = q_{\text{cv}} = h_{\text{prod}} - h_{\text{reac}} \quad (2.24)$$

The heat of combustion, Δh_c (also known as the heating value), is mathematically equivalent to the enthalpy of reaction, but with the inverse sign. The heat of combustion computed assuming that all of the water in the products has condensed to liquid is the upper or higher heating value, HHV. This scenario releases the greatest energy, therefore the title "higher." The lower heating value, LHV, represents the condition in which no water is supposed to condense.

2.1.9 Adiabatic flame temperature

Besides from the self-ignition temperature and reactant concentration limits of the mixture, another critical component is the adiabatic flame temperature, T_{af} . The energy balance between reactants and products at equilibrium determines this temperature. If the reaction zone is very narrow in comparison to the rest of the domain, the maximum temperature in the reaction zone is commonly assumed to be the flame temperature, T_{flame} .

As we'll see further on, if combustion occurs in an adiabatic burner, the flame temperature is referred to as the adiabatic flame temperature, T_{af} . This factor is the highest temperature that may be reached in a given combustion process with a given fuel, because any heat flow to the outside or incomplete combustion will reduce the reaction temperature. Additionally, it's worth noting that in many circumstances, theoretical calculations yield more accurate results than experimental measurements.

For many hydrocarbons, the maximum flame temperature occurs when slightly higher equivalence ratios than 1 are used ($\phi \approx 1.05$), due to the dissociation effect [31, 32]. In Table 2.4, we show the T_{af} values for various combinations of reactants, where the flame temperatures refer to stoichiometric mixtures and Figure 2.2 illustrates the graph that represents the relationship between T_{af} and the equivalence ratio for various fuels.

Table 2.4: Adiabatic flame temperature and Maximum flame burning speed of common reactants in a combustion reaction [33]

Reactants	Adiabatic Flame Temperature [K]	Maximum Burning Speed [m/s]
H₂ + O₂	3083	11
H₂ + Air	2380	3.1
CO + O ₂ → H ₂ O	2973	1.08
CH ₄ + O ₂	3010	4.5
C ₂ H ₂ + O ₂	3431	11.4
CO + Air	2400	0.45
CH ₄ + Air	2222	0.45
C ₂ H ₂ + Air	2513	1.58

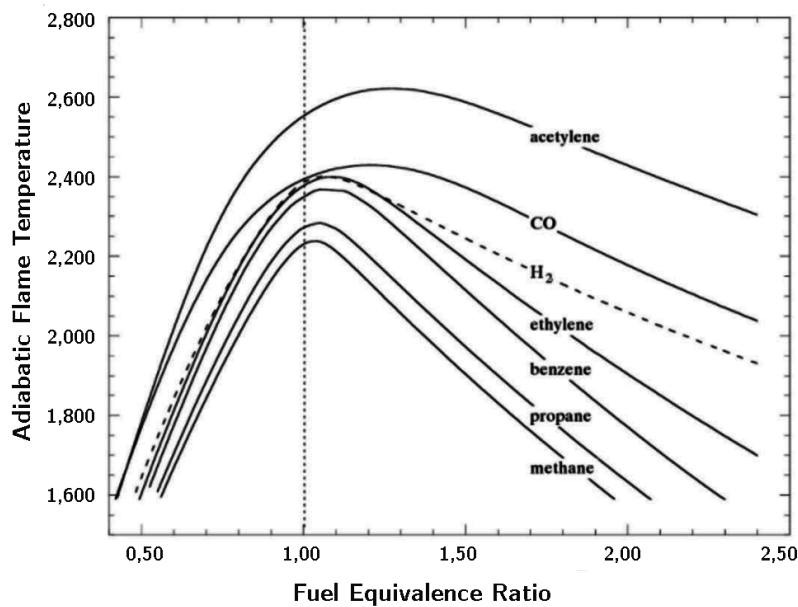


Figure 2.2: Evolution of T_{af} by varying ϕ , for various fuels [31].

2.1.10 Flame burning speed

The rate at which the flame front spreads across the fuel-air mixture is referred to as a flame's burning speed. Its speed is influenced by a number of variables, including temperature, pressure, and the chemical composition of the air-fuel mixture. It's worth noting thou that the flame speed is highly dependent on temperature, which can be varied by adjusting the equivalence ratio of the mixture. This affects the adiabatic flame temperature and thus changes the flame velocity [14]. This is illustrated in Figure 2.3 where the laminar flame speed is plotted in function of the equivalence ratio and normalized equivalence ratio, with data from multiple studies.

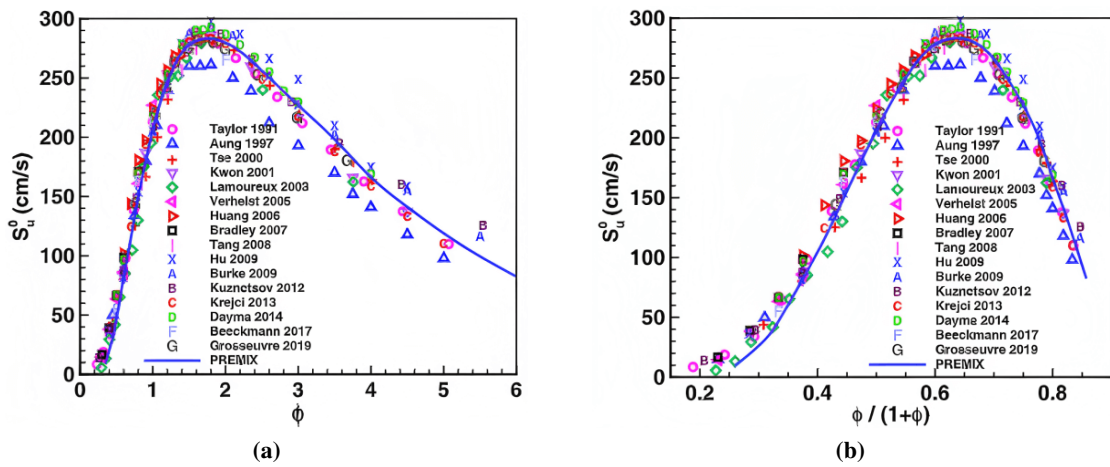


Figure 2.3: Laminar flame speed of H_2 /air at Normal Temperature and Pressure (NTP) as a function of equivalence ratio (a) and normalized equivalence ratio (b), where the symbols denote experimental results [34].

With the help of several methods, including the flat flame burner, the spherical flame burner, and the burner stabilized on a revolving disk, it is possible to evaluate the burning speed of a flame experimentally. These techniques involve determining the flame front's velocity as it passes through the fuel-air mixture [35].

The rate at which a flame burns depends on a number of variables. For instance, raising the fuel-air mixture's temperature or pressure while removing inert gases like nitrogen will result in a slower flame [36]. Flame speed can also be significantly influenced by the chemical makeup of the fuel [35].

2.2 A Review on Heat Transfer

2.2.1 Understanding heat transfer in combustion

In this Section, we extend thermodynamic analysis by delving into the modes of heat transfer. While thermodynamics deals with the end states of a process involving interactions, it does not provide insights into the nature of the interaction or its time rate. Our focus here is to explore the intricate aspects of heat transfer mechanisms.

Heat transfer, as seen in [37], is thermal energy in transit due to a spatial temperature difference. In other words, whenever there exists a temperature difference in a medium or between media, heat transfer must occur. There are three possible modes (i.e. types) of heat transfer [37], as shown in Figure 2.4:

1. Conduction: the term used to describe heat transfer across a stationary medium, which can be a solid or a fluid, when a temperature gradient is present within it;
2. Convection: refers to the heat transfer that will occur between a surface and a moving fluid with different temperatures.;
3. Radiation: encompasses the emission of energy in the form of electromagnetic waves from all surfaces with finite temperatures. Consequently, when there is no intervening medium, heat transfer occurs between two surfaces at different temperatures through radiation..

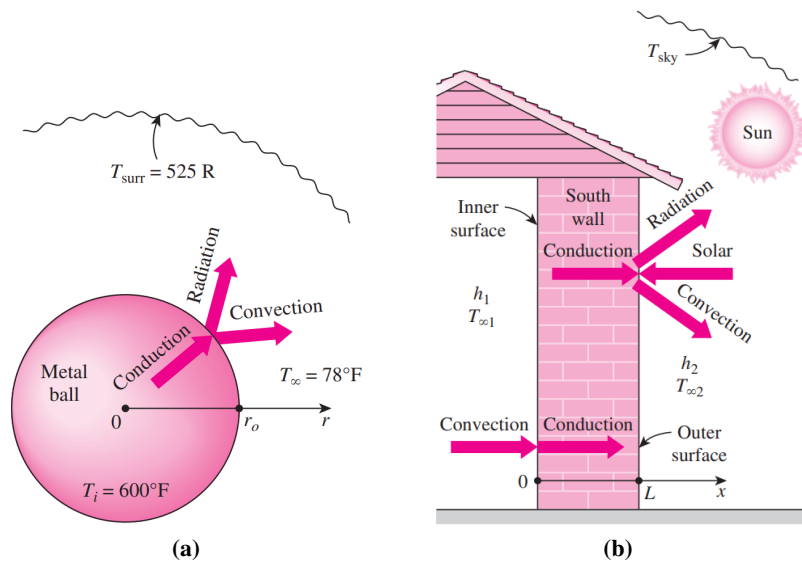


Figure 2.4: Schematics of [38] (a) Combined convection and radiation conditions; (b) Combined convection, radiation and heat flux.

2.2.2 Delving into Conduction

Conduction is a fundamental heat transfer mechanism that facilitates the flow of thermal energy from regions of higher temperature to regions of lower temperature within a body, all without causing any significant displacement of the body's molecules [39]. This process is observed in materials that are in direct physical contact, including solids, liquids, and gases [37]. As the conduction process unfolds, more energetic particles impart their energy to adjacent particles with lower energy levels, leading to the redistribution of heat throughout the medium [38].

As seen in [37], heat transfer processes can be effectively quantified through the application of suitable rate equations, enabling the computation of energy transfer per unit time. In the context

of heat conduction, the Fourier's law serves as the rate equation of reference, especially in one-dimensional plane walls applications.

$$q_x'' = -\lambda \frac{dT}{dx} \quad (2.25)$$

where q_x'' [W/m²] represents the heat flux (heat transfer rate in the x direction per unit area perpendicular to the direction of transfer) and λ [W/(m · K)] represents the thermal conductivity and is a characteristic of the wall material.

And by recognizing the heat flux as a vector quantity, we can write a more general statement of the conduction rate equation (Fourier's law) as follows [37]:

$$\mathbf{q}'' = -\lambda \nabla T = -\lambda \left(\mathbf{i} \frac{\partial T}{\partial x} + \mathbf{j} \frac{\partial T}{\partial y} + \mathbf{k} \frac{\partial T}{\partial z} \right) \quad (2.26)$$

where ∇ is the three-dimensional del operator ($\nabla = \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k}$) and $T(x, y, z)$ is the scalar temperature field.

Incorporating potential energy generation and storage within the body, the heat conduction equation in Cartesian coordinates emerges as a partial differential equation governing temperature distribution over time and space [38]. This equation is obtained through an energy balance approach, which can be done considering differential rectangular or cylindrical elements, as depicted in Figures 2.5a and 2.5b.

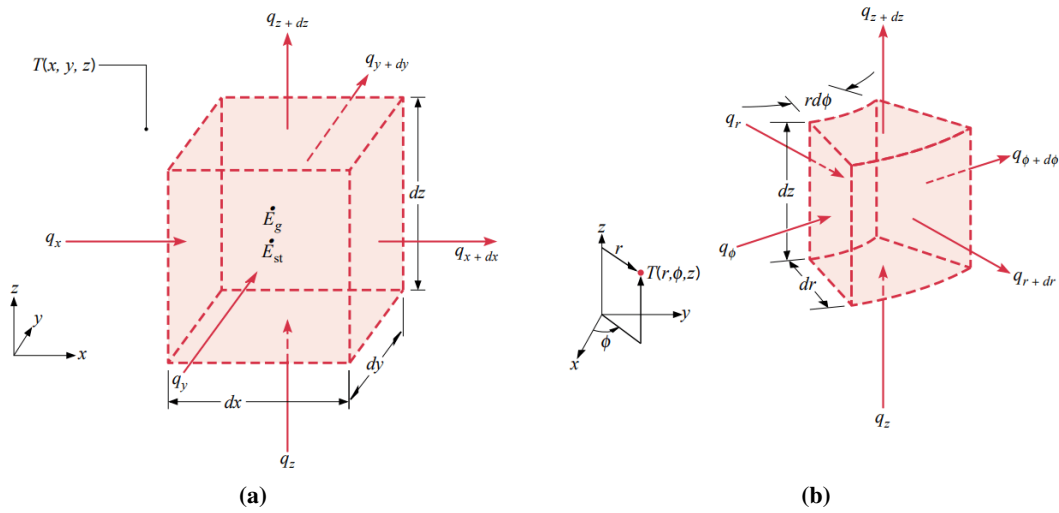


Figure 2.5: Differential control volumes [37] (a) $dx dy dz$, for conduction analysis in Cartesian coordinates (x, y, z) . (b) $dr \cdot r d\phi \cdot dz$, for conduction analysis in Cylindrical coordinates (r, ϕ, z) .

The equations for each situation are described, respectively, as follows:

$$\frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + \dot{q} = \rho c_p \frac{\partial T}{\partial t} \quad (2.27)$$

$$\frac{1}{r} \frac{\partial}{\partial r} \left(\lambda r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \phi} \left(\lambda \frac{\partial T}{\partial \phi} \right) + \frac{\partial}{\partial z} \left(\lambda \frac{\partial T}{\partial z} \right) + \dot{q} = \rho c_p \frac{\partial T}{\partial t} \quad (2.28)$$

2.2.3 Delving into Convection

Conduction and convection share a common characteristic of relying on a material medium for heat transfer. However, they differ in that convection specifically necessitates the presence of fluid motion [38]. Although convection is a complex process, the rate of heat transfer through convection, q''_{conv} [W/m²], is found to be directly proportional to the temperature difference and can be conveniently described by Newton's law of cooling as [37]:

$$q''_{\text{conv}} = h_{\text{conv}} (T_{\text{sur}} - T_{\infty}) \quad (2.29)$$

where h_{conv} [W/m²K] is the convection heat transfer coefficient, A_{sur} [m²] is the heat transfer surface area, T_{sur} [K] is the temperature of the surface, and T_{∞} [K] is the temperature of the fluid sufficiently far from the surface.

Convection can be natural/free or forced [37, 38], as shown in Figure 2.6. In natural convection, any fluid motion is caused by natural means such as the buoyancy effect, i.e. the rise of warmer fluid and fall the cooler fluid. Whereas in forced convection, the fluid is forced to flow over a surface or in a tube by external means such as a pump or fan.

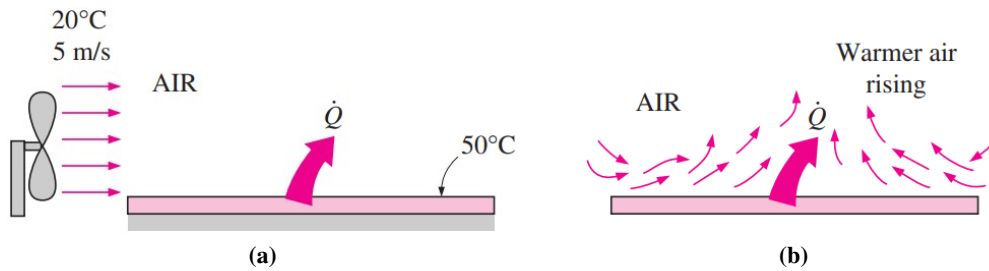


Figure 2.6: Two types of convection [38]: (a) Forced convection; (b) Free convection.

2.2.4 Delving into Radiation

As explained in [37, 38], radiation distinguishes itself from the other two heat transfer mechanisms by its independence from the presence of a material medium. Remarkably, radiation operates at the speed of light, exhibiting the fastest energy transfer, and experiences no attenuation even in a vacuum. Furthermore, radiation transfer occurs not only in gases and liquids but also within solids. In practical scenarios, all three modes of heat transfer often coexist to varying extents. However, heat transfer across an evacuated space exclusively relies on radiation. A prime illustration of this is the sun's energy reaching the Earth through radiation.

Above 0 [K], all bodies emit radiation in various wavelengths and directions. The amount of emitted radiation depends on the body's material, surface condition, and temperature [37]. To compare radiative properties, an idealized body called a blackbody is used as a standard. A blackbody is a perfect emitter and absorber of radiation. No surface can emit more energy than a blackbody at a given temperature and wavelength [38]. It absorbs all incident radiation ($\alpha_b = 1$), emits energy uniformly in all directions ($\epsilon_b = 1$), and is referred to as a diffuse emitter. In real surfaces, $0 < \epsilon_{\text{rad}} < 1$, and the radiation heat flux is given by the Stefan-Boltzmann law:

$$E_{\text{rad}}(T_{\text{sur}}) = \epsilon_{\text{rad}} \sigma T_{\text{sur}}^4 \quad (2.30)$$

where T_{sur} [K] is the surface temperature of the body and $\sigma = 5.67 \times 10^{-8} [\text{W}/(\text{m}^2 \cdot \text{K}^4)]$ is the Stefan-Boltzmann constant.

The incident radiation flux on a surface from all directions is called irradiation G . For real materials, we also consider absorptivity α_{rad} and transmissivity τ_{rad} . This leads to absorbed (G_{abs}), reflected (G_{rfl}), and transmitted (G_{tr}) portions of G . Additionally, surfaces emit radiation (E_{rad}) and reflect it, resulting in radiosity J , which represents the rate at which radiation energy leaves a unit area of the surface in all directions [38]. Refer to Figure 2.7a for the three types of radiation flux and Figure 2.7b for irradiation portions considering α_{rad} , ϵ_{rad} , and τ_{rad} .

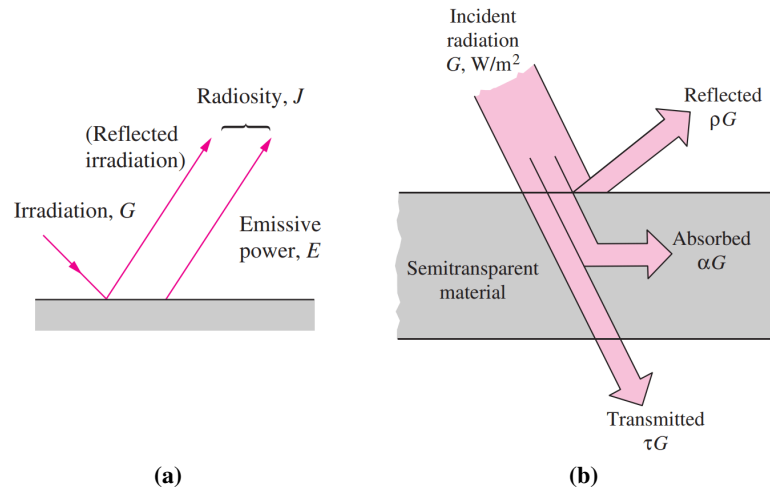


Figure 2.7: (a) The three kinds of radiation flux: emissive power, irradiation, and radiosity [38]; (b) The absorption, reflection, and transmission of incident radiation by a semitransparent material [38].

For an opaque material ($\tau_{\text{rad}} = 0$) and a grey body^(b) ($\epsilon_{\text{rad}} = \alpha_{\text{rad}}$), considering isothermal surroundings much larger than the surface, with a temperature of T_{wall} [K], the net heat flux exchanged by radiation from the surface (q''_{rad} [W/m^2]) is given by:

$$q''_{\text{rad}} = \epsilon_{\text{rad}} \sigma (T_s^4 - T_{\text{wall}}^4) \quad (2.31)$$

2.3 A Review on Microcombustion

The subsequent section builds upon the previous discourse on combustion and aims to explore the salient features pertinent to micro-combustion. Specifically, this section endeavors to explicate the concept and challenges of micro-combustion, elucidate the diverse flame types and flame behaviors associated with it, and highlight some of the present-day applications in the domains of internal combustion engines and reactors^(c).

^(b)Kirchhoff's Law [38]: The total hemispherical emissivity of a surface at temperature T equals its total hemispherical absorptivity for radiation from a blackbody at the same temperature.

^(c)In Section 2.4, a thorough examination of the current applications of microthrusters, which are associated with micro-propulsion, will be presented.

2.3.1 Definition of micro-scale Combustion

To begin with, as previously stated, several MEMS systems have been developed in recent years, and the concept of micro-scale combustion is arbitrary and thus ambiguous. This can lead to confusion, hence it is critical to define “micro-scale combustion” so that it doesn’t get mixed up with “mesoscale combustion”. Generally speaking, there are three different length scales that have been used in previous research to define “micro-scale” combustion [40]:

- i) Definition based on Physical length: A generally used characteristic to distinguish between micro-scale and meso-scale combustion is that when the length scale of the combustor is smaller than 1 mm, the combustion is referred to as micro-combustion. On the other hand, if the physical length scale is greater than 1 mm but around 1 cm, the combustion is referred to as mesoscale combustion. and is usually utilized in the development of micro-engines [41];
- ii) Definition based on the Flame quenching diameter: consists in utilizing the quenching diameter ^(d), the reference length scale for the flame [43]. Consequently, if the combustor dimensions are smaller (larger) than the quenching diameter, the combustion is referred to as micro-scale (mesoscale). This definition is more sensible in terms of the physical flame regimes and is preferred by researchers for studying the fundamental aspects of micro-combustion;
- iii) Definition based on the Device Scale: Researchers sometimes use the relative size of a device for its intended purpose compared to conventional large-scale devices as a means of defining meso and micro-scale combustion. This approach offers a third way of defining these types of combustion (often utilized by researchers who aim to design micro-thrusters for particular applications).

It’s important to keep in mind that most flows become laminar when reduced from the macro to the micro scale, and as a result, the numerical analysis of the flows is simplified when comparing with turbulent flows.

2.3.2 Challenges on microcombustion

The design and manufacture of micro burners, which have dimensions at the millimeter or submillimeter level, pose unique challenges when compared to conventional combustors, which make it not trivial to obtain a stable flame, as documented in Hossain and Nakamura [44], Ju and Maruta [40], Nakamura et. al. [45], Resende et. al. [46] and Lee et. al. [47]. These challenges extend to combustion in microscale environments, where the effects of viscosity are amplified in small channels, physical residence time of mixed gases is shortened, and the ratio of area to volume of the combustion chamber increases sharply [48, 49]. These factors have direct or indirect effects on the flame and heat release of chemical energy, thereby leading to significant differences in combustion characteristics between micro and conventional combustors [50], as will be illustrated in the following subsections.

^(d)Refers to the largest diameter of a cylindrical tube that will just quench (extinguish) the flame front of a particular fuel-air mixture [42], being a function of mixture composition and wall properties (temperature / surface reactivity) [40]

2.3.2.1 Short resistance time

Micro-combustion, characterized by its small chamber volume, exhibits a short residence time, as reported by Yun et al.[51]. This temporal constraint arises from the combined effects of diffusion and reaction times. For instance, the reaction time of H_2 or any C_nH_m species with air or O_2 falls within the range of 0.1 to 1 ms [52], which aligns with the temporal scale observed in small-scale conditions [53].

To assess the extent of fuel combustion within the combustor, one can employ the Damköhler number, denoted as Da . This dimensionless parameter represents the ratio of the residence time τ_{res} of the fuel-air mixture to the combustion time τ_c . It provides valuable insights into whether the fuel is completely consumed during the combustion process [54, 55]. The Damköhler number can be mathematically defined as:

$$Da = \tau_{res} / \tau_c \quad (2.32)$$

When the flow residence time becomes close to the characteristic combustion time ($Da < 1$), extinction will occur via incomplete combustion and the incomplete fuel is blown out, which reduces the combustion efficiency (and subsequently power generation efficiency) [56].

2.3.2.2 High heat loss ratio

Micro-combustion exhibits a notable challenge stemming from increased heat losses associated with the relatively larger surface-to-volume ratios of the combustion chamber. Consequently, it is crucial to comprehensively comprehend the underlying causes of these heat losses and explore effective mitigation strategies. The heat loss ratio of the combustor can be quantified, as presented by Li et al. [57]:

$$q\& = \frac{Q}{m} = \frac{\int_{S_{ch}} q\& dS_{ch}}{\int_{V_{ch}} \rho dV_{ch}} = \frac{\overline{q\&''}}{\bar{\rho}} = \left(\frac{S_{ch}}{V_{ch}} \right) \quad (2.33)$$

where, $q\&$ is heat loss density, $\overline{q\&''}$ is the average heat loss density, S_{ch} is the inner surface area of the combustor, and V_{ch} is the chamber volume.

Besides, the hydraulic diameter of a burner can also be employed to compare the combustion heat release rate and the heat dissipation rate:

$$\frac{E''}{E'} \propto \frac{1}{d_h^{1.2}} \quad (2.34)$$

where, E' is the mixture combustion heat release rate, E'' is the heat dissipation rate of the inner wall, and d_h is the interior wall heat dissipation rate.

As the size of the combustion chamber decreases in the micro-scale range, the surface-to-volume ratio (S/V) undergoes a rapid increase. Consequently, as indicated by Eqs. (2.33) and (2.34), the heat loss ratio of the combustor substantially amplifies with the reduction in burner size (d_h)^(e). This phenomenon accelerates the dissipation of heat from the inner wall.

^(e)For a conventional burner, the S/V is approximately 3 to 5 [m^{-1}], while it reaches 500 [m^{-1}] under the micro condition of the combustor [58]

2.3.2.3 Weak flame stability

The stability of micro-combustion depends on reactions, heat transfer, and the interaction between burned and unburned gases [59, 60]. Factors like flow fields, temperature, and species distribution in microchannels can cause combustion instabilities such as flame blowout, oscillations, and asymmetric distribution [61, 62].

High heat loss from combustor walls can lead to non-self-sustaining combustion, including thermal or radical extinction in small chambers [63]. Radical extinction occurs when active radicals are absorbed by the inner wall, hindering their reactivity. External wall heating is proposed to enhance flame stability [64].

The increased surface-to-volume ratio in micro-combustion intensifies wall heat losses and radical collisions, affecting flame extinction and micro power systems [65, 66]

2.3.3 Typical length and time scales and phenomena

Micro-combustion, akin to its conventional-scale counterpart, encompasses a plethora of physical and chemical processes that exert direct influence on the observed phenomena. These processes comprise gas-phase and surface reactions, molecular transport, thermal and mass diffusion, as well as convection and radiation effects [40]. In Table 2.5 we list some important length and time scales which strongly affect the phenomena of micro-scale and mesoscale combustion:

Table 2.5: Typical length and time scales in micro-scale combustion, adapted from Ju et al. [40]

Time Scales	Length Scales
Flow residence time, τ_{res}	Combustor scales ^(e) , d
Characteristic combustion time, τ_c	Combustor structure scales ^(f) , d_s
Diffusion time scale of gas-phase, $\tau_\alpha = d^2/\alpha_f$	Flame thickness, δ_f
Diffusion time scale of solid-phase, $\tau_s = d_s^2/\alpha_s$	Quenching diameter ^(g) , $d_0 = n\delta_f$
Time scale of heat loss ^(h) , τ_h	Mass diffusion length, δ_D
Time scale of acoustic wave ⁽ⁱ⁾ , τ_a	Thermal diffusion length, δ_α
Ignition time scale, τ_{ig}	Mean free path, λ_{fp}
Characteristic flow time, τ_f	-

Small-scale combustion is influenced by length and time scales [40], as shown in Table 2.6. For instance, when the combustor size is close to the flame thickness or quenching diameter, flame extinction or instability can occur due to wall heat loss and/or radical quenching. Moreover, there's limited fuel-oxidizer mixing. The coupling of wall heat loss and auto-ignition at isolated hot spots causes steady/unsteady flame streets to appear. Furthermore, decreasing the combustor structure

^(e)Characteristic size of combustor inner diameter

^(f)Characteristic length scale of the structure (solid phase)

^(g)The quenching diameter, which is contingent upon the wall temperature, is typically several times (n) the flame thickness. In the case of a wall temperature corresponding to room temperature, n is approximately 15.

^(h)Is a function of convective and radiative heat losses

⁽ⁱ⁾Depends both on the span-wise and streamwise dimensions of the combustor

leads to multiple flame regimes and a strong flame-wall coupling, expanding the flammability limit. Higher wall temperatures result in shorter ignition times and the possibility of weak flames or flameless combustion. Flame instability arises when ignition time approaches flow residence time and the combustor size nears the quenching limit. The Biot number governs the coupling between wall temperature and flame, while the Fourier number affects the wall temperature distribution.

In small-scale combustion, non-equilibrium transport effects become important at reduced sizes (Knudsen number > 0.01), influencing ignition and extinction. Micro-scale combustion exhibits incomplete combustion and thermal-diffusional instability when flow residence time approaches characteristic combustion time. The Lewis number effect and solid phase thermal transport significantly impact flame stability boundaries. Spinning and pulsating combustion occur for low mixture Lewis numbers. Wall confinement and high temperatures introduce strong acoustic wave effects. Understanding these phenomena requires analysis of relative length and time scales or consideration of unsteady temperature distribution in the solid phase [40].

Table 2.6: Non-dimensional parameters vs. micro-scale combustion phenomena, from Ju et al. [40]

Non-dimensional numbers	Phenomena
$d/\delta_f \sim O(10)$ or $d/d_0 \sim 1$	Flame extinction due to heat loss to the wall Wall catalytic/quenching effects, flame street & cells
$\tau_c/\tau_s = O(1)$, $d/d_0 \sim 1$	Flame-wall thermal coupling, multiple flame regime
$\tau_{ig}/\tau_{res} = O(1)$, $d/d_0 \sim 1$	Extinction and reignition instability, Weak flame Flameless combustion
$Bi = \tau_\alpha/\tau_h \gg 1$	Small wall temperature change
$Fo = \tau_c/\tau_s \gg 1$	Steady-state temperature distribution in solid phase
$Kn = \lambda/d > 0.01$	Non-equilibrium transport effect
$Da = \tau_{res}/\tau_c$ or $\tau_D/\tau_c \sim 1$	Flame extinction due to incomplete combustion
$Le = \delta_\alpha/\delta_D \sim 11$	Pulsating instability via flame structure coupling
$\tau_a/\tau_c = O(1)$	Acoustic instability

2.3.4 Flammability limits in micro-combustion and quenching diameter

The standard flammability limit defines the boundaries for lean or rich flame propagation limits in a one-dimensional, infinite, planar, and unstretched flame. Extensive research [43, 67, 68, 69, 70] has determined that radiating species like H_2O and CO_2 contribute to these limits.

The relationship between the mass burning rate (flame speed) and the adiabatic mass burning rate (flame speed) can be expressed as a function of the normalized radiative heat loss, H , divided by the total chemical heat release, as shown in Eq. (2.35).

$$U_{fl}^2 \ln U_{fl}^2 = -\beta H \quad (2.35)$$

In micro-scale combustion, heat loss occurs not only due to radiation but also due to convection and conduction losses to the channel wall. By normalizing the convective heat loss by the chemical heat release, researchers found it to be proportional to the square of the ratio of flame thickness to the channel diameter. As such, assuming a constant flame thickness for a given mixture, the flame speed is influenced by the channel diameter [40].

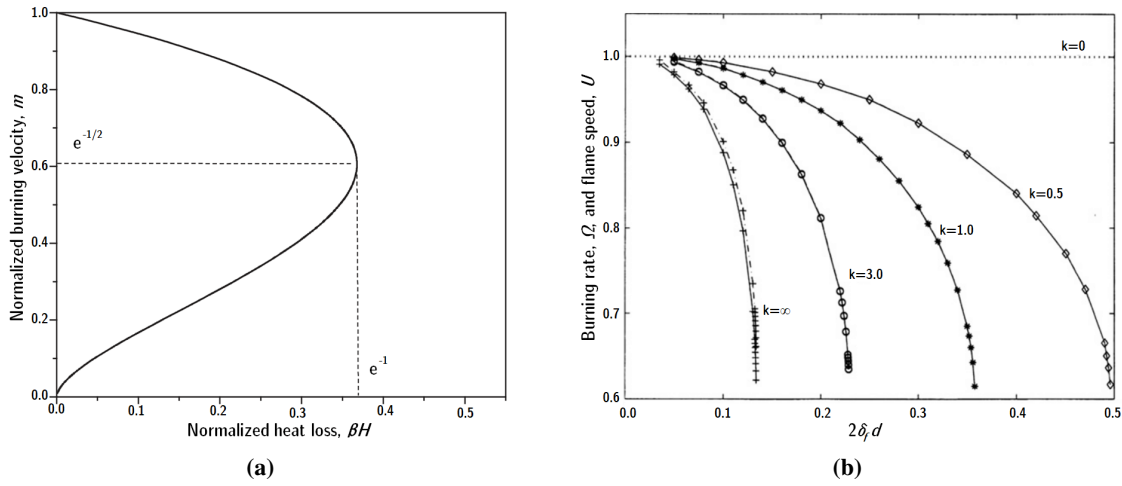


Figure 2.8: (a) The dependence of the normalized burning velocity on the normalized radiative heat loss of a one-dimensional planar flame [40]; (b) Burning rate, solid line, and normalized flame propagation speed U_{fl} , dash-dotted line, plotted against the ratio of flame thickness to channel width, d , for selected values of reduced heat transfer coefficient, k , with in a quiescent, two dimensional channel flow [71].

Further analysis from Figure 2.8a indicates that the propagation limit corresponds to a limiting tube diameter, d_0 , also known as the quenching diameter. Below this critical diameter, the flame fails to propagate in the channel, Ju et. al [40].

The size of a flame depends on how easily heat spreads (thermal diffusivity) and how fast the flame burns (flame speed), which in turn is influenced by the amount of fuel and its temperature. This means the quenching diameter, where the flame can no longer sustain itself, is determined by the fuel concentration and the properties of the fuel itself.

In Figure 2.8b shows how the flame speed in a quiescent channel depends on its width (d) and the convective heat loss (k), which is proportional to the Nusselt number (Nu), as mentioned previously. When the wall is adiabatic ($k = 0$), there is no heat loss from the flame to the wall, the flame speed does not depend on channel width (Nu = 0). With increasing heat loss, the flame speed decreases until there's a critical channel width where the flame can't propagate [71].

At high convective heat transfer ($k = \infty$), the flame extinguishes at $U = 0.6$, resulting in a quenching channel width of $2\delta_f/d_0 = 0.13$, or using the convention set in Table 2.6, $d_0/\delta_f = 15$, consistent with theory and experiments. Near-wall flame quenching occurs within 6% of the channel radius in a cold wall scenario. Additionally [71], the flow velocity and direction also affect the quenching diameter; flames are more vulnerable to heat losses when the flow moves

from the unburned to the burned side, and the quenching distance increases with higher flow rates. These findings match experimentally reported values [72].

2.3.5 Classification of flame types

Diffusion and premixed flames are two different kinds of micro combustion flames. In a premixed flame, combustion takes place after the fuel and oxidizer have been combined. The fuel and oxidizer in a diffusion flame are kept apart and only mixed as they get closer to the reaction zone [31].

The two subtypes of premixed flames are turbulent premixed flame and laminar premixed flame, as shown in the next page in Figures 2.9a and 2.9b. A laminar premixed flame is one in which the fuel and oxidizer mixture flows uniformly and without turbulence. In a turbulent premixed flame, on the other hand, the mixture of fuel and oxidizer is turbulent, meaning that it is characterized by random fluctuations in velocity and pressure [73].

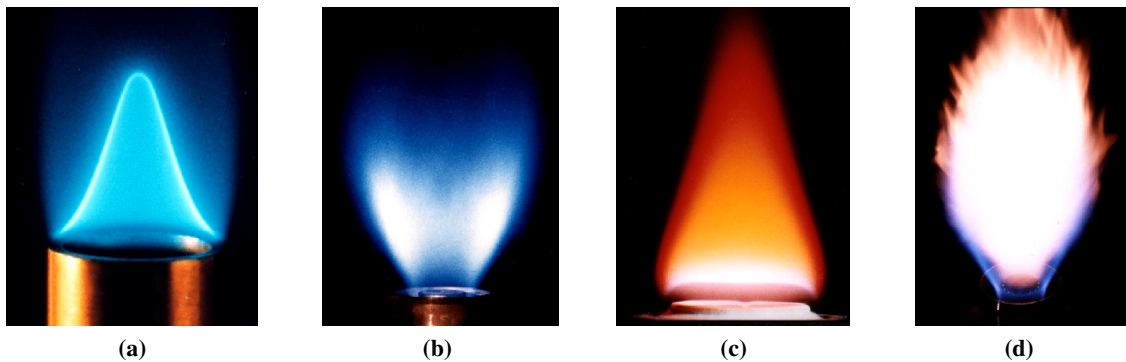


Figure 2.9: Differences in Premixed and Diffusion flames: (a) Laminar premixed flame. (b) Turbulent premixed flame. (c) Laminar diffusion flame. (d) Turbulent diffusion flame [74].

Conversely, the separation of the fuel and oxidizer is what distinguishes a diffusion flame. When approaching the reaction zone, where combustion occurs, the fuel and oxidizer are only briefly mixed. Because of natural molecular diffusion, which is fueled by the concentration gradient of the two species, the fuel and oxidizer in a diffusion flame mix together [15]. Diffusion flames can also be classified into two types: laminar diffusion flame and turbulent diffusion flame, as shown in Figures 2.9c and 2.9d.

Premixed and diffusion flames each have benefits and drawbacks. Premixed flames are commonly more efficient because they offer a more uniform mixture of fuel and oxidizer, which promotes faster combustion and less pollution. They may also have a smaller operating range and be more prone to explosions. While diffusion flames are typically more stable and capable of a wider range of operations, they may also be less effective and more polluting [31].

In the context of this dissertation, we limited the analysis to premixed flames exclusively, and all mixtures were, as such, previously mixed. Therefore, it is imperative to note that in the upcoming subsection, any discussion concerning the characteristics of micro-flames will pertain solely to premixed flames.

2.3.6 Classification of micro-flame behaviours

The microflame is a complex phenomenon that can exhibit different behaviors, which are influenced by multiple factors, such as the input velocity of the fuel-oxidizer mixture, the heat flow rate supplied to the mixture, the thermal conduction coefficient of the burner walls (i.e., boundary conditions), the burner geometry, among others. Thus, the present subsection aims to present a review of the possible behaviors of flames in microchannels, based on previous scientific research.

2.3.6.1 Flashback and blow-off

Premixed flames can experience situations where the reactant supply velocity exceeds or falls short of the flame speed, resulting in two possible scenarios for flame extinction [75]:

- i) Flashback: This occurs when the velocity of reactants supplied to the burner chamber is lower than the flame speed. As a result, the flame propagates upstream towards the fuel injection system, burning the reactants in a zone increasingly upstream, possibly self-extinguishing. ^(k)
- ii) Blow-off: In this scenario, the reactants supply velocity is higher than the flame speed. The flame moves along the channel, burning the reactants in a zone increasingly downstream until it “blows off” (possibly self-extinguishing) when the fuel flow rate exceeds a certain limit.

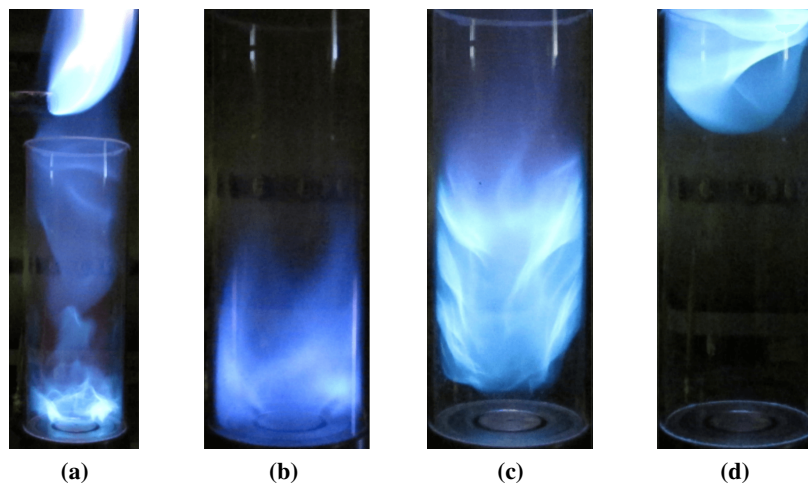


Figure 2.10: Flashback and Blow-off for flames with fixed swirl: a) flashback; b) before flashback; c) stable flame; d) after blow-off [77].

2.3.6.2 Steady versus non-steady flames

Combustion can be classified as Steady or Non-steady/Unsteady, which can be latter divided into Periodic, Quasi-Periodic and Chaotic. Non-steady flames show fluctuations in their behavior, such as changes in their burning rate or flame shape that happen over time, in contrast to steady flames, which keep a consistent burning pace [78].

^(k)It is important to acknowledge that flashback can be triggered by combustion instabilities as well. Combustion instability-induced flashback is connected to the phenomenon of the instantaneous axial flow velocity experiencing significant reductions, sometimes even reaching negative values, during large-amplitude oscillations [76].

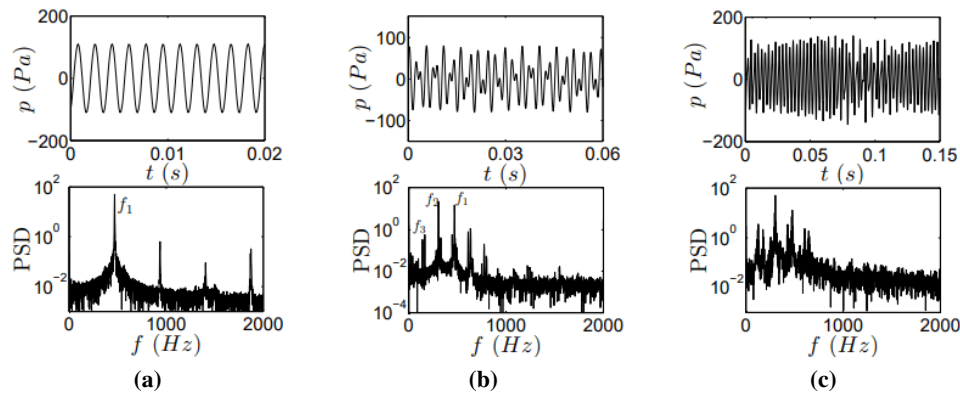


Figure 2.11: Time-spectrum (up) and Power Series (down) for different Non-steady combustion modes in ducted premixed flames: a) Periodic; b) Quasi-periodic; c) Chaotic [79].

As illustrated in Figure 2.11, Non-steady flames can exhibit different types of dynamics, including periodic, quasi-periodic, and chaotic behavior [80]:

- i) Periodic flames, which are characterized by fluctuations in their behavior that occur periodically over time, in a constant pattern;
- ii) Quasi-periodic flames, in which the oscillations present irregular periodicity and recurrence are observed;
- iii) Chaotic combustion, that can occur when steady combustion waves lose stability and transition to non-steady chaotic burning, exhibiting highly irregular and unpredictable behavior.

The transition from steady to non-steady burning can be predicted using nonlinear stability theory [78].

2.3.6.3 Mild combustion

Mild combustion, also called flameless combustion, is a combustion mode that is distinguished by a relatively small temperature rise and an incomplete but considerable fuel conversion. It is generally observed at low inflow velocities and exhibits an axisymmetric shape. This mode has been identified in numerous research studies, and is typically characterized by a lack of a distinct temperature peak, as documented in [81]. It is a potentially beneficial flame type for applications requiring a weak heat source in microsystems.

On the other hand, the combustion process is contingent upon two critical factors [82, 83]: the reactants must be preheated above the temperature at which they will self-ignite, and enough inert combustion products must be incorporated into the reaction area to saturate the flame.

Furthermore, it is noteworthy to mention High Temperature Air Combustion, a technique that often leads to mild combustion scenarios, characterized by the synergistic utilization of highly preheated air and exhaust gas recirculation (EGR) in furnaces, resulting in high thermal efficiency and low NO_x emissions [84, 85].

The phenomenon of interest was first observed in micro-scale systems in Maruta et. al. [86]. The authors conducted a comprehensive investigation into the combustion characteristics of such

systems employing experimental, numerical and analytical techniques. Specifically, a narrow cylindrical quartz channel with a fixed temperature gradient was utilized, possessing an inner diameter of 2 [mm]. For sufficiently low velocities in the range of 2 – 3 [cm/s], it was observed that a sharp temperature gradient did not form between the chamber's walls and the gas phase. The article by Pizza et al. [87] explored the combustion modes that occur in the three-dimensional combustion of premixed hydrogen and air in open cylindrical microtubes^(f). The researchers identified a particular type of mild combustion in both narrow and wider tubes with diameters of 1.0 [mm] and 1.5 [mm], respectively, when using the lowest air inlet velocities, which were $0.5 [\text{cm} \cdot \text{s}^{-1}] \leq U_{\text{in}} \leq 1.0 [\text{cm} \cdot \text{s}^{-1}]$. The maximum temperature increase ranged from 1.5 [K] and 2.5 [K] (for U_{in} of $0.5 [\text{cm} \cdot \text{s}^{-1}]$ and $1.0 [\text{cm} \cdot \text{s}^{-1}]$, respectively).

The findings were consistent with the antecedent investigations conducted by the authors in their prior 2D study [88], wherein the phenomenon of Mild Combustion was also observed for low inlet velocities. The authors examined the dynamics of premixed Hydrogen/Air flames in a microchannel that is confined between two parallel, infinitely wide plates, and maintained a constant length-to-height aspect ratio of $L/h = 10 [-]$.

2.3.6.4 Stable flames

Upon initiation of combustion, the flame undergoes movement either upstream or downstream before stabilizing at a particular location on the burner, as reported numerically by several studies [89, 90] and experimentally observed in Maruta et. al. [86]. This constitutes the simplest form of micro-flame behavior and is illustrated schematically in Figure 2.12.

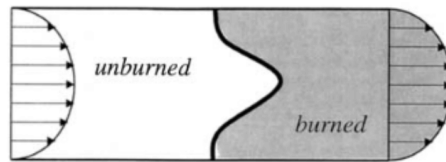


Figure 2.12: Schematic representation of a stable micro-flame [91].

Typically, flames of this type exhibit a reduction in flame temperature as inlet velocity increases, which can impact heat transfer to the wall [92]. Additionally, distinct velocity profiles can influence flame propagation and structure [93]. As seen in Norton et. al. [94], an increase in inlet velocity necessitates a greater distance for incoming gases to preheat, leading to downstream stabilization of the flame. This stabilization results in higher wall temperatures at the flame location and lower heat losses, ultimately leading to increased reaction rates and elevated flame temperatures, exceeding the adiabatic flame temperature [92].

This phenomenon, which can exhibit symmetric and asymmetric characteristics (or both, depending on the axis, if in 3D settings), has been observed both numerically, experimentally, and analytically in multiple studies such as Lewis and Von Elbe [70], Kurdyumov et. al. [95, 96],

^(f)The wall temperature was controlled by gradually increasing it from the temperature of the incoming mixture T_{in} to a final value of 960 [K] over the initial 1/20 length of the domain. This was achieved by applying a hyperbolic tangent function to smoothly ramp up the wall temperature

Dogwiller et. al. [97] and Tsai [98]. The previously mentioned articles by Pizza et al. [87, 88] and the experimental observations by Maruta et al. [81, 86] also corroborate since the phenomenon was also identified in these studies.

2.3.6.5 FREI: Flames with repetitive extinction and ignition

Flames with repetitive extinction and ignition (FREI) refer to a specific type of flame behavior characterized by the repeated extinguishing and reignition of the flame, and this phenomenon is observed in various systems, including micro flow reactors and lean premixed hydrogen-air combustion [40, 99, 100].

In the region characterized by the FREI phenomenon, a distinctive behavior of the flame is apparent: it ignites in a downstream region, propagates towards the unburned gases, and eventually extinguishes in an upstream region. Over the course of simulation, it becomes evident that the flame consistently occupies the same region, with the phenomenon recurring cyclically. Within the scope of this investigation, given that the employed burner possesses an undulating geometry (expounded upon in Section 4.7), a unique behavior is observable due to the emergence of vortices within the microchannel cavity. Following ignition, the flame is transported through these vortices to an upstream position, ultimately leading to its cessation.

Maruta et al. [86] first captured experimentally FREI flames in a straight micro-channel. These flames exhibit cyclic behavior with luminescence starting at "ignition," moving upstream to "extinction," and then reigniting after a delay. This cyclic process, illustrated in Figure 2.13b contrasts with the stable flame behavior shown in Figure 2.13a. Furthermore, other experimental investigations established that the dynamics of FREI also manifest in curved mesoscale channels [101] and later in mesoscale cylindrical combustors featuring a backward-facing step [102].

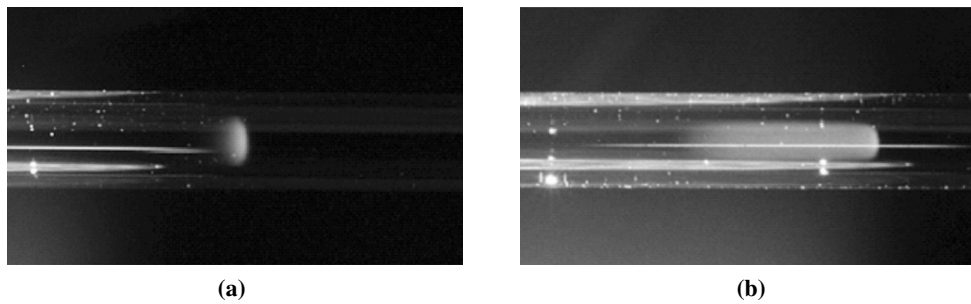


Figure 2.13: Direct photographs of [86]: (a) stable flame; (b) FREI.

Numerous advancements in the computational field have been achieved in probing this phenomenon utilizing lean hydrogen/air premixed flames, allowing a better understanding of the FREI phenomena. Minaev et al. [103] provided a theoretical interpretation of FREI. They analyzed non-stationary behavior of near-limit premixed flames in a microchannel with a temperature gradient. Their theoretical work resulted in a 1D nonlinear evolutionary equation for the flame front, explaining flame stabilization, nonlinear oscillations, and the repetitive extinction-ignition phenomena observed in experiments. Later, Jackson et al. [104] numerically investigated FREI dynamics

in a thermally active semi-infinite channel. They found stable solutions at specific flow rates, instability leading to oscillations or extinction-reignition flames at higher flow rates, in alignment with experimental observations. The studies by Pizza et al., as mentioned earlier, observed FREI dynamics in planar micro combustors with prescribed wall temperature at various channel heights [88] and also in 3D cylindrical microtubes [87]. Miyata et al. [105] performed direct numerical simulation to investigate FREI characteristics in a narrow circular channel, where they varied the wall temperature gradient and the inflow temperature in their study.

In a subsequent study, Alipoor and Mazaheri [99] scrutinized the FREI phenomenon through a singular simulation, affording a more intricate analysis of alternating extinction and ignition. In pursuit of this, contour maps of hydroxide radical (OH) concentrations were examined along the channel for various time instances, as shown in Figure 2.14. Furthermore, an investigation into heat release rate profiles, fluid and wall temperatures, and molar concentrations of pertinent species central to the reaction was undertaken. Subsequently, flame bifurcation was evaluated from a hydrodynamic standpoint utilizing flow velocity vectors.

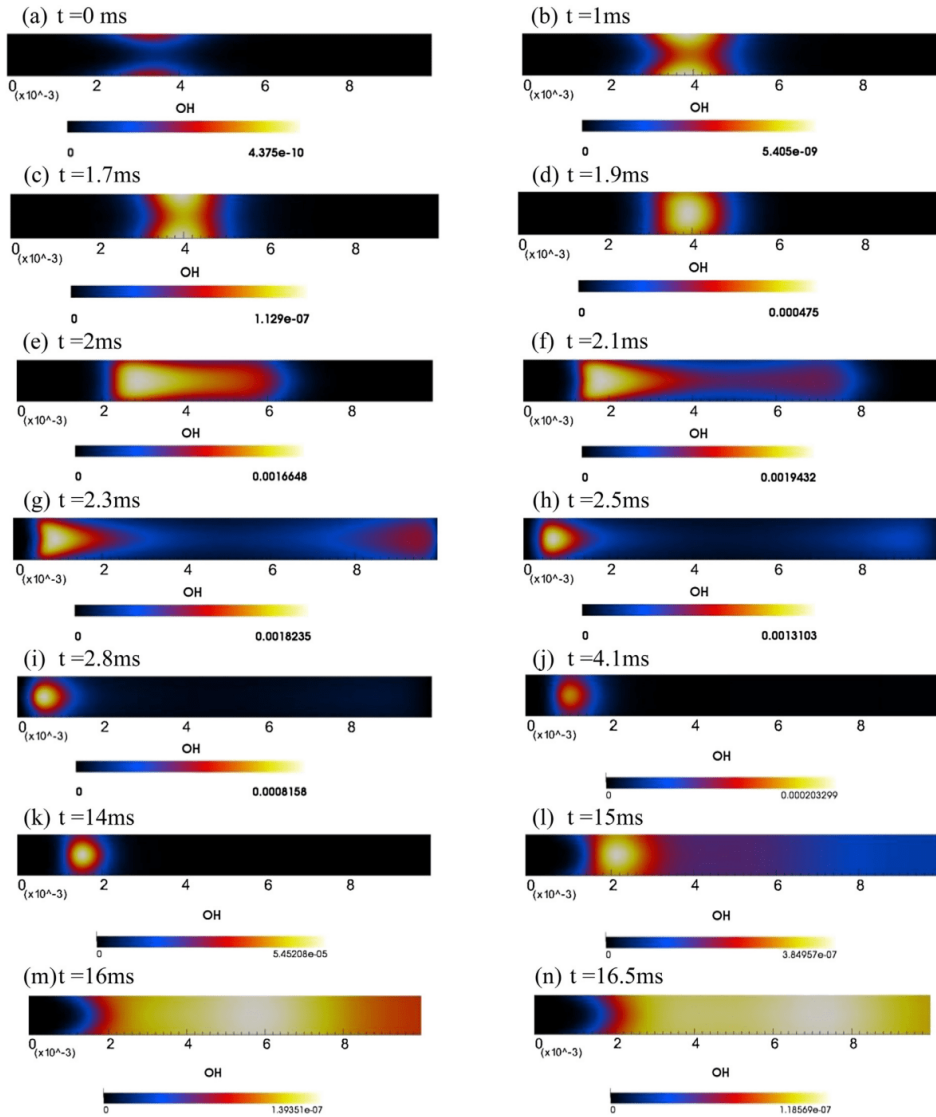


Figure 2.14: Repetitive extinction-ignition dynamics using hydroxide mass fraction (Y_{OH}) [99].

Subsequently, the same authors [106] delved into flames featuring equivalence ratios ranging from 0.5 up to the stoichiometric condition of $\phi = 1$, in microchannels with widths spanning 0.4 to 1 mm. The accrued findings illustrated that augmentations in equivalence ratio and burner width increased the amplitude of the FREI phenomenon while reducing its frequency. Furthermore, this examination illuminated that the phenomenon engenders fluid recirculation zones and flame bifurcation due to the presence of heavier species. These species exhibit an elevated heat absorption capacity, thereby inducing temperature reduction.

Later, Alipoor and Mazaheri [107] conducted a comprehensive study concerning these flames within a heated microchannel possessing a hyperbolic temperature profile. Within this inquiry, three distinct flame behaviors were observed, including the FREI phenomenon. This phenomenon manifested under low velocities near the lower flammability limit. In pursuit of a deeper comprehension of the phenomenon's causality, diverse simulations were performed, manipulating three key parameters: inlet velocity, equivalence ratio, and microchannel width. Elevating the velocity led to escalated reaction intensity, consequently inducing rapid flame front extinction. Increasing the equivalence ratio from 0.5 to 0.6 resulted in enhanced flame speed due to the augmented burning rate of the flame front, thus validating its accelerated extinction.

Beyond hydrogen utilization as a fuel, the prospect of employing alternative fuels in microcombustion studies is viable. The FREI phenomenon was also observed in the research conducted by Biswas [108]. In this instance, a CH₄/air mixture was employed, with ignition achieved through spark insertion into the burner. The combustion of this mixture under stoichiometric conditions was examined within both a linear microchannel and a microchannel characterized by a contraction (convergent-divergent).

Additionally, other computational investigations have been conducted to enhance the comprehension of the FREI phenomenon across diverse fuel types. Nakamura et al. [109], Tsuboi et al. [110], and Miyata et al. [105] undertook analyses involving CH₄ and air mixtures. Initially, they employed a one-dimensional model, subsequently validated against their experimental findings. Subsequently, they exclusively utilized direct numerical simulations to scrutinize the impact of boundary conditions—such as inlet temperature and wall temperature gradient—on the flame dynamics. The combustion characteristics of n-heptane-air were subject to experimental and numerical inquiry by Yamamoto et al. [111], wherein they also noted the manifestation of FREI dynamics.

2.3.6.6 PFB: pulsatory flame burst

The phenomenon known as Pulsatory Flame Burst (PFB) is a specific flame behavior characterized by burst-like flame pulsation due to flow and combustion interactions. As of currently, PFB only occurs in undulating geometries with premixed hydrogen and air, and the flame bursts involve the ignition, propagation, bifurcation (splitting), and extinction of the flame in a cyclic manner. Unlike FREI, where the flame extinguishes upstream, in PFB, a new flame emerges before the current one extinguishes. This prevents complete extinction, marking a significant difference.

PFB though initially observed without distinction from FREI, was first identified by Macedo in the course of micropropulsion studies conducted with wavy geometries [112], involving various inlet velocities and equivalence ratios, using a mixture of H_2 and air. The geometry used is similar to our research, and it was incorporated different wall conditions (hyperbolic and linear temperature profiles, as well as adiabatic conditions). Under the linear profile and adiabatic conditions, some simulations exhibited the phenomenon of PFB. This suggests that the microchannel geometry recirculates combustion energy, preventing flame extinction by flame lifting at higher speeds. Regarding propulsion capacity, it was found that increasing both the inlet velocity and equivalence ratio contribute to higher propulsion indicators. This underscores the significance of PFB, as pulsating flames exhibit substantial peaks in specific impulse.

Only in a subsequent study by Resende et al. [113], PFB was accurately identified and named. This investigation delved into stable and pulsatory flame burst behaviors within an undulating geometry, utilizing premixed hydrogen and air (with an equivalence ratio of $\phi = 1.0$) and applying a linear temperature profile along the wall. The findings revealed that, at a lower inlet velocity (4 [m/s]), the flame maintained stability, while at higher velocities, it exhibited pulsatory burst dynamics. The interplay between fluid dynamics and combustion response proved crucial, particularly due to vortices generated by the nonlinear burner geometry. With increased inlet velocity, the heat release rate transmitted through the vortices diminished, leading to ignition delay. This was evident through reduced pulsatory burst frequency and heightened peak heat release rate, albeit not substantial enough to amplify the maximum temperature amplitude. In Figure 2.15 and 2.16 it's presented the results of a typical PFB flame, as reported in [113].

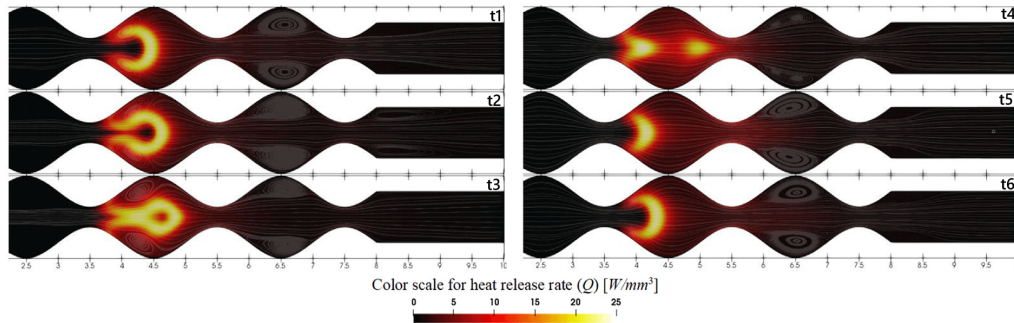


Figure 2.15: Streamlines of the flow field and heat release rate distribution for the pulsatory flame burst dynamics with $U_{in} = 6$ [m/s], with 10 ms intervals [113].

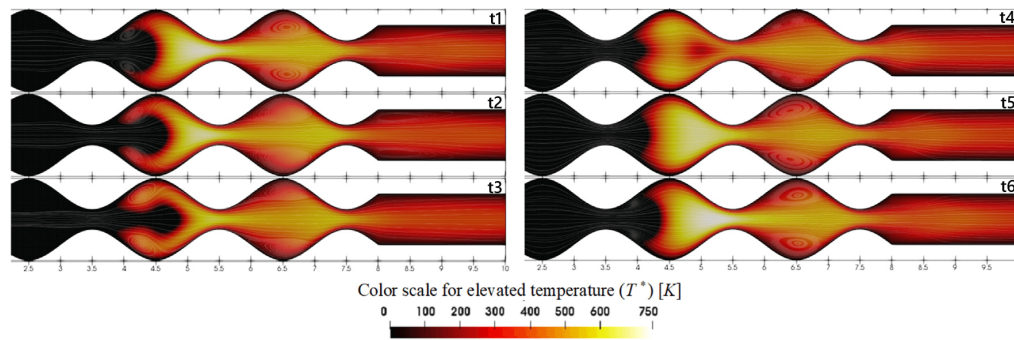


Figure 2.16: Streamlines of the flow field and temperature distribution for the pulsatory flame burst dynamics with $U_{in} = 6$ [m/s], with 10 ms intervals [113].

2.3.7 Investigations in microcombustion

Li et al. [114] conducted numerical investigations into the combustion characteristics of hydrogen/air premixed flames in microtubes and parallel-plate microchannels with hydraulic diameters less than one millimeter. The results showed that microtubes lead to higher flame and wall temperatures, in comparison to parallel-plate microchannels. In subsequent studies, Li et al. [115] performed a similar investigation using methane as the fuel, finding higher temperatures in parallel-plate microchannels. Moreover, the upper flammability limit of the hydrogen/air mixture was higher than that of methane due to hydrogen's faster burning rate.

The wall thickness of the burner, flame thickness, and hydraulic diameter are of the same order of magnitude in microcombustion chambers. Therefore, heat transfer through the wall and heat recirculation have a significant impact on combustion sustainability and its characteristics. Ronney [116] demonstrated that for burners with counterflow zones and heat recirculation, heat conduction through the wall in the direction of flow has a crucial effect on flammability limits, particularly in flows with low Reynolds numbers.

To investigate the effect of heat recirculation on flammability limits, Kim et al. [117] experimentally studied the use of Swiss-roll microburners with channel widths smaller than the extinction diameter for propane/air combustion. Here it was found that a stable propane/air flame could be observed in channels with dimensions smaller than the quenching diameter for a wide range of inlet velocities and equivalence ratios, primarily due to heat recirculation. Kuo and Ronney [118] also numerically investigated heat recirculation in a Swiss-roll microburner and suggested that heat conduction along the burner wall, dividing the reactant flow from the reaction product flow, reduces the reaction temperature and extends extinction limits.

Recently, the use of catalyst-containing surfaces [119, 120] has been studied for potential application in Swiss-roll burners. In Pizza et al. [121, 122], it was found that instabilities in hydrogen/air premixed flames in parallel-plate burners could be avoided through the use of catalysts. Zhou et al. [123] experimentally and numerically tested three microburners with copper, alumina, and quartz catalysts, confirming the advantages of catalyst utilization in combustion.

Flow recirculation zones, as well as low-velocity zones achievable through combustion chamber design, are highly effective techniques for flame stabilization. One common technique involves the insertion of a backward-facing step in the burner walls. In this regard, Yang et al. [124] experimentally investigated the enhancement of a thermophotovoltaic microcombustion system's efficiency using a backward-facing step in the combustion chamber. They concluded that the step insertion is useful for controlling the flame position and extending flammability limits. An experimental study on wall temperature and radiation heat flux from cylindrical microburners with a backward-facing step, conducted by Li et al. [125], revealed that optimal efficiency occurs at an equivalence ratio of 0.8, regardless of burner dimensions and flow velocity. Furthermore, it was found that the backward-facing step is helpful in stabilizing flame positions. Khandelwal et al. [126] experimentally investigated flame stabilization in a microtube with three steps and found that flammability limits increase with the number of steps inserted in the reaction zone. Farazpour et al. [127] conducted a numerical study on the effects of microburner geometry and inlet velocity on flame position and radiation efficiency. The results showed that the presence of

the backward-facing step stabilizes the flame at high velocities, increases the average outer wall temperature, and anchors the flame closer to the burner inlet.

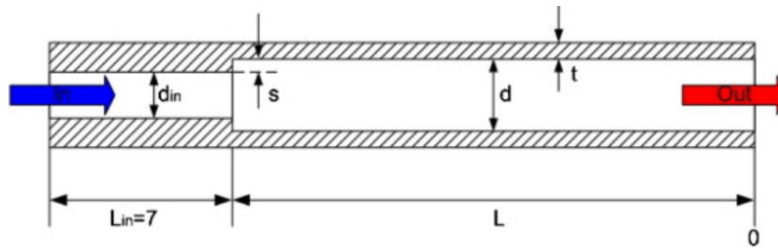


Figure 2.17: Example of a Backward-Facing Step Insertion in a Microcombustor, used in Li et al. [125].

Fan et al. [128] explored the impact of obstacles (bluff body) on hydrogen/air premixed flames. They investigated triangular and circular obstacles, concluding that the insertion of obstacles increases combustion flammability limits.

Yang et al. [129] studied hydrogen/air premixed flames in a convergent-divergent microtube. They simplified the geometry to two dimensions and used experimental temperature distribution data on the microtube's outer surface as thermal boundary conditions in numerical simulations. Their findings showed stable combustion for equivalence ratios ranging from 0.6 to 2.2 and inlet velocities from 3.4 m/s to 41.4 m/s. Comparing these results with a regular microtube, they observed broader flammability limits in the convergent-divergent microtube. Later, Biwas et al. [130] numerically investigated extinction and flame propagation behaviors of methane/air premixed flames in straight and convergent-divergent microchannels with diameters ranging from 1 to 10 mm. They examined the effects of microchannel diameter, equivalence ratio, inlet velocity, and exit-to-throat area ratio. Adiabatic wall conditions with conjugate heat transfer were considered. Their results indicated that flames extinguish more readily in convergent-divergent microchannels than in straight microchannels under adiabatic conditions.

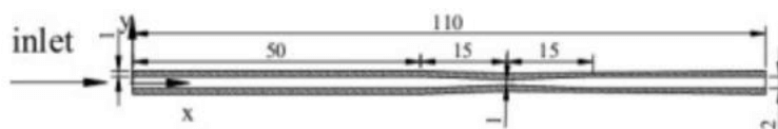


Figure 2.18: Schematics of the microburner used in Yang et al. [129].

Recently, Abbaspour and Alipoor [131] conducted numerical investigations into hydrogen/air premixed flame characteristics and behaviors in heated convergent-divergent microtubes. Results showed that the convergent-divergent section led to decreased flame temperature due to increased flow velocity and convective heat transfer, resulting in oscillating flames. However, this geometry also contributed to flame stability. When the flame stabilized near the outlet section, reduced flame wall instability and increased upper flammability limits were observed due to enhanced heat recirculation in the convergent-divergent section.

In recent years, studies have explored microburners with nonlinear geometries. Wan et al. [132] numerically studied hydrogen/air mixture combustion in a microburner with wall cavities, varying cavity depth and other reaction parameters. As the mixture velocity increased, the flame separated into two distinct zones, leading to significant fuel leakage from the reaction zone and a sharp

decrease in hydrogen conversion rate. They concluded that excessively deep cavities are detrimental when the burner is used as a heat source for thermoelectric or thermophotovoltaic devices, as flame separation results in more temperature peaks along the burner with lower intensities, reducing flame temperature. Yang et al. [133] conducted a similar study, focusing on burners with double cavities.

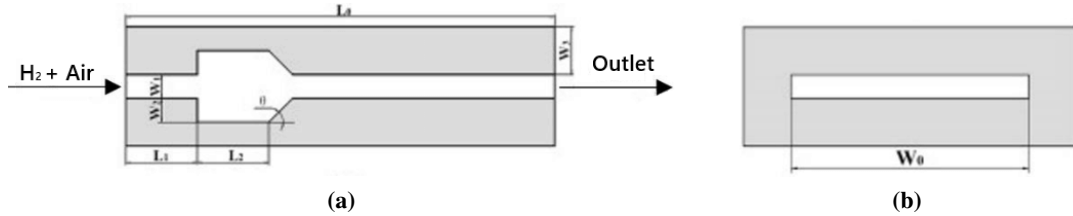


Figure 2.19: Microcombustor with Cavity Schematic [132]: (a) Longitudinal Plane; (b) Transverse Plan.

Various studies have examined flame dynamics in combustion chambers with diameters close to extinction diameters. These studies often assume negligible wall thickness in microburners, creating a significant difference in heat propagation rates between the fluid and walls. A constant temperature profile is typically used as the temperature boundary condition on the wall. Pizza et al. conducted numerous numerical studies on the dynamics of hydrogen/air premixed flames in heated meso channels [134], microchannels [88], and microtubes [87]. Different flame dynamics were observed, including Flame Reverse (FREI), mild combustion, swirling flames, and stable symmetrical flames. Later, Alipoor and Mazaheri [107] presented flame dynamics maps for hydrogen/air premixed flames based on three parameters: inlet velocity, equivalence ratio, and microchannel width, which are shown below in Figure 2.20.

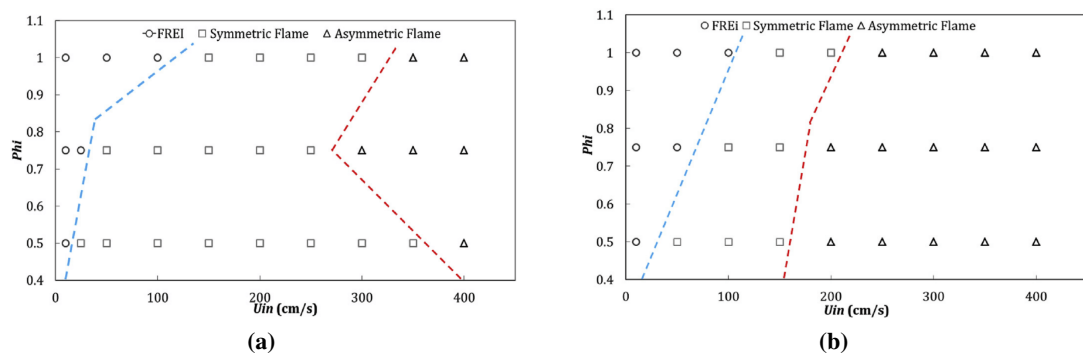


Figure 2.20: Flame dynamics diagrams [107]: Effect of U_{in} and ϕ for a channel width of: a) 0.6 mm; b) 0.8 mm.

This study focuses on microcombustion in the field of micropropulsion, a critical component of nanosatellite propulsion systems. Chen et al. [135] developed a hydrogen-based micropropulsion system using catalytic microcombustion to provide power for microsatellites' maneuvers. They experimentally and numerically studied this system's performance, investigating parameters like fuel/air mixture flow rate, equivalence ratio, and nozzle contraction ratio. They used a platinum catalyst-coated tube with a 500 μm diameter and 1 cm length as the reactor, inserted into a quartz tube with various converging-diverging nozzle ratios. It explored different flame behaviors and intrinsic properties, including temperature and mass concentration of key species (H_2 , OH , H_2O).

Boyarko et al. [136] aimed to understand the physics and chemistry of combustion processes in microreactors for microspacecraft propulsion systems. These microspacecraft are designed to have a mass of less than 50 kg, with propulsion systems capable of delivering impulses of 1-10 mN. Micropropulsion systems exhibit distinct behavior compared to larger-scale systems due to differences in flow rates and heat loss variations to the surroundings. The study analyzed flames in a microtube, chosen for its ease of manufacturing from catalytic materials and its simple geometry, suitable for simulations to validate the case under investigation. Experimentally, they explored the role of catalyst-coated tube surfaces in 0.4 mm and 0.8 mm diameter tubes, with a focus on rich hydrogen and oxygen mixtures.

2.3.7.1 Investigations in wavy wall geometries

The literature on wavy wall geometries in microcombustion is notably limited. The initial research into this subject was led by Mansouri [137]. This study utilized numerical analysis to evaluate the impact of a newly devised micro-channel characterized by wavy walls on the performance of a Micro-Thermo-Photovoltaic system. This investigation proved crucial due to the substantial influence of burner geometry on the system's power output. The study involved a two-dimensional numerical simulation using premixed CH₄/air combustion, maintaining a constant velocity of $U = 1$ [m/s] and an equivalence ratio of $\phi = 1$ across various wavy number configurations. The goal was to gain insights into flame behavior under varying kinetic mechanisms and wave-like designs.

Mansouri [138] later extended the study, examining how equivalence ratio, inlet velocity, and burner height affect wavy burner geometry's performance. The results showed an impressive 8.3% increase in conversion efficiency compared to flat burners, suggesting the adoption of undulating shapes in future micro-combustor designs and studies.

In their study, Han et al. [139] explored the impact of energy conversion improvement and NO_x emissions in the context of thermophotovoltaic applications using ammonia/hydrogen mixtures. Among three distinct wavy combustor designs, it was observed that NO_x emissions decreased notably in the wave-shaped design with smooth arcs. Furthermore, this particular design exhibited superior temperature uniformity at velocities exceeding 12 m/s.

In a recent study by Resende et al. [140], flame dynamics within a wave-shaped combustor featuring substantial divergence and convergence variations were investigated. The study employed a hydrogen/air mixture and revealed a pronounced interaction between fluid dynamics and chemical reactions. Specifically, the vortices within the convex regions were identified as acting as a resistance to heat loss flux. Later, the study was extended (Resende et. al [113]), which as mentioned before, investigated stable and pulsatory flame burst phenomena in an undulating geometry using premixed hydrogen and air with $\phi = 1.0$. Notably, this work introduced a linear temperature profile along the wall, allowing for an analysis of flow dynamics without imposing fixed flame locations. Two flame configurations were observed (stable for the lowest inlet velocity and PFB). The study emphasized the importance of the interaction between fluid dynamics and combustion, especially due to vortices formed by the burner's nonlinear geometry.

2.4 A Review on Micropropulsion

In this Section, we will delve into the fundamental concepts of propulsion that are crucial for a thorough understanding of the results presented in the following sections. The theoretical knowledge presented in the works of [141, 142, 143] forms the basis for our discussion here.

2.4.1 Overview on micropropulsion systems

As seen in Webster's Dictionary [144], Propulsion can be defined as: "The action or process of drive something forward or onward by or as if by means of a force that imparts motion". In other words, the propulsion system is a mechanical system which turns different forms of energy into kinetic energy.

The limitations of conventional propulsion systems to deliver small and precise impulses for small satellites have necessitated the development of specific propulsion systems tailored to micro-scale applications [145, 146]. In comparison to conventional propulsion systems, micropropulsion systems (MPS) exhibit two general characteristics^(m):

- i) They possess the capability to generate relatively minor thrust with magnitudes ranging up to 100mN and impulse values of μNs – mNs;
- ii) They display a relatively low volume and weight profile, often weighing in at kilograms or lower orders of magnitude.

MPS based on the use of propellants have traditionally been classified according to the state of the propellant, namely gas, solid, or liquid. However, recent advances in the development of propellantless technologies, such as the Solar Sail, have prompted the need for additional classification schemes. Figure 2.21 provides a concise summary of the classification schemes utilized.

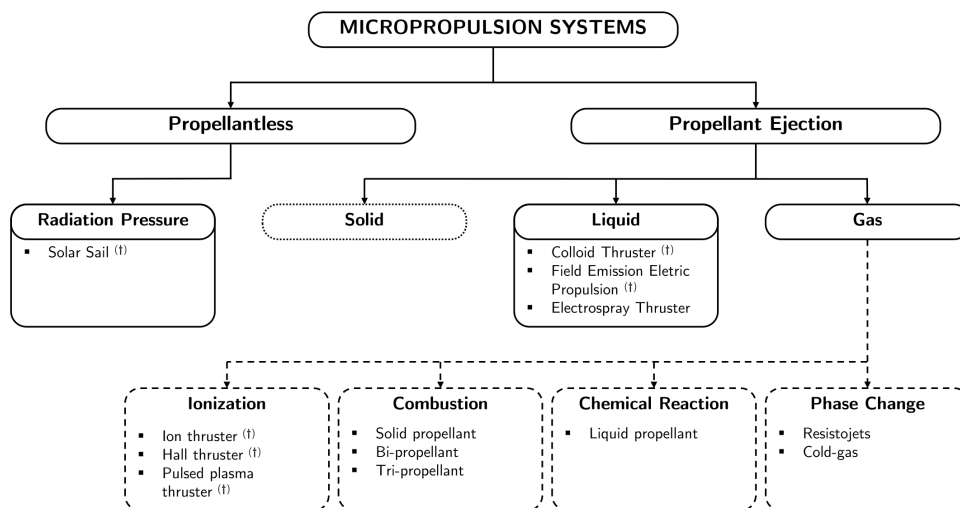


Figure 2.21: Classification of micropropulsion concepts (based on [9]): the systems highlighted with (+) are manufactured with conventional methods whereas the ones without made using MEMS and silicon technologies.

^(m)Though, notably, a propulsion system that solely possesses the first characteristic outlined below, is commonly referred to as a micropropulsion system.

As shown in Figure 2.21, another relevant categorization of MPS pertains to the manufacturing techniques employed, with some systems utilizing MEMS and silicon technologies (this research focuses specifically on such systems), while others utilize conventional methods.

2.4.2 Micropropulsion systems performance

MPS performance is commonly assessed under the framework of ideal rocket conditions. Nevertheless, it is crucial to acknowledge that these conditions rely on a set of assumptions that may not perfectly align with the realities of MPS. One such assumption is the neglect of friction forces [143]. Hence, a cautious approach is required when applying these idealized models to micropropulsion scenarios. Therefore, the set of equations presented here (the indices correspond to those depicted in Figure 2.22) serves to provide insights into the ideal performance of micropropulsion systems. When analyzing the performance of the thruster, two key parameters are of major interest: specific impulse and thrust. These equations offer valuable information regarding the performance characteristics of such micropropulsion systems.

2.4.2.1 Thrust and specific impulse

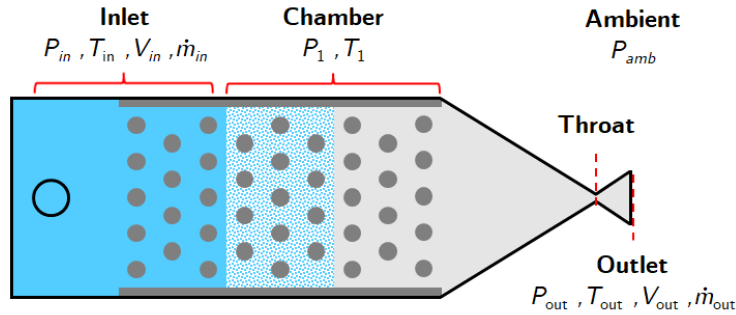


Figure 2.22: Diagram of a MPS showing the variables and their indexes (adapted from [9]).

In aircraft, thrust is normally explained through the application of Newton's third law of action and reaction. A gas, or working fluid, is accelerated by the engine, and the reaction to this acceleration produces a force on the engine. The general derivation of the thrust equation shows that the amount of thrust generated depends on the mass flow rate through the engine and the gas exit velocity [147].

From Newton's second law, force can be defined as the change in momentum of an object over time. Momentum is equal to the mass of the object times its velocity. When dealing with a gas, the thrust equation is given as:

$$F = \dot{m}_{out} \cdot v_{out} - \dot{m}_{in} \cdot v_{in} + (P_{out} - P_{in}) \cdot A_{out} \quad (2.36)$$

where $\dot{m}_{out}$ and $\dot{m}_{in}$ are the mass flow rates at the outlet and inlet of the propulsion system, v_{out} and v_{in} are the respective average fluid velocities at the outlet and inlet of the propulsion system, P_{out} and P_{in} are the outlet and inlet pressures, and A_{out} is the area of the outlet section.

In several cases, the outlet and inlet pressures of the propulsion system are equal to atmospheric pressure. In this case, the term $(P_{\text{out}} - P_{\text{in}})$ becomes zero, and the equation can be simplified as:

$$F = \dot{m}_{\text{out}} \cdot v_{\text{out}} - \dot{m}_{\text{in}} \cdot v_{\text{in}} \quad (2.37)$$

It has been observed that the mass flow rate at the exit is equal to the sum of the mass flow rate at the inlet and the mass flow rate of fuel. By using the fuel-to-air equivalence ratio, ϕ , the following relation is obtained:

$$\dot{m}_{\text{out}} = (1 + \phi) \cdot \dot{m}_{\text{in}} \quad (2.38)$$

Let us introduce a new variable termed specific impulse I_{sp} , which serves as a measure of efficiency with respect to propellant consumption.

$$I_{\text{sp}} = \frac{\int_0^t F dt}{g \int_0^t \dot{m} dt} \quad (2.39)$$

where the constant $g = 9.80665 \text{ [m/s}^2\text{]}$ represents the gravitational acceleration on Earth at sea level. Despite being expressed in seconds, it does not indicate a measure of time; rather, it denotes the thrust per unit weight of propellant. For optimal propellant consumption efficiency, this value should be as high as possible.

Assuming constant velocity and pressure at the outlet and inlet, it becomes possible to simplify Eq.(2.39). Through algebraic manipulations and by employing Eq.(2.38), we arrive at Eq. (2.40), wherein I_{sp} solely relies on the engine's velocity difference.

$$I_{\text{sp}} = \frac{F}{\dot{m}_{\text{in}}} = (1 + \phi) \cdot v_{\text{out}} - v_{\text{in}} \quad (2.40)$$

The definition of this new variable brings several advantages in the analysis of propulsion systems. Firstly, the specific impulse is an indicator of the efficiency of the mechanism. Different engines will always have different values of specific impulse. The engine with a higher specific impulse will be more efficient since it produces more thrust for the same airflow. Secondly, as it is a specific property, the inlet mass flow rate can be omitted in all intermediate calculations, greatly simplifying the mathematical procedure. Thirdly, it is a variable that facilitates the design of the propulsion mechanism.

2.4.2.2 Thrust key indicators

In contemporary propulsion systems, multiple components such as turbines, compressors, and combustion chambers are commonly integrated. Typically, several compressors are employed in series to progressively increase the air pressure. Subsequently, the combustion chamber facilitates the reaction between fuel and air, followed by the installation of a turbine ahead of the propulsor's exit section. Propulsion is achieved through the difference between the inlet and outlet velocities, generating the desired thrust force.

Two highly relevant indicators in the realm of propulsion mechanisms emerge, although they are not addressed in this dissertation. The first indicator is the Engine Pressure Ratio (EPR), defined as the ratio of the total pressure across the engine. As previously explained, modern engines consist of various components, and in this case, the EPR becomes the product of pressure ratios across all propulsion system components. Consequently, the EPR can be simplified and calculated as follows:

$$\text{EPR} = \frac{P_{\text{tot,out}}}{P_{\text{tot,in}}} \quad (2.41)$$

The second indicator is the Engine Temperature Ratio (ETR), which, analogously to the previous indicator, represents the ratio of the total temperature across various engine components. Similar to the previous case, given the complexity of modern engines, the ETR becomes the product of temperature ratios across the engine's components. Hence, the ETR is calculated using the following expression:

$$\text{ETR} = \frac{T_{\text{tot,out}}}{T_{\text{tot,in}}} \quad (2.42)$$

2.4.3 Conventionally manufactured micropropulsion systems

2.4.3.1 Pulsed plasma thruster

The PPT is an electromagnetic electric thruster, that relies on an electromagnetic field to accelerate the plasma to produce thrust. It is based on the principle of the Lorentz force, which creates a force that accelerates the plasma to generate thrust. In other words, it is generated a high voltage discharge between the cathode and the anode rod sleeve, which in turn heats the propellant (usually Teflon) making it decompose, which is then ionized to create a plasma. Specifically, the joint action of the magnetic pressure and the gas dynamic pressure in the thin layer of ionized gas accelerates the gas to produce thrust.

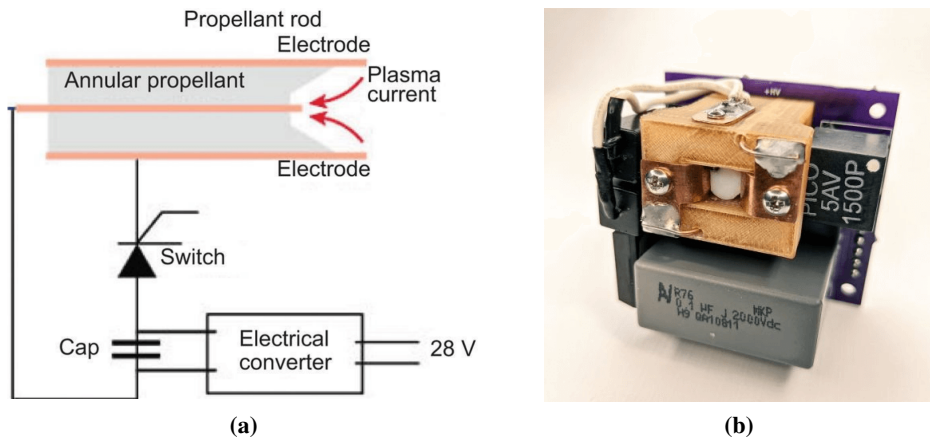


Figure 2.23: Pulsed Plasma Thruster: (a) Working principle [148]; (b) Prototype by AIS [149].

PPT operates in a pulsed manner due to the generation of sparks. As a result, continuous operation is not possible, hence the term "pulsed." Figure 2.23a illustrates the working principle of the PPT, while Figure 2.23b showcases a working prototype developed by AIS [149].

This system has garnered considerable interest among researchers owing to its straightforward design, cost-effectiveness, durability, and capacity for generating low-level outputs. Its track record of successful operation in space dates back to 1964 [150]. Recently, it has been used in CubeSat [151, 152, 153, 154] and micro-satellite [155, 156] missions successfully.

2.4.3.2 Field emission electric propulsion

This type of devices use a liquid propellant ejection system and must employ high-density substances to optimize thruster efficiency. As such, FEEP can be defined as an electrostatic electric propulsion system, that employs a high-voltage electrostatic field to accelerate charged ions for generating thrust. In Figure 2.24a we illustrate the fundamental principles of typical FEEP operation, while in Figure 2.24b we showcase a working prototype developed by TU Dresden.

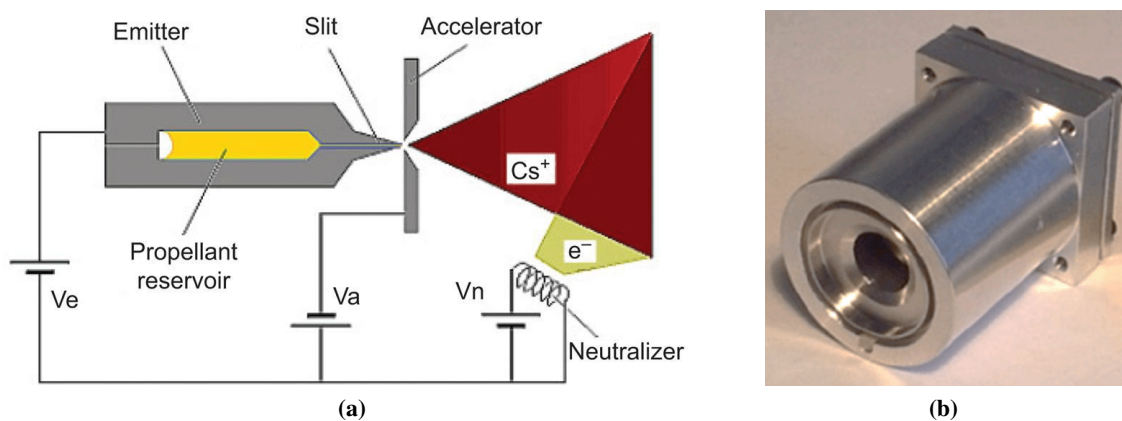


Figure 2.24: Field emission electric propulsion: (a) Working principle [157]; (b) Prototype by TU Dresden [158].

FEEP consists of a transmitter with a propellant reservoir chamber, an accelerating electrode, and a neutralizer. It employs low melting point metals (e.g., cesium, indium) as propellants, stored as solids until liquefied by heating. Capillary action transports the liquid metal to the emitter outlet slit. With 8-15 kV applied between the emitter electrode and the accelerating electric field, metal ions overcome surface tension and gain acceleration, producing thrust [141]. Additionally, a positive voltage on the transmitter and a negative voltage on the accelerator create an electric field, enabling electron beams to discharge metal ions, minimizing pollution plume effects.

2.4.3.3 Other relevant micropropulsion system technologies

Besides FEEP and PPT, there are other conventionally manufactured MPS options available, such as:

- Colloid Thruster: an electrostatic electric MPS similar to FEEP, that uses high voltage and conductive liquids to accelerate charged particles, producing thrust. The thruster comprises

charged particle emitters, extraction electrodes, an accelerating network, and a neutralizer to prevent ionic contamination on satellites. Different electrode potentials generate particle streams of varying polarities.

- **Hall thruster & Ion Thruster:** devices that generate thrust by ejecting ions at high velocities. They can achieve high specific impulse, but typically produce low thrust levels. There are two main types: Hall thrusters and ion thrusters. Hall thrusters use the Hall effect to trap electrons, ionize the propellant, and then accelerate and exhaust it to create thrust. Ion thrusters, on the other hand, use charged grids to accelerate the ionized propellant [159, 160, 161]. This propulsion technology has already seen implementation in space missions and is capable of delivering thrust within the appropriate range for CubeSat missions.
- **Solar sail:** is a spacecraft propulsion method that utilizes sunlight momentum to drive the craft forward [162]. It consists of a lightweight, reflective-coated sail with extreme thinness (down to 4.5 microns) and substantial size (hundreds of meters or kilometers) [163]. Photons from the Sun impart momentum to the sail, propelling the spacecraft and this continuous acceleration allows for high speeds over time. Solar sails have various advantages, including cost-effectiveness, sustainability, applicability to small satellites, and potential for long operating lifetimes [164]. This technology shows great promise for efficient and lightweight space travel.

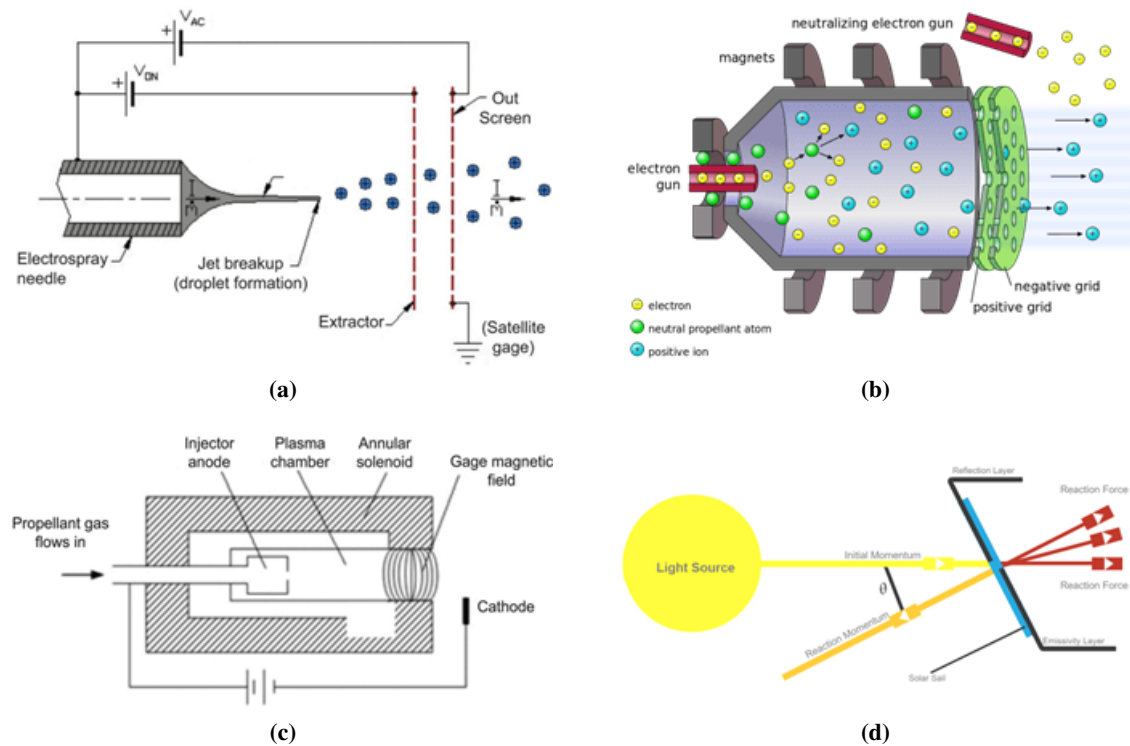


Figure 2.25: Working principle of: (a) Colloid thruster [165]; (b) Ion thruster [166]; (c) Hall thruster [165]; (d) Solar sail [167].

2.4.4 Micro-Electro-Mechanical Systems

The focus of this Section is a comprehensive investigation of MEMS micropropulsion systems, specifically with regards to their suitability for implementation in nano- and picosatellites. As mentioned in the preceding chapter, the utilization of MEMS holds great potential for the development of highly compact spacecraft, owing to their ability to fabricate extremely small features and seamlessly integrate electronics [168]. More specifically, we delve into systems characterized by the incorporation of MEMS (Micro-Electro-Mechanical Systems) and silicon technologies specifically in the construction of the thruster component. It is noteworthy that some systems may incorporate MEMS elements, such as sensors, but these singular components do not categorically define the entire system as MEMS micropropulsion.

2.4.4.1 MEMS Manufacturing

Many of these systems operate within the micro to nanometer scales, and they fluidly combine mechanical and electrical components into a unified device. In the context of micropropulsion, the mechanical aspects encompass features like fluidic channels and structural components, while the electrical aspects involve components such as resistive heaters, sensors, and so on [169]. Nevertheless, defining precise boundaries between these mechanical and electrical components within MEMS can be challenging due to the intricate processes occurring within these devices.

The fabrication of these devices, as shown in Figure 2.26, typically encompasses a sequence of iterative procedures, commencing with a silicon wafer, and then involving these processes [9]:

1. **Deposition:** This step entails the deposition of minute layers of materials onto the surface of the silicon wafer.
2. **Patterning:** Patterning is employed to imprint a specific design onto the surface, thereby safeguarding certain regions while exposing others to shape the device's features.
3. **Etching:** Etching serves the purpose of material removal from the exposed areas, employing either isotropic or anisotropic techniques.

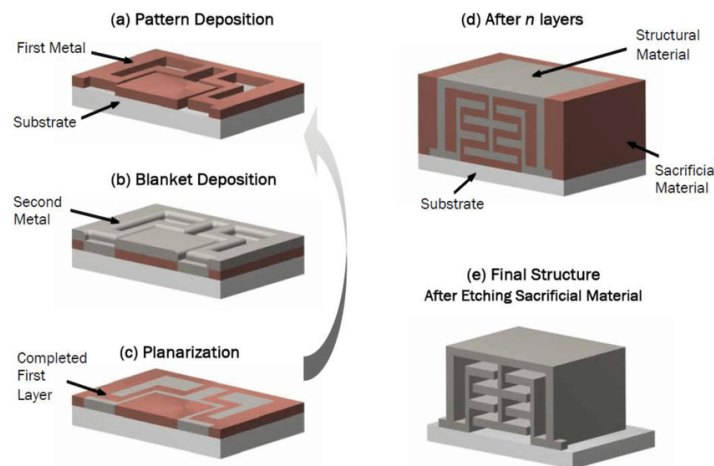


Figure 2.26: Metal MEMS fabrication process [170].

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Chapter 3

Governing Equations and Numerical Modelling

*“To not know math is a severe limitation
to understanding the world.”*

Richard Feynman

The objective of this chapter is to introduce the governing equations involved in the combustion process, along with the numerical approach utilized to solve them. The chosen numerical framework draws upon the works of [11, 12]. While a comprehensive discussion of all the numerical methods employed within this framework exceeds the scope of this document, a concise overview will be provided.

Particularly, two distinct solvers will be presented. Firstly, we will explore the *laminarSMOKE* solver developed by Cuoci et al [11, 12]. This solver is designed to address the equations presented in subsection 3.2.1. Notably, *laminarSMOKE* originated from the *pisoFoam*^(a) solver, which deals with unsteady, compressible, non-reacting flows, and is part of the standard OpenFOAM solver collection.

To enable the utilization of the *laminarSMOKE* solver for simulating reacting flows under stationary or unsteady conditions in both simple and complex geometries, at the micro-scale, in an autonomous manner, independent of third-party information, it becomes necessary to incorporate heat transfer considerations at the wall during the gas phase calculations. This entails solving the energy equations concurrently for both the solid and gas phases, presented in subsection 3.2.2 a method termed the Conjugate Heat Transfer (CHT) problem.

The Conjugate Heat Transfer problem involves the intricate interaction between thermal conduction in the solid domain and the convection taking place in the fluid domain that is in contact with the solid. The newly developed solver is denoted as *chtlaminarSMOKE*, as it represents a tailored version of the original *laminarSMOKE* solver, specifically designed for addressing CHT problems.

^(a)The prefix "PISO" designates the implementation of an Implicit Pressure-Based Algorithm with Splitting of Operators.

3.1 Computational Fluid Dynamics

These solvers fall under the domain of Computational Fluid Dynamics (CFD)^(b). They consist of a C++ library commonly applied in simulation applications, built upon the OpenFOAM and OpenSMOKE++ framework. These solvers are rooted in mathematical techniques for modeling physical events involving fluid flow, and they subsequently utilize computational resources to obtain numerical solutions. The mathematical model used will differ depending on the problem's content, such as heat transmission, mass transfer, phase change, chemical reaction, and so on.

3.1.1 Perspective

Prior to 1960, the approach to solving fluid dynamics problems was twofold, involving theory and experimentation. However, the landscape of fluid dynamics research and practice underwent a significant transformation with the advent of high-speed digital computers and the concurrent advancement of precise numerical techniques tailored for solving physical problems on these computing platforms. This revolution gave rise to Computational Fluid Dynamics (CFD) as a crucial third dimension in the field, as articulated by Anderson [171]. The three distinct dimensions for tackling fluid dynamics challenges are [171]:

1. **Theoretical Approach:** This involves using governing equations and mathematical models to analytically solve fluid dynamics problems, yielding mathematical representations of system behavior;
2. **Experimental Technique:** This method interfaces laboratory equipment and instruments with full-scale physical models of the system under study. Experimentation with physical models provides robust results, although sometimes, cost or practicality constraints necessitate testing on a reduced scale;
3. **Numerical Technique:** This forms the foundation of CFD, where a set of partial differential equations (PDEs) is solved through computational processes to obtain solutions to fluid dynamics problems. CFD is widely applied in various stages of engineering processes, including conceptual design, product development, optimization, debugging, and system redesign.

3.1.2 Main concept

More concretely, we can describe CFD as a tool used to estimate solutions to differential equations. In this method, a suitable set of conservation equations is solved for each specific flow problem [172]. Before delving into the governing equations, it is essential to establish notations for the Partial Differential Equations (PDEs).

Figure 3.1 illustrates the motion of an infinitesimally small fluid element as it moves through a Cartesian space defined by unit vectors i , j , and k along the x , y , and z axes, respectively, with the vector velocity field $\mathbf{v}$ defined as:

$$\mathbf{v} = u\mathbf{i} + v\mathbf{j} + w\mathbf{k} \quad (3.1)$$

^(b)CFD are the techniques of mathematically modeling a physical event involving fluid flow and solving it numerically utilizing computing power.

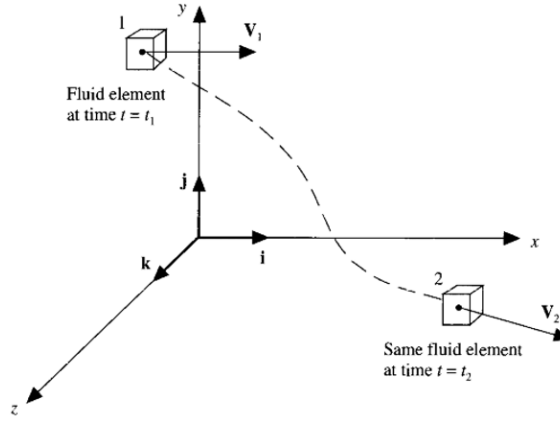


Figure 3.1: Movement of a Fluid Element in Fluid Flow ([171])

Considering an unsteady flow where u , v , and w are both functions of space and time t , the velocity components x , y , and z are given, respectively, by:

$$u = u(x, y, z, t) \quad v = v(x, y, z, t) \quad w = w(x, y, z, t) \quad (3.2)$$

and the density of the flowing fluid as a function of space and time is also given by:

$$\rho = \rho(x, y, z, t) \quad (3.3)$$

From Figure 3.1, the fluid element is located at point 1 and 2 at time t_1 and t_2 respectively. Thus, the densities of the fluid element at these points are given, respectively by:

$$\rho_1 = \rho(x_1, y_1, z_1, t_1) \quad \rho_2 = \rho(x_2, y_2, z_2, t_2) \quad (3.4)$$

Expanding equation (3.3) in a Taylor series about point 1 and ignoring higher order terms and doing the proper simplifications (as shown in [171]), we can obtain the following equation:

$$\frac{d\rho}{dt} \equiv u \frac{\partial \rho}{\partial x} + v \frac{\partial \rho}{\partial y} + w \frac{\partial \rho}{\partial z} + \frac{\partial \rho}{\partial t} \quad (3.5)$$

Simplifying this equation, an expression for the substantial derivative $\frac{d}{dt}$ in the Cartesian coordinate can be obtained as:

$$\frac{d}{dt} \equiv u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} + w \frac{\partial}{\partial z} + \frac{\partial}{\partial t} \quad (3.6)$$

Furthermore, by recognizing $\mathbf{v}$ as a vector quantity, Equation (3.6) can be simplified to:

$$\frac{d}{dt} = \frac{\partial}{\partial t} + (\mathbf{v} \cdot \nabla) \quad (3.7)$$

The significant derivative (denoted as d/dt) measures how a fluid element changes over time as it moves. This captures the rate of change in time for a fluid element in motion. In contrast, the local derivative, represented as $\partial/\partial t$, describes the rate of change at a fixed position in the fluid. Additionally, $\mathbf{v} \cdot \nabla$ represents the convective derivative, which reflects the time rate of change resulting from a fluid element's migration from one point to another within a flow field that has changing flow parameters [171, 172].

3.2 Governing Equations

We will now focus on an in-depth examination of the fundamental equations that govern the dynamics of both gas phase and gas-solid phase combustion phenomena (the latter are the scenarios characterized by the presence of a physical enclosure encompassing the combustor).

3.2.1 Gas phase equations

The focus of this research revolves around the examination and analysis of reactive, laminar flows^(c). Mathematically, these flows are characterized and represented by the conservation equations governing continuous, multicomponent, compressible, and thermally-perfect mixtures of gases, which are treated as Newtonian fluids.

The essential equations encompass the total mass conservation, Eq. (3.8), mixture momentum conservation, Eq. (3.9), individual species mass fractions conservation, Eq. (3.10), and mixture energy conservation, Eq. (3.11). These equations are articulated as follows:

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) = 0 \quad (3.8)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla(\rho \mathbf{v} \mathbf{v} + \rho \mathbf{I}_3) = \nabla \tau_{st} + \rho \mathbf{g} \quad (3.9)$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho Y_k \mathbf{v}) = \nabla(\rho Y_k \mathbf{V}_k) + \dot{\Omega}_k \quad k = 1, \dots, NC \quad (3.10)$$

$$\rho C_P \frac{\partial T}{\partial t} + \rho C_P \mathbf{v} \nabla T = -\nabla \mathbf{q}'' - \rho \sum_{k=1}^{NC} C_{P,k} Y_k \mathbf{V}_k - \sum_{k=1}^{NC} h_k \dot{\Omega}_k \quad (3.11)$$

where t is the time, ρ is the mixture density, P the pressure, $\mathbf{v}$ the mixture velocity vector, τ_{st} the fluid stress tensor, $\mathbf{g}$ the acceleration vector due to gravity, Y_k the mass fraction of species k , $\mathbf{V}_k$ is the diffusion velocity of species k , $\dot{\Omega}_k$ the formation rate of species k , T the temperature, C_P and $C_{P,k}$ are the specific heat at constant pressure of the mixture and of the individual species k , respectively, $\mathbf{q}''$ the heat flux vector and h_k the individual species enthalpy.

The density of the mixture is determined utilizing the ideal gas equation of state, while the heat flux vector, encompassing both conduction and radiation, is computed using the next equation:

$$\mathbf{q}'' = -\lambda \nabla T + \mathbf{q}_{rad}'' \quad (3.12)$$

where λ is the mixture thermal conductivity and the radiative heat flux is represented by $\mathbf{q}_{rad}''$. To determine the diffusion velocities of species k , it is essential to incorporate both Fick's law and thermal diffusion, which is commonly referred to as the Soret effect:

$$\mathbf{V}_k = -\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k \Theta_k}{X_k} \frac{1}{T} \nabla T \quad (3.13)$$

^(c)As mentioned earlier, we'll assume purely laminar flows, since in microchannels, flows are typically laminar due to the dominance of viscous forces at small scales, resulting in low Reynolds numbers.

where X_k denotes the mole fraction and Θ_k represent the thermal diffusion ratio of species k . Additionally, D_k corresponds to the individual-species mixture-averaged diffusion coefficient, which can be coupled to the binary diffusion coefficients Γ_{jk} through the following expression:

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k}^{NC} \frac{X_k}{\Gamma_{jk}}} \quad (3.14)$$

To ensure mass conversation, the approach introduced by Coffee and Heimerl [173] is adopted. This method involves substituting the velocity term $\mathbf{V}_k$ in Equations Eq. (3.10) and Eq. (3.11) with a corrective diffusion velocity, denoted as $\mathbf{V}_k^C$. The corrective diffusion velocity is precisely defined as follows:

$$\mathbf{V}_k^C = \mathbf{V}_k + \mathbf{V}_C \quad (3.15)$$

where $\mathbf{V}_C$ is a constant correction factor, which is independent of the species but can vary spatially and temporally, used in order to satisfy mass conservation. The calculation of this correction factor is done using the following equation:

$$\mathbf{V}_C = - \sum_{k=1}^{NC} Y_k \mathbf{V}_k \quad (3.16)$$

The modeling of radiative heat transfer in this study is based on the assumption of optically thin radiation, where the self-absorption of radiation is disregarded. Only the following major radiating species are considered: H_2O , CO , CO_2 , and CH_4 . The contribution of radiative heat transfer to the energy equation is described as follows:

$$\nabla \mathbf{q}_{\text{rad}}'' = -4\sigma a_P (T^4 - T_{\text{sur}}^4) \quad (3.17)$$

here, T_{sur} represents the temperature of the environment, and σ denotes the Stefan-Boltzmann constant. The Planck mean absorption coefficient, denoted as a_P , is defined as follows:

$$a_P = p_{\text{H}_2\text{O}} a_{P,\text{H}_2\text{O}} + p_{\text{CO}_2} a_{P,\text{CO}_2} + p_{\text{CO}} a_{P,\text{CO}} + p_{\text{CH}_4} a_{P,\text{CH}_4} \quad (3.18)$$

where p_k represents the partial pressure of species k . The extinction coefficient $a_{P,k}$ for species k is estimated using the RADCAL software [174].

3.2.2 Gas-solid phases equations

When using CHT, it's necessary to solve both the governing equations for the fluid and solid domains. For the fluid domain, the equation is the same as the one presented in Eq. (3.11), and for the solid domain, the energy equation is represented by:

$$\rho_s C_{P_s} \frac{\partial T_s}{\partial t} = \dot{q}_s - \nabla (\lambda_s \nabla T_s) \quad (3.19)$$

where ρ_s is the density of the solid [kg/m³], C_p is the specific heat of the solid [J/(kgK)] is the temperature of the solid [K], $\dot{q}_s$ is the heat source inside the solid [W/m³], λ_s is the thermal conductivity of the solid [W/(mK)] and t is time [s].

In the context of Conjugate Heat Transfer (CHT) problems, it is imperative to ensure the preservation of temperature and heat flux continuity at the shared interface. This fundamental requirement is exemplified by the governing equations (3.20) and (3.21) as follows:

$$T_f = T_s \quad (3.20)$$

$$\lambda_f \frac{\partial T_f}{\partial n} = -\lambda_s \frac{\partial T_s}{\partial n} \quad (3.21)$$

3.3 Numerical Model

3.3.1 Gas phase computational approach and modeling

We shall now delve into a comprehensive examination of the numerical solver, *laminarSMOKE*, as introduced earlier. The use of conventional computational fluid dynamics (CFD) methods employing segregated algorithms proves to be unsuitable for tackling reacting flows with detailed kinetics. The challenges arise from the inherent stiffness and significant nonlinearities characterizing the transport equations of species and energy in such systems. In contrast, coupled algorithms offer several advantages in handling stiff, large systems of nonlinear equations, with fully coupled and operator-splitting methods being the two primary approaches.

Nevertheless, adopting fully coupled methods presents certain limitations, particularly when dealing with cases involving intricate kinetics, as is the focus of this study. In such scenarios, the number of coupled equations to be solved becomes exceedingly large, rapidly demanding extensive computational resources. This issue is further compounded when employing high-order approximations for spatial derivatives.

The operator-splitting method is adopted in the *laminarSMOKE* code to effectively handle the complex reacting processes with detailed kinetics. This technique involves partitioning the governing equations into subequations, separating transport and reaction terms in the energy and species equations. Notably, it allows for the isolation of convective and diffusive transport terms (nonstiff processes) from chemical reactions terms (stiff processes), reducing computational overhead associated with expensive matrix operations, which are typically encountered in fully coupled algorithms.

The method of operator splitting employed in the code of *laminarSMOKE* shall now be briefly outlined. In this instance, the method of lines (MOL) approach has been embraced, whereby, subsequent to spatial discretization, the transport equations governing energy and species may be reformulated in the ensuing manner:

$$\frac{d\psi}{dt} = \mathbf{C}(\psi, t) + \mathbf{D}(\psi, t) + \mathbf{R}(\psi) \quad (3.22)$$

where the primary variables are represented by the vector ψ , which encompasses both mass fractions and temperature. The terms $\mathbf{C}(\psi, t)$ and $\mathbf{D}(\psi, t)$ are vectors corresponding to the rates of change of ψ caused by transport processes, specifically convection and diffusion, respectively. Additionally, $\mathbf{R}(\psi)$ represents the vector of rates of change of ψ due to chemical reactions.

To numerically solve Eq. (3.22), we discretize the time domain into incremental steps denoted by Δt . The solution is then progressively approximated at each time step. Notably, each term on the right-hand side of Eq. (3.22) contributes to the overall change in ψ during the numerical time step.

Given the complexity of the chemical kinetics mechanisms present in this study, the stiff operator, arising from the chemistry, must be positioned as the final step in the splitting process to ensure both stability and accuracy. To address this requirement, we adopt the Strang splitting scheme [175], which effectively groups the convection and diffusion terms together, separating them from the stiff chemical reaction term. This approach enables us to perform numerical integration in three substeps, ensuring a robust and accurate solution.

Algorithm 1 *laminarSMOKE* numerical integration

1: **Substep 1:** we integrate the reaction term over half of the time step, $\Delta t/2$, by solving a stiff ordinary differential equation (ODE):

2:

$$\frac{d\psi^a}{dt} = \mathbf{R}(\psi^a) \quad (3.23)$$

3: where the initial condition $\psi^a(0)$ corresponds to the final state of the previous time step, and the solution at $\Delta t/2$ is denoted as $\psi^a(\Delta t/2)$.

4: **Substep 2:** we integrate the reaction term over half of the time step, $\Delta t/2$, by solving a stiff ordinary differential equation (ODE):

5:

$$\frac{d\psi^a}{dt} = \mathbf{R}(\psi^a) \quad (3.24)$$

6: where the initial condition $\psi^b(0)$ is set to the final state obtained from Substep 1, $\psi^a(\Delta t/2)$, and the solution at Δt is denoted as $\psi^b(\Delta t)$.

7: **Substep 3:** similar to Substep 1, but the initial condition is set to the final state of Substep 2, $\psi^b(\Delta t)$. The solution obtained here becomes the initial condition for Substep 1 in the subsequent time step.

Substeps 1 and 3, pertaining to the reaction kinetics, exhibit no spatial dependence and, therefore, do not necessitate the imposition of boundary conditions. Conversely, the transport operators $\mathbf{C}(\psi, t)$ and $\mathbf{D}(\psi, t)$ incorporate spatial dependencies, demanding the specification of appropriate boundary conditions, as detailed in Subsection 4.3.2. To tackle these equations, several numerical methods are employed, as documented in [11, 12].

Regarding the solution procedure, the species and energy equations are addressed using the Strang splitting algorithm. Meanwhile, the continuity and momentum equations are handled via a segregated approach. To ensure mass conservation at each time step, the PISO algorithm [176] is implemented. Moreover, the time step is automatically adjusted during computations to maintain a suitably small maximum Courant number, thereby mitigating potential stability concerns.

The overall numerical algorithmic framework adopted in the *laminarSMOKE* code is depicted in Figure 3.2.

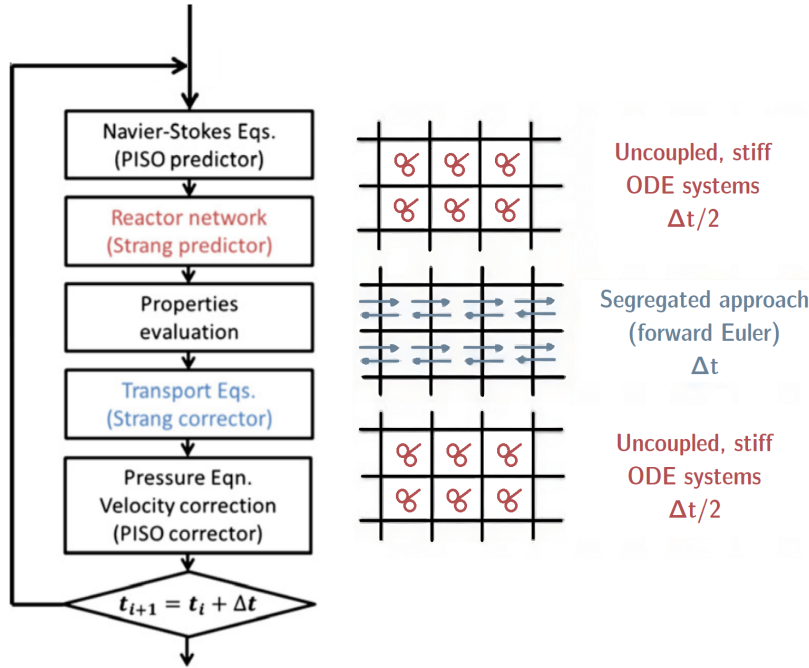


Figure 3.2: Numerical algorithm adopted in the *laminarSMOKE* code [177].

3.3.2 Gas-solid phases computational approach

Some possible different ways to solve CHT problems, as well as some advantages and downsides related to them, will be briefly presented here. As such, there are two prominent methods used which are: the Conjugate Approach and the Coupled Approach.

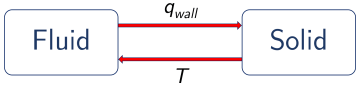
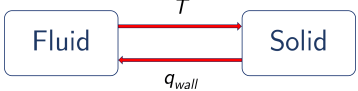
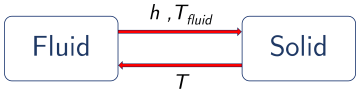
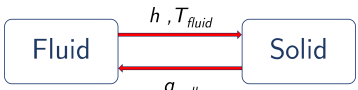
The Conjugate Approach employs a unified solver, typically based on the Finite Volume Method, for both fluid and solid domains. This is the prevalent approach adopted in both commercial and open-source software. One option under this approach is to set the velocity to zero and maintain a constant density for the solid domain. Consequently, only the energy equation needs to be dealt with in this region. Alternatively, an expression representing Eqs. (3.11) and (3.19) can be utilized, with fluid or solid properties being incorporated based on their respective positions within the entire domain. An advantageous aspect of this method is the absence of solution interpolation at the fluid and solid interface, which contributes to reduced computational time. However, a limitation is its inability to apply different numerical methods for each domain, which would have been particularly beneficial for the solid domain, given its typically higher time constant.

In contrast, the Coupled Approach involves separate solvers for each domain. The Finite Element Method is commonly preferred for the solid domain, while the Finite Volume Method continues to be utilized for the fluid domain. As a result, information exchange at the interface of the coupled domains is necessary. This approach offers several advantages: (1) the possibility of leveraging already validated codes; (2) enabling the use of distinct solvers, accommodating the differing time constants of the solid and fluid domains through appropriate techniques for each;

(3) leveraging the higher time constant of the solid domain, permitting the use of steady-state FEM, which converges solutions rapidly. Unlike the Conjugate Approach, where the solid domain is solved at every time step, the Coupled Approach solves it only after several time steps, when updates to the interface boundary conditions are necessary.

However, certain downsides should be taken into account: (1) for transient simulations, the iterative process of exchanging information between domains can be complex; (2) when dealing with non-matching meshes between the two domains, interpolating information at the interface may significantly increase computational time, potentially offsetting the advantage of using distinct solvers for each domain. The coupling algorithms currently employed are classified based on the type of information they exchange at the interface, with the fluid being the reference point for naming these different methods. These methods include:

Table 3.1: Overview of the coupling algorithms based on Nettis [178]

Flux Forward Temperature Back (FFTB)	
The imposition of heat flux acquired on the fluid side of the interface upon the solid domain, along with the transmission of temperature distribution from the solid side to the fluid domain, as depicted in Figure 3.3, represents a stable approach, contingent on the condition $Bi < 1$.	Figure 3.3: FFTB Algorithm [178]
Temperature Forward Flux Back (TFFB)	
Stands in contrast to FFTB, wherein the temperature distribution acquired on the fluid side is enforced upon the solid domain, while the heat flux obtained on the solid side is transmitted to the fluid domain, as exemplified in Figure 3.4. This method ensures stability when the condition $Bi > 1$ is satisfied.	Figure 3.4: TFFB Algorithm [178]
Heat Transfer Coefficient Forward Temperature Back (hFTB)	
Encompasses a hybrid approach, combining Neumann and Dirichlet boundary conditions, as described by the heat transfer equation: $q_{wall} = h_{conv}(T_{wall} - T_{fluid})$. Subsequently, the solution is computed, and the resulting temperature distribution is imposed on the fluid domain, as depicted in Figure 3.5.	Figure 3.5: hFTB Algorithm [178]
Heat Transfer Coefficient Forward Flux Back (hFFB)	
Bears a remarkable resemblance to hFTB, differing solely in the aspect that the heat flux is imposed upon the fluid domain, rather than the temperature distribution, as exemplified on the right in Figure 3.6.	Figure 3.6: hFFB Algorithm [178]

As reiterated in Section 2.3, the Biot number, given by Eq. (3.25), corresponds to the ratio of conductive resistance (L/λ_s) to convective resistance on the flow boundary surface ($1/h$).

$$Bi = \frac{h_{conv}L}{\lambda_s} \quad (3.25)$$

For FFTB and TFFB, convergence occurs when temperature and heat flux are balanced on both sides of the interface. However, certain situations may require the introduction of a relaxation factor during the iterative process to enhance stability. In such instances, hFTB and hFFB offer an alternative approach, utilizing the convective heat flux coefficient h to facilitate relaxation through the application of a Robin boundary condition on the solid side.

3.3.3 Gas-solid phases numerical modeling

The numerical model utilized in this study for gas-solid phases is named *chtlaminarSMOKE*. It is an adapted version of the *laminarSMOKE* solver specifically designed to handle CHT problems. The overall numerical procedure implemented in this modified solver is depicted in Figure 7.5.

The numerical solver employs a Coupled Approach that utilizes the FFTB algorithm for managing the interactions between the solid and fluid domains. This algorithm was chosen due to the nature of the cases investigated in this thesis, which involved situations where $Bi < 1$.

To address transient forced convection, the fluid region was solved using the laminar Navier-Stokes equations, while the solid region was solved using the Laplace equations, according to [179].

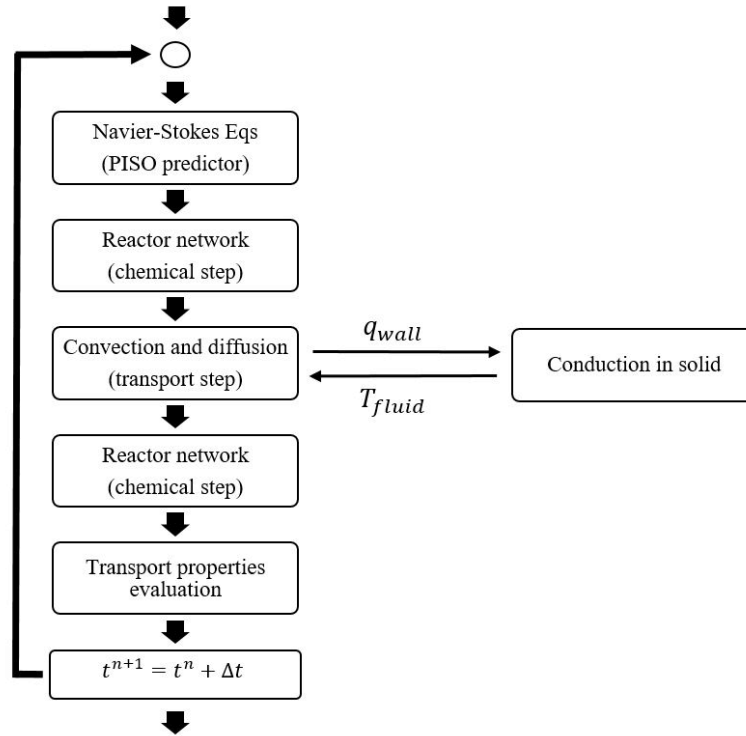


Figure 3.7: Numerical algorithm adopted in the *chtlaminarSMOKE* code [13].

It's crucial to ensure the continuity of temperature and heat flux at the common interface, as represented by Eqs. (3.20) and (3.21). To achieve this, an iterative process of flux-forward and temperature-backward loops is performed until the temperature and heat flux differences at the common interfaces of the two domains fall below the desired numerical error. Once convergence is attained, the physical time step is incremented, as demonstrated in Eqs (3.26) and (3.27).

$$-\lambda_s \frac{\partial T_s^{n+1}}{\partial n} = \lambda_f \frac{\partial T_f^n}{\partial n} \quad (3.26)$$

$$T_f^{n+1} = T_s^n \quad (3.27)$$

The *Policy_cht* file, which serves as the primary file for the solver and defines the interface for interacting with OpenFOAM and its data types, can be found in Appendix A.

3.4 Kinetic mechanism

In the realm of combustion phenomena, a mere stoichiometric chemical reaction, as discussed in Section 2.1.1, fails to capture the complexity of the process. The combustion entails the production of multiple species, arising from intricate recombination and interactions between radicals and stable species during the entire process.

To effectively solve the governing equations, it becomes imperative to accurately identify all species participating in the chemical reactions and have access to their thermophysical properties for the calculations.

At Politecnico di Milano, more precisely within the CRECK Modelling Group, extensive efforts have been made to develop detailed kinetic mechanisms that comprehensively describe these chemical reactions. The proposed mechanisms underwent validation, as documented in references [180, 181, 182]

For this study, hydrogen flames were simulated using the *POLIMI_H2CO_NOX_1412* mechanism, which encompasses 32 species and 173 reactions. The chemical reactions pertinent to the H₂ kinetic mechanism is presented in Appendix B.

3.5 Additional Remarks

Within the context of this research, the CRECK Modelling Group has developed two slightly distinct versions of the *laminarSMOKE* code, tailored for different applications, and both were extensively employed:

- i) *laminarSimpleSMOKE*: This version is specifically designed to achieve steady-state conditions rapidly. In most cases, it does not involve any time derivatives or provide any time-related information.
- ii) *laminarPimpleSMOKE*: On the other hand, this code variant is intended for simulating transient flows. It offers the flexibility to impose desired time steps, provided that it does not result in the Courant number surpassing its maximum allowable value. This capability enables the simulation of time-dependent phenomena effectively.

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Chapter 4

Software Framework and Methodology

*“The function of good software is to make
the complex appear to be simple.”*

Grady Booch

4.1 Introduction

The numerical simulations conducted in this study were carried out utilizing the widely adopted OpenFOAM platform, an open-source Computational Fluid Dynamics (CFD) tool extensively employed in both commercial and academic domains within the engineering and scientific communities.



Figure 4.1: OpenFOAM® Logo.

OpenFOAM is implemented as a C++ library, encompassing diverse code structures for tasks such as solving linear systems, ordinary differential equations, dynamic meshing, and general physical models. Leveraging the extensive capabilities of this library, executables or applications can be developed. These applications can be classified into two categories: solvers and utilities. Solvers are dedicated to performing calculations aimed at solving specific fluid mechanics problems, while utilities encompass tasks related to mesh preparation, simulation case selection, result processing, and other data manipulation operations, in addition to addressing the primary problem at hand.

It's built upon the Finite Volume Method, and is a highly customizable and extensible numerical solver package. It offers an extensive set of capabilities for resolving intricate fluid flow phenomena encompassing turbulence, chemical reactions, heat transfer, and more. Notably, OpenFOAM empowers users to efficiently manipulate existing features such as solvers and utilities, tailoring them to their specific research requirements.

In the ensuing sections, we will elucidate key features utilized for conducting simulations in this study. Additionally, we will outline essential aspects of the software that users should be well-versed in, as detailed in the OpenFOAM User Guide [183].

4.2 Structure

In order to conduct a simulation using the OpenFOAM software, it is imperative to establish and arrange the necessary data for the simulation case within three distinct subdirectories, each encompassing a multitude of files, as shown schematically in Figure 4.2.

- i) *constant*: plays a pivotal role in the simulation process within OpenFOAM. It serves as a repository for not only the fixed parameters that remain constant throughout the simulation, such as physical properties, but also encompasses the detailed description of the case's mesh structure within the *polyMesh* subdirectory.
- ii) *system*: this directory allows the user to configure parameters pertaining to the simulation procedure. Within this directory, a minimum of three files must be present. Firstly, the *controlDict* file grants the user the ability to define aspects such as the initiation and termination times, as well as the time steps utilized during the calculations. Secondly, the *fvSchemes* file provides the user with the ability to specify the discretization schemes employed in the simulation, while the *fvSolution* file enables the selection of appropriate equation solvers. Moreover, the *decomposeParDict* file can be employed to facilitate the division of all fields involved in the calculations, harnessing the potential of parallel processing and thereby reducing computational time.
- iii) First time instant: The initial time step within the simulation (typically 0) encompasses various individual files associated with specific fields. These files, dictated by the user, encompass crucial information such as initial and boundary conditions. In the context of this study, common fields include velocity, temperature, concentration of molecules for all relevant species, and so on.

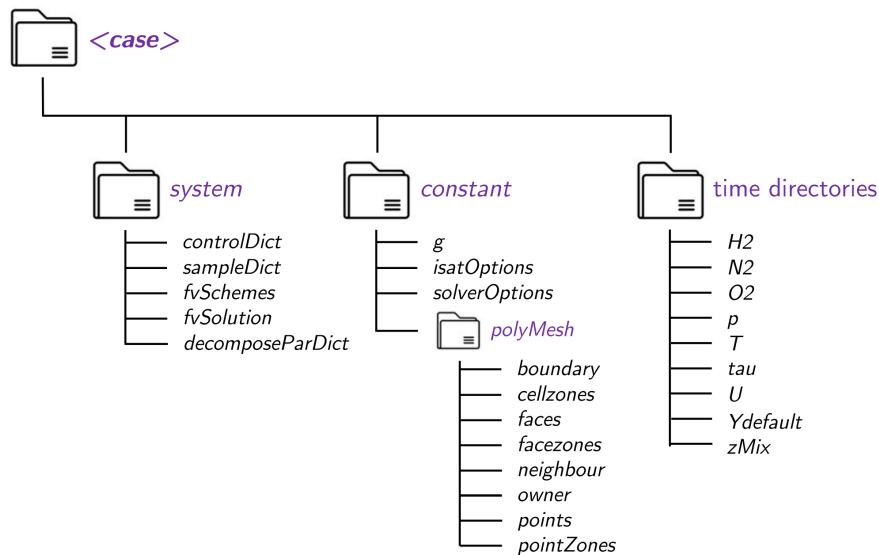


Figure 4.2: Case directory structure.

Upon initiation of the simulation, this structure undergoes a dynamic transformation. New folders are generated at the same level as the three previously introduced files. These folders represent the newly computed time instances and bear a striking resemblance to the folder of the initial

time instant. In essence, they contain nearly identical files, albeit with properties corresponding to their respective time instances and additional specific fields, such as new species resulting from chemical reactions.

Consequently, as the simulation progresses, the user can examine the information pertaining to the calculated time instances by consulting the files contained within the newly created folders. At the end of the simulation, a collection of folders is obtained, each corresponding to a distinct time instant and encompassing various computed fields.

4.2.1 File Structure for CHT

In line with prior discourse, the utilization of gas-phase modeling was limited exclusively to the adiabatic scenario, while for all other cases involving a physical wall, gas-solid phase modeling was adopted, treating them as conjugate heat transfer (CHT) problems. Consequently, although the current file structure has been employed for gas phase modeling, substantial modifications are required to accommodate CHT problems. In order to execute a simulation effectively utilizing the *chtLaminarSMOKE* solver, the organization of the case folder must adhere to the configuration depicted in Figure 4.3.

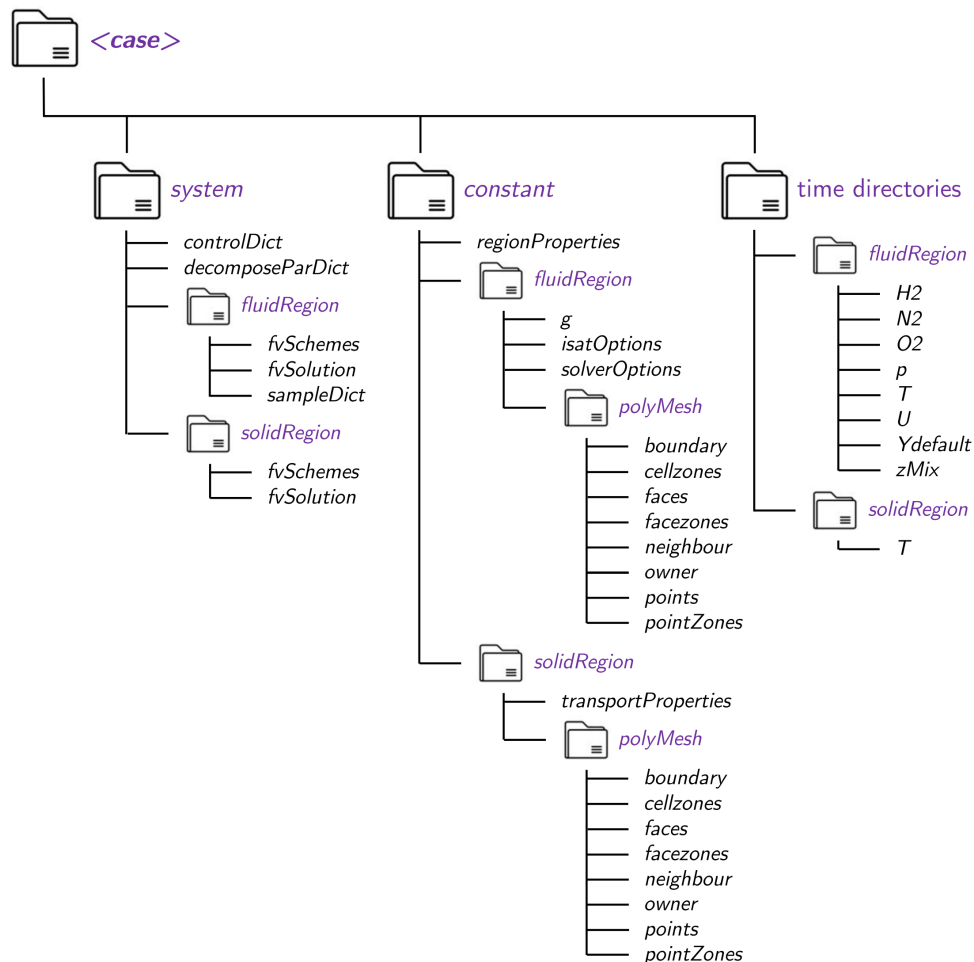


Figure 4.3: Case directory structure adapted for CHT.

It is imperative to highlight certain notable aspects that the user of this computational solver ought to acknowledge. The construction of the computational mesh follows an identical procedure to that employed in the Finite Volume Method. The implementation of the solver's code necessitates the creation of distinct case folders for both the fluid and solid meshes, treating each one as an individual case in its own right.

In the folder *constant/regionProperties*, it's defined the different regions of the simulation domain. This way after executing the *blockMesh* utility, the code will automatically differentiate between the different regions in the simulation

After executing the *blockMesh* utility for the distinct fluid and solid cases, the ensuing step entails duplicating the *polyMesh* folder into the *fluidRegion* and *solidRegion* folders, correspondingly situated within the constant directory of the conjugate heat transfer (CHT) case. Additionally, in the *blockMeshDict* file pertaining to both the fluid and solid domains, it is crucial to designate the boundaries of the shared interface as walls and precisely label them as "fluid interface" and "solid interface," correspondingly. By following this approach, the code will automatically compute the temperature gradient from the fluid domain to the solid domain and vice versa, regardless of the specified thermal boundary conditions at the interface shared by both domains.

The transport properties of the solid material, including thermal conductivity, density, specific heat, and thermal diffusivity, need to be specified in the *transportProperties* file located within the *constant/solidRegion* directory. For the solid-side energy equation solution in *chtLaminarSMOKE*, the solver requires either the input of thermal conductivity or thermal diffusivity, depending on the compiled version being employed. In Eq. (4.1), the thermal conductivity tensor, denoted as λ_s , is presented. The tensor should be filled appropriately, depending on the desired conduction directions and the dimensional characteristics of the geometry under investigation.

$$\lambda_s = \begin{bmatrix} \lambda_{xx} & 0 & 0 \\ 0 & \lambda_{yy} & 0 \\ 0 & 0 & \lambda_{zz} \end{bmatrix} \quad (4.1)$$

Finally, the adoption of a pseudo-transient approach presents a viable option for conducting a computational investigation. Specifically, by assigning a suitable value to the variable S_0 within the *transportProperties* file, one can effectively modulate the transient term within the solid energy equation, as shown in Eq. (4.2). This manipulation serves to augment the time step, thereby enabling a swifter solution convergence within the solid domain. Notably, the solid domain tends to exhibit significantly greater time constants in comparison to the fluid domain.

$$s_0 \rho_s C_{p,s} \frac{\partial T_s}{\partial t} = -\nabla \cdot (\lambda_s \nabla T_s) \quad (4.2)$$

The heat flux lost to the outside was modelled combining both the convection and radiation terms. The equation used was:

$$q'' = h_{\text{conv}} \cdot (T - T_{\text{wall}}) + \sigma \cdot \epsilon_{\text{rad}} \cdot (T^4 - T_{\text{wall}}^4) \quad (4.3)$$

where q'' represents the heat flux, which is the amount of heat energy transferred per unit time and per unit area, h_{conv} is the convective heat transfer coefficient, a measure of how effectively heat is transferred through convection between the object and its surrounding medium, T and T_{wall} are the temperatures of the object and the surrounding walls respectively and σ and ϵ_{rad} are the Stefan-Boltzmann constant and the emissivity of the object.

Additionally, the heat flux was given by the temperature gradient equation:

$$\nabla T = -\frac{q''}{\lambda_s} \quad (4.4)$$

where ∇T represents the temperature gradient and λ_s the thermal conductivity of the object (combustor walls). This is included in the T file of the solid regions ($0/\text{solidRegion}/T$).

4.3 Pre-Processing

4.3.1 Mesh Generation

In accordance with previous discussions, the numerical solutions in OpenFOAM are founded on the Finite Volume Method, which necessitates the subdivision of the physical domain into a discrete mesh.

Within the OpenFOAM framework, there are multiple open-source mesh generators specifically designed for its use. These mesh generators are distributed across the two main development branches: vanilla OpenFOAM and foam-extend. Among them are *blockMesh*, *snappyHexMesh*, *foamyHexMesh*, *foamyQuadMesh*, and *cfMesh*. These tools primarily fall under the category of mesh utilities rather than core mesh generators, which are the focus of this subsection.

In this subsection, we will briefly discuss *blockMesh* and *snappyHexMesh*, reviewing their applications and working principles. Generally, the primary objective of these mesh generators is to create the *polyMesh* data structure, as described in the preceding section, in a user-friendly manner. Both mesh generators operate similarly, where they read input from a dictionary file and produce the final mesh, which is then stored in the *constant/polyMesh* directory.

4.3.1.1 *blockMesh*

To generate such a mesh, the user is required to either construct a *blockMeshDict* file from scratch or modify another file from a different case within the *constant/polyMesh* subdirectory. This file contains the geometric representation of the mesh.

Initially, the user must identify all existing vertices using Cartesian coordinates, with each vertex being assigned a corresponding label. Subsequently, the blocks are assembled, each consisting of eight vertices, in the configuration of a hexahedron, as illustrated in Figure 4.4.

The geometric representation of each block within the mesh consists of a user-defined number of cells. It is important to consider that increasing the number of cells, thus refining the mesh, will result in longer processing times for the software to complete the simulation. Additionally,

each block can have a cell expansion ratio, allowing the cells to gradually expand relative to the previous cell in a specified direction.

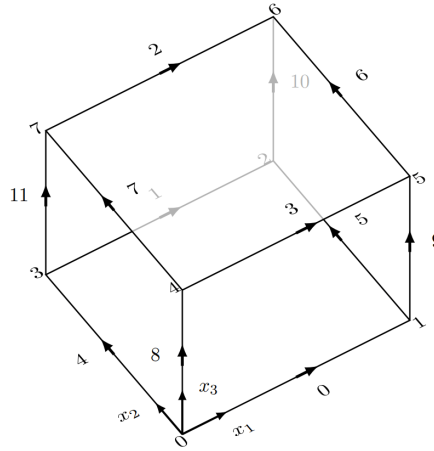


Figure 4.4: A *blockMesh* base block with vertex and edge naming convention [184].

By default, each edge of a block is assumed to be straight. However, it is possible to specify a curved edge if desired. This flexibility enables the user to tailor the mesh geometry to suit their specific requirements, taking into account both processing time considerations and the desired shape of the edges.

4.3.1.2 *snappyHexMesh*

In addition to *blockMesh*, OpenFOAM offers a more advanced tool known as *snappyHexMesh*. This utility can be regarded not merely as a mesh generator, but rather as a mesh sculptor that operates on an existing base mesh. When compared to *blockMesh*, *snappyHexMesh* eliminates the need for laborious tasks such as block addition and connection. However, this convenience comes at the cost of reduced control over the final mesh structure. *SnappyHexMesh* enables the effortless generation of hexadominant meshes, requiring only two components: a hexahedral background mesh and one or more geometries in a compatible surface format.

Moreover, *snappyHexMesh* supports the incorporation of localized mesh refinements defined by various volumetric shapes (refer to Table 4.1), the application of boundary layer cells such as prisms and polyhedra, and the ability to execute operations in parallel.

Table 4.1: List of cell selection shapes [184]

Shape	Name	Parameters
Box	<i>searchableBox</i>	min, max
Cylinder	<i>searchableCylinder</i>	point1, point2, radius
Disk	<i>searchableDisk</i>	origin, normal, radius
Plane	<i>searchablePlane</i>	point, normal
Plate	<i>searchablePlate</i>	origin, span
Sphere	<i>searchableSphere</i>	centre, radius
Collection	<i>searchableSurfaceCollection</i>	geometries
SurfaceWithGaps	<i>searchableSurfaceWithGaps</i>	gap, geometries

In short, in the file `snappyHexMeshDict(a)`, which is located in the "system" folder, numerous options are available to the user, catering to their specific objectives:

- i) Mesh refinement;
- ii) Mesh adjustment to conform to provided geometries;
- iii) addition of boundary layers near specified patches

An illustration showcasing the application of the *snappyHexMesh* utility is presented in Figure 4.5. The specific features, namely i), ii), and iii), are individually depicted in Figures 4.5b, 4.5c, and 4.5d, respectively.

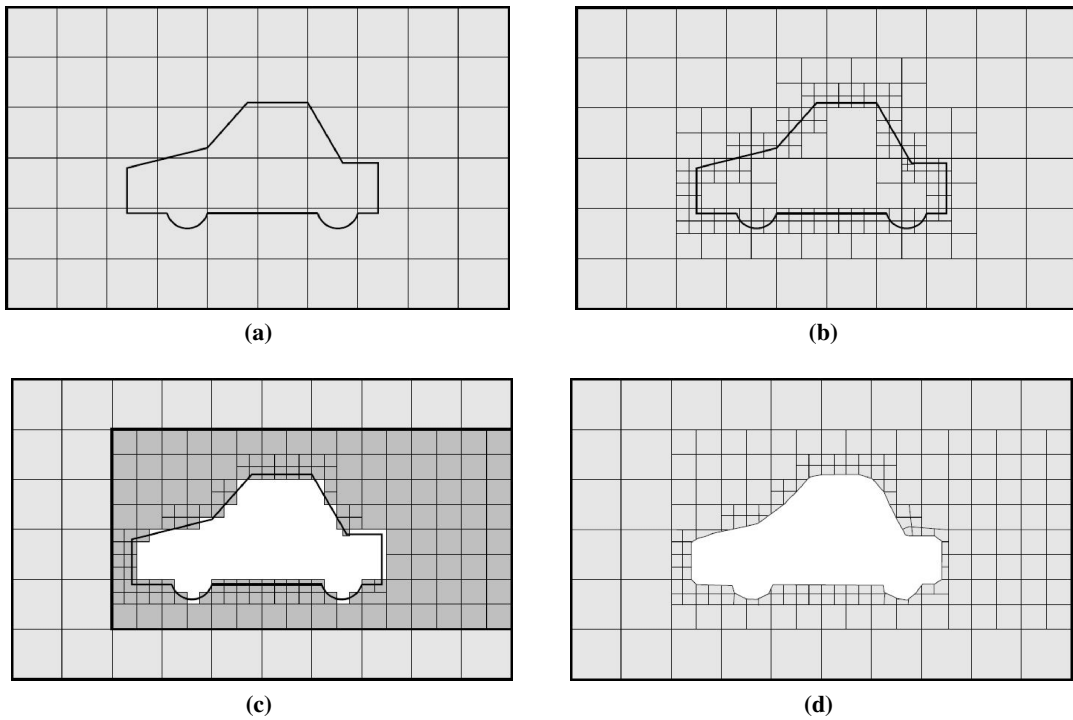


Figure 4.5: Application examples of *snappyHexMesh*: (a) creation of the background mesh; (b) cell splitting by surface; (c) cell splitting by region and cell removal; (d) final surface snapping [183].

4.3.2 Boundary Conditions

Boundary conditions play a pivotal role in addressing problems within the realm of CFD. In order to close the equations system governing the flow and ensuring a well-defined starting point for the numerical simulation in OpenFOAM, it is essential to establish the boundaries and define the initial conditions. As such, the careful selection and accurate implementation of boundary conditions assume paramount significance for achieving reliable and meaningful results.

In openFOAM, the domain boundaries are partitioned into distinct patches or regions. Each patch is associated with a keyword that characterizes its interaction with the simulated external

^(a)the dictionary which contains all of the parameters required by *snappyHexMesh*.

domain. These keywords represent boundary types, which play a crucial role in defining the behavior of the system. The designated names assigned to each patch are subsequently utilized to define the initial conditions and corresponding boundaries of the field data files at the onset of the simulation. This ensures accurate representation and proper initialization of the simulated field dynamics.

The main BC ^(b) provided by OpenFOAM used were:

- i) *fixedValue*: This condition, also known as the Dirichlet boundary condition, imposes a constant value of the function throughout the surface patch for all time steps in the simulation.
- ii) *fixedGradient*: This condition imposes a constant gradient throughout the surface patch for all time steps. In the case where the imposed gradient is zero, the condition can be simplified to *zeroGradient*. This boundary condition is often referred to as the Neumann boundary condition.
- iii) Robin BC: This condition combines aspects of both the Dirichlet and Neumann conditions. It allows for a combination of fixed values and gradients to be imposed on the surface patch, taking into account both the function's values and its derivative.

The thermal boundary conditions, if applied to the previous presented cases, are exemplified in Figure 4.6, and take the following form:

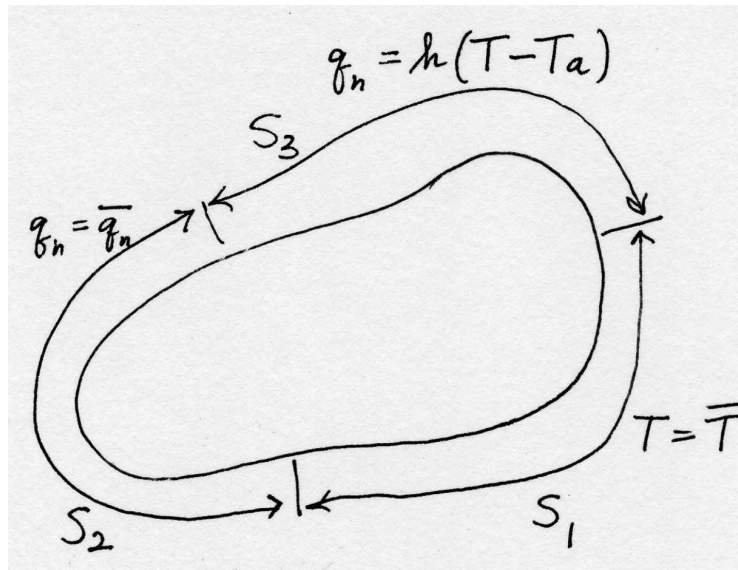


Figure 4.6: The subdivision of the surface for the purpose of the boundary condition application [177].

Given that OpenFOAM does not allow the introduction of a boundary condition in the form of an expression or function, a tool called *swak4foam* was developed to overcome this obstacle. This tool enables the use of more complex boundary conditions, such as a hyperbolic or linear temperature profile. In fact, this tool is of utmost importance in the present study, as will be demonstrated later in the conducted simulations. Further information about the *swak4foam* tool can be found in [185].

^(b) Additional pertinent BC are provided in Appendix C for further reference.

4.3.3 Discretisation and solution of equations

In accordance with the contents presented in Chapter 3, the flows under investigation in this study are mathematically described by a set of partial differential equations that depend on both temporal and spatial dimensions. Due to the variables being continuous, a process known as discretisation is employed to transform them into discrete entities. In the realm of CFD analysis, discretisation is a crucial step, enabling the numerical solution of these variables.

It should be noted that the discretisation process inherently introduces a certain degree of error. Therefore, it is imperative to employ numerical methods that effectively minimize these errors to a negligible level. The specifications for achieving such discretisation schemes, specifically pertaining to Finite Volume methods, are defined within the *fvSchemes* dictionary, which is located in the system directory. Likewise, the settings for solving the equations, including tolerances and algorithm controls, are established in the *fvSolution* dictionary, also located within the system directory.

In addition, the ordinary differential equations associated with the kinetic mechanisms are resolved through the utilization of the OpenSMOKE framework.

4.3.4 Simulation control

In the context of solver execution, various parameters are defined and configured within the controlDict file, which is located in the system subdirectory. This file specifies important simulation details such as the start and end times, the time increment between calculations, the intervals at which the software records field values, and the desired precision for these values.

It is crucial to ensure numerical stability and temporal accuracy in each computational cell. To achieve this, the Courant number (Co) must always be maintained at a value below 1. The Courant number is defined as follows:

$$Co = \frac{\delta t \cdot |U|}{\delta x} \quad (4.5)$$

where δt represents the time step, $|U|$ represents the magnitude of velocity, and δx the cell size in the direction of the velocity. To maintain $Co < 1$ throughout the simulation, it is common practice to select δt based on the worst-case scenario, considering the combined effect of the highest flow velocity and the smallest cell size. Alternatively, simulations can be conducted using an adjustable time step mode, where a new time step is calculated at each time instant, ensuring that the maximum Courant number in the mesh does not exceed a predefined maximum value.

4.3.5 Flame ignition

The combustion phenomenon begins with the ignition of the mixture, marking the onset of the chemical reaction. For this to occur, as seen in Subsection 2.1.5, it is required that the mixture reaches a certain temperature. Consequently, there are two possible ways to achieve mixture

ignition: either through an external heat source supplying heat to a small portion of the mixture (e.g., a spark), or by raising the mixture temperature to meet or exceed its self-ignition temperature, which can be accomplished by imposing a temperature gradient on the wall.

In this study, we focus on investigating premixed flames, which involve gases pre-mixed before combustion. There will be two types of flame ignitions that will be used:

- i) Imposed Temperature: it's introduced an imposed temperature gradient on the burner wall during the initial time step. By defining a desired temperature profile function in the burner wall section of the *T* file within the initial time step folder, we aim to mimic the experimental results of a stable flame;
- ii) Spark: the ignition of the mixture is initiated by a spark located just before the entry into the first cavity of the microchannel. The spark is implemented through the spark function in the *solverOptions* file, located in the *constant* folder. To activate this function, the first line of the code is set to "on". It is then necessary to specify the spark's position within the burner, i.e., its Cartesian coordinates, the ignition time, duration, temperature, and its size.

4.4 Simulation

After completing all the previously outlined steps in the preprocessing section of the case under study, the user is ready to initiate the simulation. The OpenFOAM applications can run the simulation either as foreground or background processes. In the foreground simulation, the progress is displayed in the terminal window, providing the user with the current time, maximum Co number, and initial and final residuals for all fields. As a background or secondary process, the user can request these information to be saved in a file while utilizing the terminal window for other tasks. The latter approach was adopted in executing all simulations in this study, given the significantly high number of simulations and the need to perform multiple tasks in parallel. Thus, to monitor the ongoing simulations (in HPC cluster as will be explained in Section 4.6), the command:

```
1 $ squeue -u up202102696
```

was used with the appropriate username (in this case “up202102696”), which displayed the list of all ongoing or queued simulations.

Numerical simulation is a computationally intensive process, primarily dependent on mesh refinement. Therefore, in this work, tools were employed to reduce processing time, such as utilizing multiple processors interconnected to divide the burner geometry equally among the processors. Sets of up to 8 processors were used during for the non-CHT cases (adiabatic)^(c). This decision was made during the simulation preprocessing phase by modifying the parameters in the *decomposeParDict* file located in the system folder.

^(c)The current implementation of the chtlaminarSMOKE code does not support parallel processing for simulations due to difficulties in separating the nodes for the fluid and solid meshes. As a result, the code does not have the capability to effectively distribute computational tasks across multiple processors or cores. Consequently, simulations using chtlaminarSMOKE can only be performed sequentially on a single processing unit, limiting its utilization of parallel processing architectures.

4.5 Post-Processing

The primary tool provided by OpenFOAM for processing the collected information from a numerical simulation is paraFOAM^(d), which utilizes ParaView.



Figure 4.7: ParaView® Logo.

ParaView is an open-source application [186, 187] that enables the visualization of simulation results. It offers an intuitive interface that allows users to observe the computed fields in different cells at various time steps. Given that the analysis involves a temporal aspect, ParaView facilitates the creation of animations, enabling users to gain a deeper understanding of the dynamic behavior over time, particularly during the ignition phase of the mixture. Furthermore, ParaView provides a wide range of data analysis tools, including the ability to create macros, temporal plots, and position graphs.

4.5.1 ParaView Overview

Upon launching ParaView, the software interface presents the user with a window as depicted in Figure 4.8.

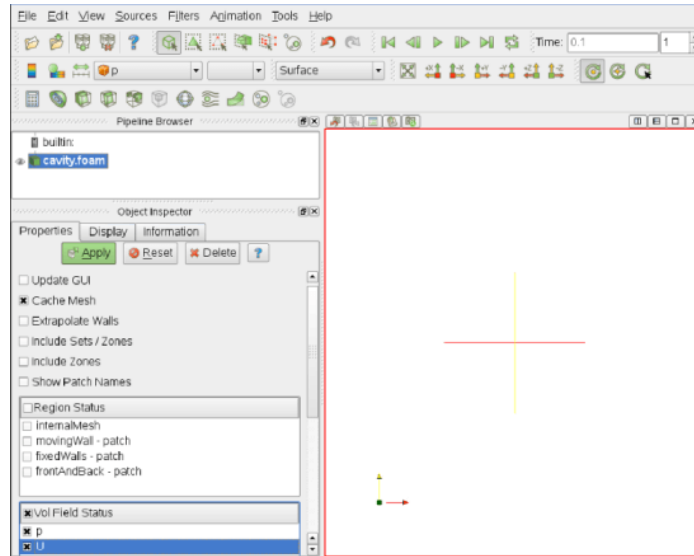


Figure 4.8: The paraFOAM window [186].

The left panel of the window governs the control of the case and encompasses the following components:

- i) Pipeline Browser: This section lists the modules currently open in ParaView. The selected modules are highlighted in blue, and the visibility of their graphics can be toggled on or off by clicking the eye button adjacent to each module;
- ii) Properties panel: Within this panel, users can configure various input parameters for the case, including times, regions, and fields;

^(d)paraFOAM is a script that launches ParaView, utilizing the default reader module from OpenFOAM. It is sometimes used interchangeably with the OpenFOAM reader module itself.

- iii) Display panel: The Display panel provides controls for manipulating the visual representation of the selected module, such as adjusting colors and other visual attributes;
- iv) Information panel: This panel furnishes case-related statistics, such as mesh geometry and size.

ParaView adopts a tree-based structure, allowing the user to apply filters to the top-level case module, thereby creating sets of sub-modules. For instance, a contour plot depicting pressure distribution may serve as a sub-module of the case module, containing all the relevant pressure data. One of ParaView's key strengths lies in its ability to generate multiple sub-modules, enabling users to selectively display the desired modules to create customized images or animations. By adding solid geometry, meshes, and velocity vectors to a pressure contour plot, users can activate or deactivate any of these components as needed.

The general workflow of ParaView revolves around the user's selection of specific settings followed by clicking the green "Apply" button located in the Properties panel. Supplementary buttons include:

- Reset button: used to reset the GUI (Graphical User Interface) if necessary;
- Delete button: deletes the currently active module from the workspace.

Additionally, ParaView offers a range of functions accessible through both the top pull-down menus and the toolbars located below them. Users have the option to select specific toolbars from the main "View" menu. The default layout, depicted in Figure 7.4, displays all available toolbars, each labeled accordingly. The buttons on the toolbars are designed with intuitive icons, and users can obtain concise descriptions of their functions by enabling tooltips in the "Help" menu.

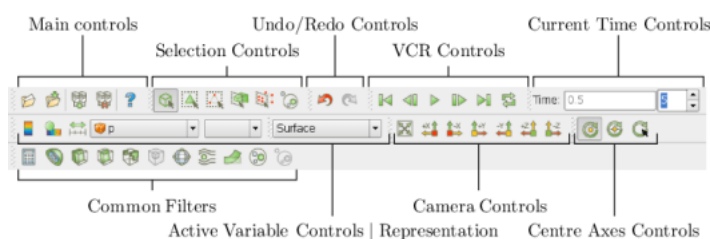


Figure 4.9: Toolbars in ParaView [186].

4.6 Computational Resources

The simulations performed in this study involve highly intricate calculations and iterations, demanding significant computational resources to achieve multiple results within a relatively short timeframe (approximately four months). Moreover, these complex simulations require parallel execution to expedite the process, necessitating access to suitable computational infrastructure capable of handling such demands. To address this need, the Faculty of Engineering of the University of Porto (FEUP) granted access to High Performance Computing (HPC) resources. These resources are organized in a cluster of machines, built upon technology similar to that found in conventional desktop or laptop computers, but equipped with more potent CPUs, increased RAM, and faster network capabilities compared to typical consumer-level machines. A comprehensive

guide detailing the steps to run a simulation on an HPC (High-Performance Computing) system can be found in Appendix D.

The specific cluster utilized for this research, named Avalanche [188], consists of 29 nodes, with each node housing 16 cores and having a RAM capacity ranging between 64 GB and 128 GB. Interconnectivity among the nodes is facilitated through a high-speed 40 Gbps InfiniBand network. The central storage capacity amounts to 10 TB, while each node is equipped with 500 GB of local storage. The clusters operate on the Scientific Linux operating system, specifically version 7.

4.7 Model Configuration

In all simulations conducted in this study, the inlet temperature of the mixture remains constant at $T_{\text{in}} = 300$ [K], at atmospheric pressure. The mixture always consists of the same species, with a fixed equivalence ratio of $\phi = 1$. Specifically, the mixture comprises the fuel H_2 and the oxidant (air), composed of O_2 and N_2 . A schematic representation of the case study and the remaining boundary conditions are depicted in the diagram shown in Figure 4.10.

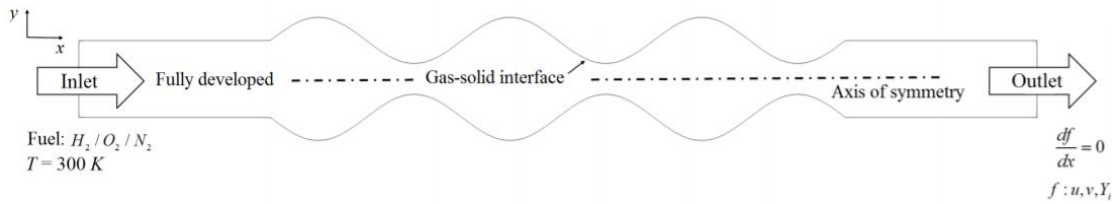


Figure 4.10: Schematic illustration of the computational domain.

4.7.1 Used Meshes

Two different meshes are used, as mentioned before, for the cases using CHT (finite wall of materials) and the adiabatic cases:

1. For the gas-phase simulations (no wall), the simulations are performed in an undulating symmetric micro-channel burner^(e) with a length of 10 [mm] and a height ranging from 0.30 to 1.28 [mm] at the center of the chamber. At both the inlet and outlet, a uniform height of 0.8 [mm] is maintained over a length of 2 [mm]. The mesh is represented in Figure 4.11a.
2. In the gas-solid phase simulations involving finite material walls, we introduce two additional meshes. The *fluidRegion* mesh is essentially similar to the one utilized in the gas phase simulations, but with an extra cavity and a slightly longer outside nozzle section measuring 4 [mm]. This decision was motivated by the need to increase the chances of flame stabilization, given the significant heat loss observed in certain materials. As explained in Section 2.3.2, stabilizing the flame becomes more challenging under such conditions. Furthermore, two^(f) *solidRegion* meshes (*solidRegion1* and *solidRegion2*) are employed to represent the finite material walls of the combustor. These meshes have a resolution similar

^(e)This geometric configuration was established by applying a sinusoidal function, specifically $\sin(x)$, to delineate the profiles of the upper and lower boundaries of a parallel plate structure. This approach was utilized to emulate the inlet and outlet regions of the aforementioned geometry.

^(f)The division of solid meshes was necessary to ensure consistent heat flux distribution. The presence of separate meshes helped mitigate numerical errors that were encountered when utilizing a single mesh.

to that of the other meshes and each possesses a thickness of 0.15 [mm]. Consequently, the total length of the combustor is 14 [mm]. The mesh is represented in Figure 4.11b.

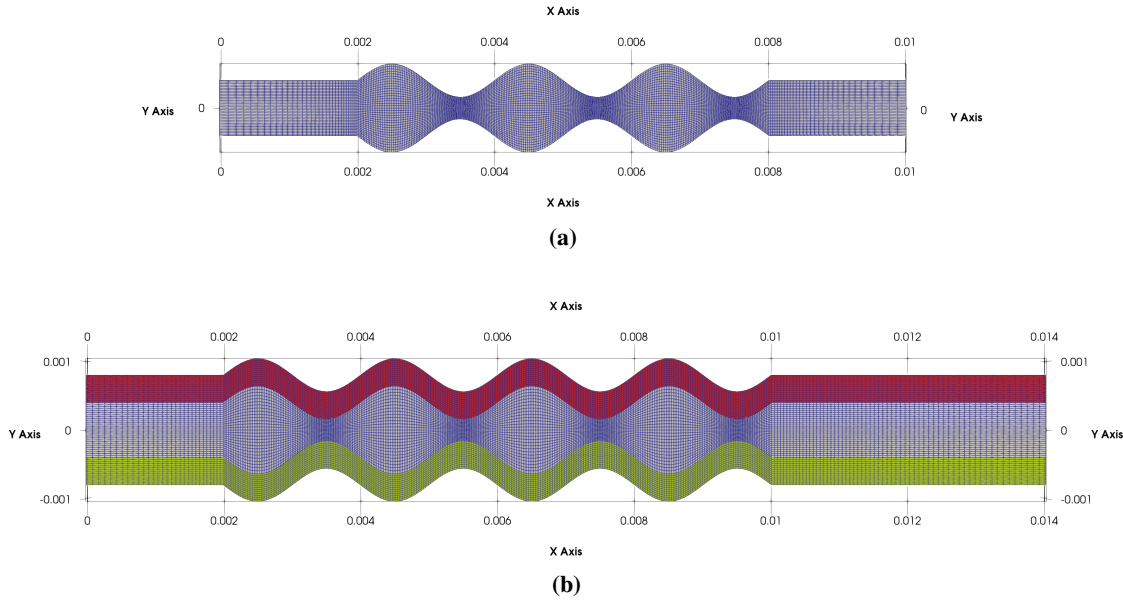


Figure 4.11: Used meshes with resolution: (a) Gas phase modelling (only *fluidRegion*). (b) Gas-solid phase modelling (*fluidRegion* mesh in blue, *solidRegion1* mesh in red and *solidRegion2* in yellow).

The meshes used in this study have a higher refinement in the contraction regions compared to the cavity regions of the microchannel. Mesh refinement is a crucial parameter that needs to be carefully determined at the beginning of each simulation. Insufficient mesh refinement can lead to significant errors in the calculated parameters within each finite volume, while excessive refinement requires high computational resources or results in extensive simulation times.

In this analysis based on the finite volume method, a mesh resolution of 10,836 cells was employed throughout the microchannel for the *fluidRegion*^(g), with equidistant spacing at the center. This resulted in finer resolution in smaller areas, where the smallest cells had dimensions of 25 by 9 micrometers, a resolution that is similar to the mesh resolution of Alipoor and Mazaheri [99]. It has also been previously employed in related studies, notably, Resende et al. [189, 190] utilized this mesh resolution to investigate the impact of N₂ dilution on H₂ and air mixtures in a microchannel. Their findings demonstrated the ability of this mesh resolution to accurately capture the intricate physics involved in the system. The meshes used to represent the solid walls contained a total 5740 cells each, with a similar resolution to the one used in the *fluidRegion*.

Table 4.2: Employed mesh specifications for the computational regions

Mesh Region	N° cells in domain [-]	N° points in domain [-]	Memory (t_0) [Mb]
<i>fluidRegion</i> (adiabatic)	10836	22348	1.014
<i>fluidRegion</i> (CHT)	11480	23838	1.074
<i>solidRegion1</i> & <i>solidRegion2</i>	5740	12330	0.555

^(g)for the the gas-solid phase simulations, due to the increase in length, the mesh resolution contained 11480 cells.

Part III

Investigatio de Materia

INVESTIGATIO :: (noun) *the action of investigating something or someone; formal or systematic examination or research*

MATERIA :: (noun) *the matter from which a thing is or can be made*

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Chapter 5

Characterizing the Thermal Behavior of Different Materials using a Spark

*“A spark is a little thing, yet it
may kindle the world.”*

Martin Farquhar Tupper

5.1 Case Introduction

Investigating flame dynamics in microchannels is crucial for optimizing performance and ensuring safety. To achieve this, we will employ a spark ignition method to study the influence of different materials on flame behavior, starting from an equilibrium state where the combustor wall temperature (T_{wall}) matches the ambient temperature (T_{amb}).

However, a crucial challenge in this investigation arises due to the limitation of computational resources and the timescale required for simulations to reach steady-state conditions. In most cases, the transient term $\frac{dT}{dt_0}$ would substantially prolong the simulation duration, as the walls of the microchannel would need to be heated to a sufficiently high temperature to sustain the flame. To address this issue, we made an informed decision to turn off the transient term $\frac{dT}{dt_0}$ in the simulation file *transportproperties*, of *solidRegion1* and *solidRegion2*, for all the materials. This approach allowed us to focus on the critical aspects of flame dynamics without being hindered by lengthy simulation times during the spark ignition phase. Further explanation in Section 5.2.

To facilitate the ignition process and ensure the undisturbed flow and combustion dynamics, we introduced a well-defined heat source inside the microchannel, as shown in Figure 5.1.

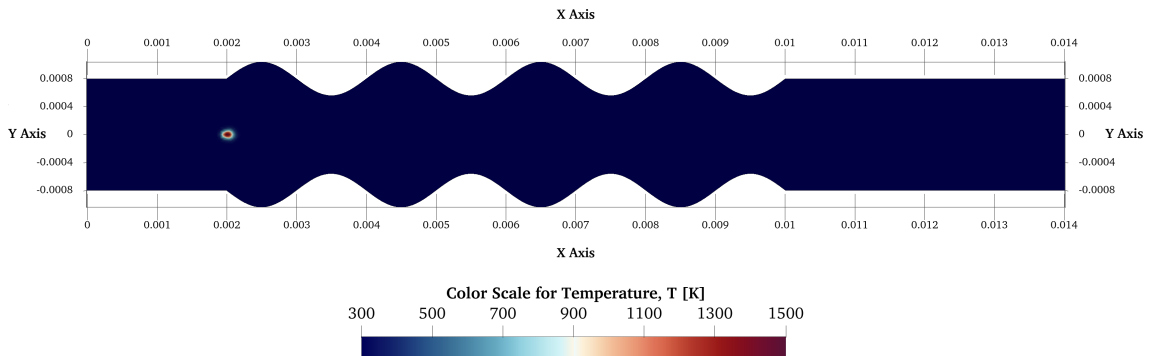


Figure 5.1: Graphical representation of the spark imposed within the microchannel with walls.

This heat source was carefully designed to ignite the mixture while preserving the inherent behavior of the flow and combustion processes. The implementation of the spark inside the combustor, was done by employing a function defined in the *solverOptions* file. The function allowed us to specify essential parameters such as spark duration, spatial localization, characteristic dimensions (diameter), and temperature. This function is shown in Listing 5.1:

```

1 Spark
2 {
3     spark                on;
4     position              (0.002  0.0 5e-5);
5     time                  0.;
6     temperature           1500;
7     duration              0.0005;
8     diameter              0.1e-3;
9 }

```

Code Listing 5.1: Imposed Spark Function in C++.

In this study we investigated the flame dynamics with a set of ten different structural materials, each belonging to one of four distinct groups: Steels, Ceramics, Thermal Conductors, and Amorphous materials. The selection of materials was made based on their relevance and common usage in aerospace applications. In Table 5.1, the utilized materials are listed alongside a comprehensive summary of their key heat transfer properties, namely: thermal conductivity (λ_s), density (ρ), specific heat capacity (C_p), thermal diffusivity (α_T), and emissivity (ϵ_{rad}).

Table 5.1: Chosen materials for this study and their key heat transfer properties

Group	Material	λ_s [W/(mK)]	ρ [kg/m ³]	C_p [J/(kgK)]	α_T [m ² /s]	ϵ_{rad} [—]	Ref.
Adiabatic	Adiabatic	0	n.a.	n.a.	n.a.	n.a.	[191]
Amorphous	Borosilicate Glass	1	2230	830	5.40×10^{-7}	0.3	[192]
	Fused Silica	1.47	2200	670	9.97×10^{-7}	0.3	[193]
Ceramic	LTCC	2.8	2950	710	1.34×10^{-6}	0.75	[194]
	HTCC	20	3670	790	6.90×10^{-6}	0.75	[195]
Steel	Stainless Steel High Carbon	16.2	7750	510	4.10×10^{-6}	0.5	[196]
	Stainless Steel	25	7700	470	6.91×10^{-6}	0.5	[197]
Conductor	Silicon	130	2321	700	8.00×10^{-5}	0.5	[198]
	Aluminium	200	2750	860	8.46×10^{-5}	0.1	[199]
	Copper-Tungsten	250	11300	200	1.06×10^{-4}	0.4	[200]

As shown in the table, we decided to adopt α_T , the thermal diffusivity, as a key indicator of the material's thermal characteristics, when assessing the performance of a MPS. It basically represents the material's ability to conduct heat relative to its heat storage capacity per unit volume. A higher α_T implies more efficient heat conduction and faster heat transfer compared to heat retention within the material. Can be calculated using the other shown key material properties, as indicated by Eq. (5.1).

$$\alpha_T = \frac{\lambda_s}{\rho \cdot C_P} \quad (5.1)$$

Among the Steels category, two types of stainless steel were chosen for studying: AISI 310, which has a higher carbon percentage, and AISI 430. The Ceramics group comprises two distinct materials: High Temperature Co-fired Ceramic (HTCC) and Low Temperature Co-fired Ceramic. For the Thermal Conductors category, materials who conduct heat exceptionally well, three materials were selected: pure Silicon, an aluminium alloy, and a copper-tungsten alloy. Finally, two amorphous materials, Borosilicate glass and fused silica glass, were studied in detail.

Furthermore, a comparative analysis was performed with an adiabatic material, allowing us to better understand the specific properties and behavior of each material in relation to this reference point. The research methodology involved simulations to study various properties of these solid materials.

For each material, a series of five simulations were performed, varying the inlet speed, V_{in} , at five different values: 4, 6, 8, 10, 12 [m/s]. In Table 5.2, these simulations are presented along with their corresponding velocities used.

Table 5.2: Series of simulations done utilizing the spark initial condition

Group	Name	U4 [m/s]	U6 [m/s]	U8 [m/s]	U10 [m/s]	U12 [m/s]
Adiabatic	Adiabatic	Ad4Sp	Ad6Sp	Ad8Sp	Ad10Sp	Ad12Sp
Amorphous	Fused Silica	FS4Sp	FS6Sp	FS8Sp	FS10Sp	FS12Sp
	Borosilicate Glass	BG4Sp	BG6Sp	BG8Sp	BG10Sp	BG12Sp
Ceramic	LTCC	LT4Sp	LT6Sp	LT8Sp	LT10Sp	LT12Sp
	HTCC	HT4Sp	HT6Sp	HT8Sp	HT10Sp	HT12Sp
Steel	Stainless Steel High Carbon	CS4Sp	CS6Sp	CS8Sp	CS10Sp	CS12Sp
	Stainless Steel Low Carbon	SS4Sp	SS6Sp	SS8Sp	SS10Sp	SS12Sp
Conductor	Copper-Tungsten	CT4Sp	CT6Sp	CT8Sp	CT10Sp	CT12Sp
	Silicon	Si4Sp	Si6Sp	Si8Sp	Si10Sp	Si12Sp
	Aluminium	Al4Sp	Al6Sp	Al8Sp	Al10Sp	Al12Sp

5.2 Simulation settings

We adopted a pseudo-stationary approach (which was previously explained in Subsection 4.2.1) by turning off the transient term dT/dt_0 due to the vast disparity between the timescales of chemical reactions and heat transfer. This streamlines the solution process within the solid material, leading to a notable reduction in simulation time. While this approximation does not capture the complete transient behavior, it still offers valuable insights, especially given our primary objective of comprehending heat transfer across diverse solid materials.

Conversely, in specific scenarios such as heat exchangers or flows involving substantial dissipation, it is common practice to employ distinct time steps for different equations within the simulation. This trade-off may result in the loss of intricate details, but it effectively balances the trade-off between simulation speed and accuracy.

The policy file⁽¹⁾ of the *chtLaminarSMOKE* solver, as previously mentioned, is shown in Appendix A, in Listing A.1. Furthermore, the more relevant *system* files, namely *fvSchemes*, *fvSolution*, and *controlDict*, each are showcased in Listings A.2, A.3, and A.4, respectively.

Of particular significance are the *constant* files, particularly the *transportProperties* file (as depicted in Listing A.5), which delineates crucial heat transfer attributes for both *solidRegion1* and *solidRegion2* and the file *solverOptions*⁽²⁾ (refer to Listing A.6) which orchestrates the calibration of configuration parameters, thus governing the operational behavior of the *chtLaminarSMOKE* solver within the domain of the *fluidRegion*.

Table 5.3 presents the *T* files *boundaryField* details across the three regions, outlining the specific Boundary Conditions employed for each individual mesh face, for the initial timestep.

Table 5.3: *T* *boundaryField* of the for both *fluidRegion* and *solidRegion1* and *solidRegion2* for the initial timestep

<i>fluidRegion</i>		<i>solidRegion1</i> & <i>solidRegion2</i>	
Face	Boundary Condition	Face	Boundary Condition
inletfuel	type <i>fixedValue</i> value uniform 300	adiabaticwall	type <i>fixedGradient</i> uniform 0
outlet	type <i>zeroGradient</i>	defaultfaces	type <i>fixedGradient</i> uniform 0
axis	type <i>symmetry</i>	outerwall	type <i>groovyBC</i> valueExpression "0" fractionExpression "0" gradientExpression "gradT"
fluid_interface fluid_interface2	type <i>fixedValue</i> uniform 300	solid_interface1 solid_interface2	type <i>fixedGradient</i> uniform 0
front & back	type <i>empty</i>	front & back	type <i>empty</i>

As an additional remark, the *outerwall* of the *solidRegion*, characterized by a *groovyBC*, was done utilizing Equations (4.3) and (4.4).

⁽¹⁾Configuration file used to define various settings and options for a solver.

⁽²⁾This file serves the crucial function of configuring kinetics models, physicalModel settings, and conjugate heat transfer (CHT) configurations, among other essential parameters.

5.3 Dynamics of adiabatic materials

This section explores flame dynamics in adiabatic materials and involves numerical analysis of flame behavior, temperature, NO_x emissions and heat release rates for different inlet velocities.

In the adiabatic material simulations, a null temperature gradient is enforced along the entire burner wall, preventing any heat exchange between the channel's interior and exterior. By achieving adiabatic conditions during the combustion process, the adiabatic flame temperature should be attained. This temperature represents the inherent maximum flame temperature associated with the chemical process, as exemplified in Section 2.1.9. Also, as explained in Chapter 3, the used solver for the adiabatic simulations will be *laminarSmoke*, since only gas-phase modelling is needed.

5.3.1 Stability map

In conjunction with the investigation conducted by Macedo [112], where the behavior of an adiabatic material was studied using a spark similar to the one employed in our research, operating at equivalence ratios of $\phi = 0.7, 1.1, 1.3$, we present the stability map⁽³⁾. We augment this study by incorporating the outcomes for $\phi = 1.0$. Results shown in Figure 5.2.

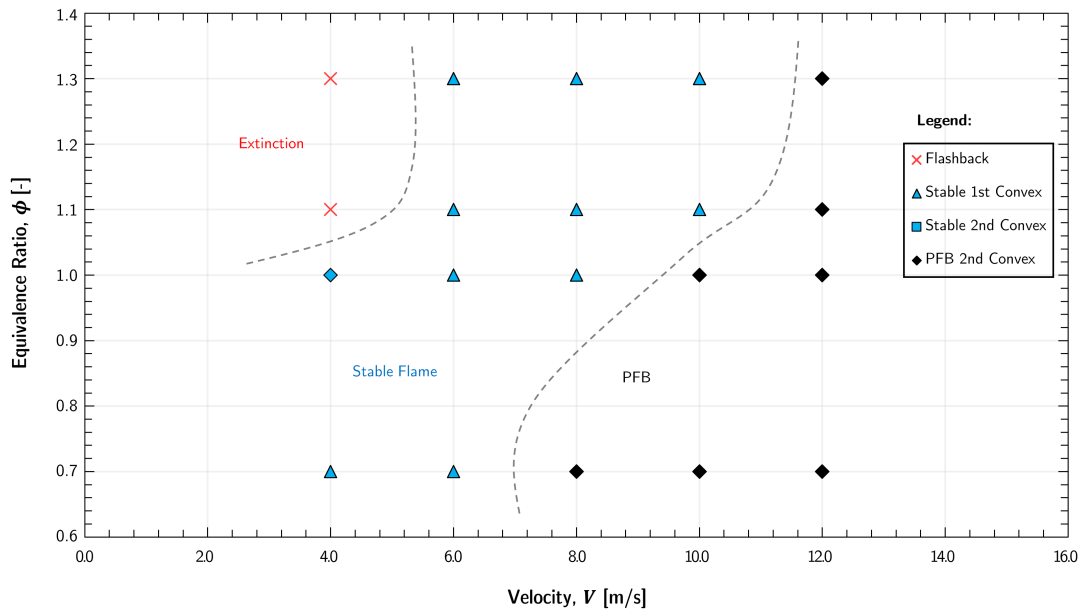


Figure 5.2: Stability map for the various simulations conducted with the adiabatic microchannel ($\phi = 0.7, 1.1, 1.3$ from [112]).

5.3.2 Flame behaviour in adiabatic materials

As depicted in Figure 5.2, the adiabatic simulations (Ad4Sp to Ad12Sp) showcased two distinct dynamics. Among the five simulations conducted, Ad4Sp, Ad6Sp, and Ad8Sp demonstrated stable flames⁽⁴⁾, while the remaining two simulations displayed PFB dynamics.

⁽³⁾This map aims to delineate the transition zone of flame behavior concerning the inlet velocity and equivalence ratio.

⁽⁴⁾Notably, Ad4Sp's flame achieved stabilization in the 2nd convex zone, while the other two achieved it in the 1st cavity.

5.3.2.1 Stable flame dynamics

In Figure 5.3, we observe the flame structure for the stable cases. The figure presents the distribution of the heat release rate, q''' , along with the streamlines of the flow field. Notably, 2 of the flames exhibit a configuration anchored in a distinct V-shape at the initial stage of the convexes zones, and one ($U_{in} = 4$ [m/s]) anchors in the second stage. The highest concentration of the flames are concentrated along the centerline of the burner. This observation suggests a robust and coherent flame structure under these conditions.

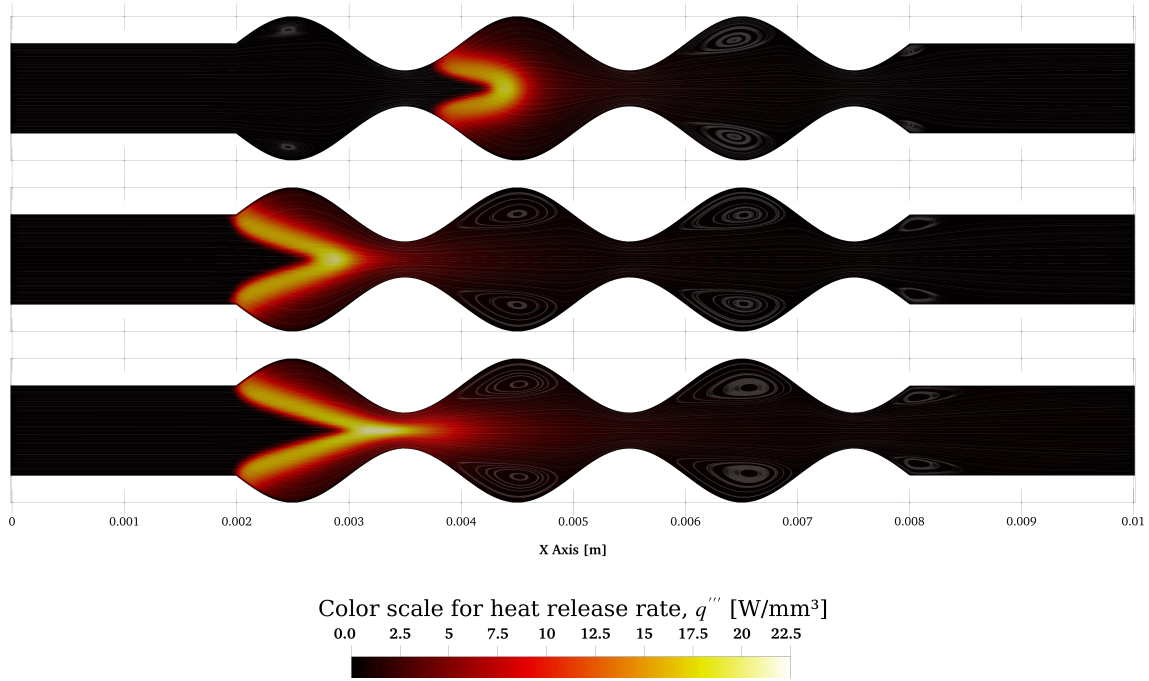


Figure 5.3: Streamlines of the flow field and distribution of heat release rate for stable cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).

To facilitate a thorough analysis of the simulation, we will now introduce a newly defined parameter known as "flame length," denoted as ℓ_f ⁽⁵⁾. This variable is specially important since it provides insights into the spatial progression of combustion and the visible extent of the flame front (dynamic nature of the flame's growth)⁽⁶⁾.

From Figure 5.3 and the analysis conducted using *ParaView* data, it's clear that for Ad4Sp, the flame is anchored around the 2nd convex zone ($x \in 4, 5$ [mm]). Specifically, ignition occurs at $x_i = 3.75$ [mm], extending to the middle of the convex zone with a flame length of $\ell_f \approx 0.50$ [mm]. Notably, the simulation shows average and maximum heat release rates of $q'''_{avg} = 1.164$ [W/mm³] and $q'''_{max} = 19.094$ [W/mm³], respectively.

⁽⁵⁾The flame length is a parameter we defined to quantify the visible extent of combustion within a microchannel configuration resembling a triangular flame front. It is measured from the initial anchoring point of the flame (x_i), located near the wall of the microchannel where combustion initiates, to the point (x_f) along the centerline of the chamber where the flame becomes observable. As such, $\ell_f \approx x_f - x_i$.

⁽⁶⁾The "flame front" refers to the boundary or interface between the unburned mixture of fuel and oxidizer and the burned combustion products in a combustion process, i.e. leading edge of a flame propagating

As for the two situations, Ad6Sp and Ad8Sp, where the flame anchored on the 1st convex zone ($x \in 2, 3$ [mm]), with $x_i = 1.95$ [mm] for both cases and flame lengths of $\ell_f \approx 0.70$ [mm] and $\ell_f \approx 0.95$ [mm], for $U = 6$ [m/s] and $U = 8$ [m/s] respectively. In regard to the heat release rates, for Ad6Sp we observe $q'''_{avg} = 1.797$ [W/mm³] and $q'''_{max} = 20.503$ [W/mm³], and for Ad8Sp we observe $q'''_{avg} = 2.711$ [W/mm³] and $q'''_{max} = 21.533$ [W/mm³].

Utilizing the computational visualization tool *ParaView*, the "Integrate Variables" filter is employed to ascertain the integral of the amount of heat released distributed across the entirety of the simulated mesh at a specified temporal juncture. This yields the integrated heat release rates, denoted as q_{tot} , for the triad of scenarios, evaluated at the final temporal point. Consequently, the cumulative integrated heat release rates manifest as 0.423 [W], 0.640 [W], and 0.850 [W], sequentially corresponding to the progression from Ad4Sp through Ad8Sp.

In sum, it can be seen that higher inlet velocities engenders a stronger, more pronounced and well-defined flame configuration (sharper), possibly since increased U_{in} likely promotes more fuel concentration downstream (resulting in higher values of q''' and q_{tot}). Notably, a positive correlation emerges, whereby augmenting the values of the inlet velocity parameter (U_{in}) corresponds to an elongation of the resulting flame length, ℓ_f .

Furthermore, an escalation in both average and maximum heat release rates is observed, with a more pronounced effect on the average rates⁽⁷⁾. This can be primarily attributed to the longer flame structure and increased quantities of fuel and air within the microchannel (constant volume across all simulations) as the value of U_{in} is elevated.

We will now show in Figure 5.4, the distribution of temperature for the three different cases.

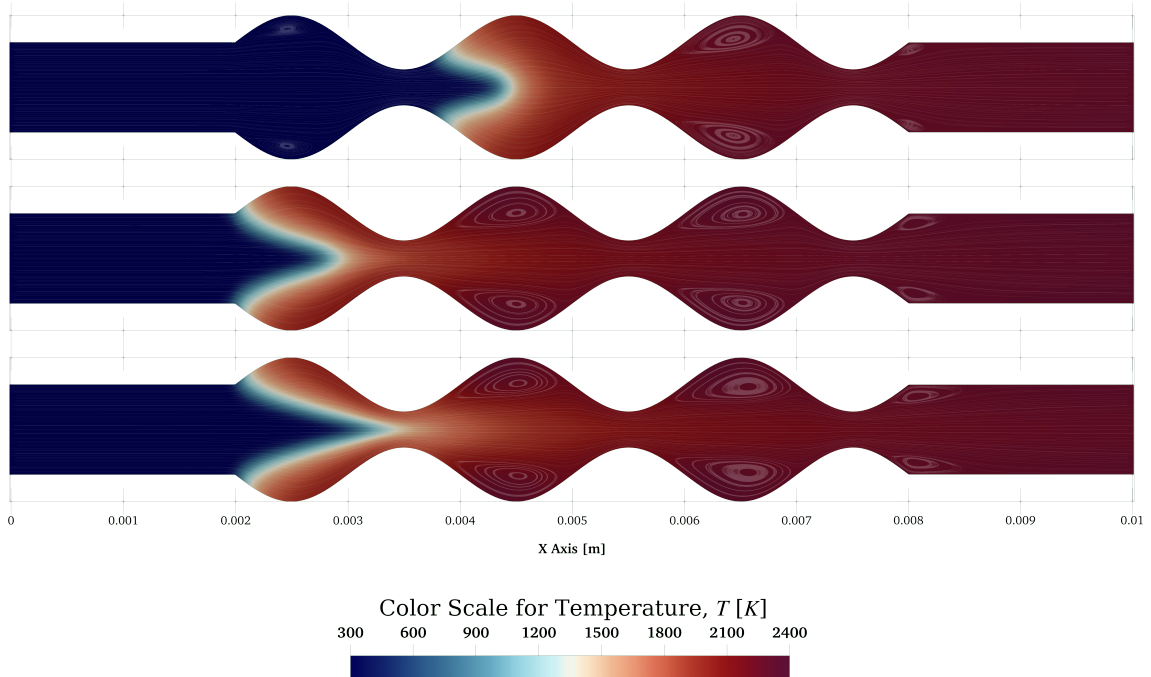


Figure 5.4: Streamlines of the flow field and distribution of temperature for stable cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).

⁽⁷⁾It's noteworthy that findings in [112] indicate that alterations in U_{in} yield a significantly more substantial impact on the amplification of q''' and q_{tot} values compared to variations in ϕ .

As evident from the data, a consistent trend is observed across all scenarios, whereby temperatures exhibit a progressive elevation culminating at the outlet face of the microchannel. As explained previously, the air/fuel mixture is supplied at a base temperature of 300 K, and by referring back to Fig 5.3, where it's possible to discern the propagation of the flame front, we can see that in this zone there's a discernibly acute escalation in temperature. This observed phenomenon aligns seamlessly with the theoretical prognoses rooted in combustion kinetics, wherein the rapid exothermic reactions inherent to combustion lead to a conspicuous thermal surge.

To facilitate the ongoing analysis, we proceed by presenting the evolution of temperature (T) and the heat flux (q''') along the central axis of the microchannel (x-axis), in Figure 5.5.

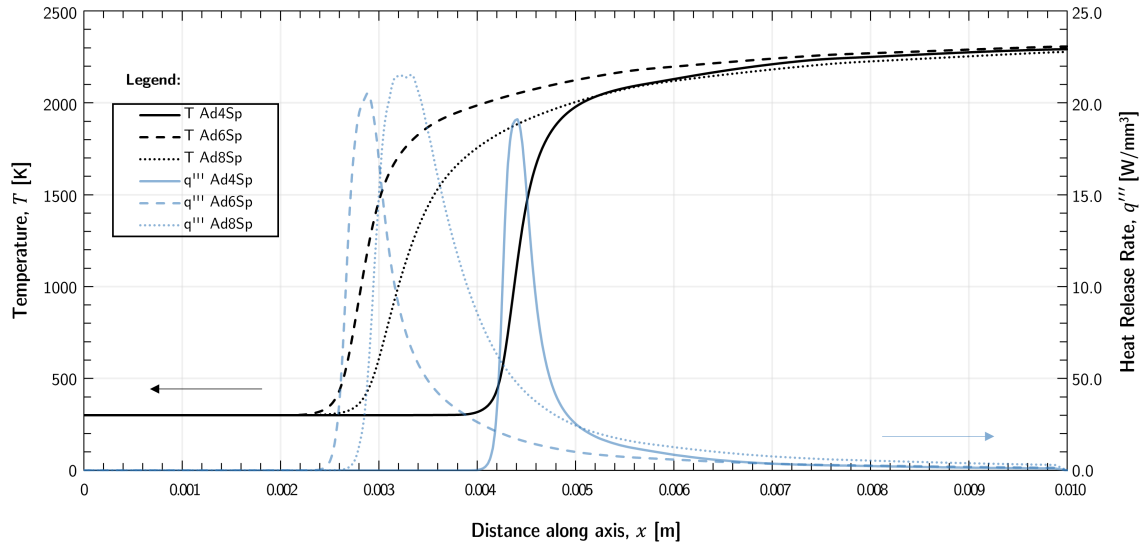


Figure 5.5: Heat release rate and temperature profiles along the x axis (centerline) for the adiabatic stable cases.

In the context of the three scenarios, the temperature evolution along the microchannel's centerline displays a resemblance to a logarithmic curve, featuring a sharp ascent around the flame front followed by a gentler climb until reaching a plateau close to the adiabatic flame temperature. As anticipated, the steepness of the curve for scenario Ad4Sp starts at a considerable higher distance than the other two, simply due to the flame being anchored in the second convex zone. Additionally, we can see that reduced values of U_{in} lead to an initial rapid temperature rise that gradually levels off, ultimately aligning with the plateau observed in the other curves (theoretically close to the adiabatic temperature see in Section 2.1.9). Moreover, it's worth noting that despite Ad8Sp and Ad6Sp anchoring at similar distances, the former, due to an increase on U_{in} experiences a delayed initial steep ascent, mainly attributed to the higher ℓ_{fl} , has observed previously.

In relation to the evolution of heat release along the microchannel centerline, the presented curves exhibit a parabolic morphology characterized by an initial exponential ascent culminating at the maximum q''' point. This trajectory is succeeded by a logarithmic decline, ultimately approaching a value of zero. The parabolic curve aligns with the steep increase in the temperature curves, which is to be expected since this region corresponds to the locale of peak heat release emanating from the combustion dynamics. From a comprehensive analysis of these curves, several significant observations can be extrapolated:

- i) With increasing U_{in} , the curves exhibit a noticeable broadening, implying a wider and dispersed flame—a trend that aligns well with prior observations.
- ii) Although the exponential segments of the curves maintain a semblance of similarity, the higher U_{in} , the higher q'''_{max} along the centerline.
- iii) Higher values of U_{in} , as previously demonstrated, results in elongated ℓ_{fl} , a characteristic evident in the progression of q''' since the logarithmic trend requires a prolonged duration to converge towards 0.

Concluding our analysis of temperatures and heat release rates, we present in Table 5.4 the maximum and average values observed for both temperature (T) and heat release rate (q''') across the three cases. Furthermore, the temporal evolution of T_{avg} , T_{max} , q'''_{avg} , and throughout the simulation from 0 [ms] to 2.40 [ms] is depicted in Figure 5.6.

Table 5.4: Maximum and average values for temperature and heat release rate for the adiabatic stable cases

Scenario	ℓ_{fl} [mm]	T_{avg} [K]	T_{max} [K]	q'''_{avg} [W/mm ³]	q'''_{max} [W/mm ³]	q_{tot} [W]
Ad4Sp	0.50	1451.25	2299.96	1.164	19.094	0.423
Ad6Sp	0.70	1879.78	2321.74	1.797	20.503	0.640
Ad8Sp	0.95	1790.27	2321.39	2.711	21.533	0.850

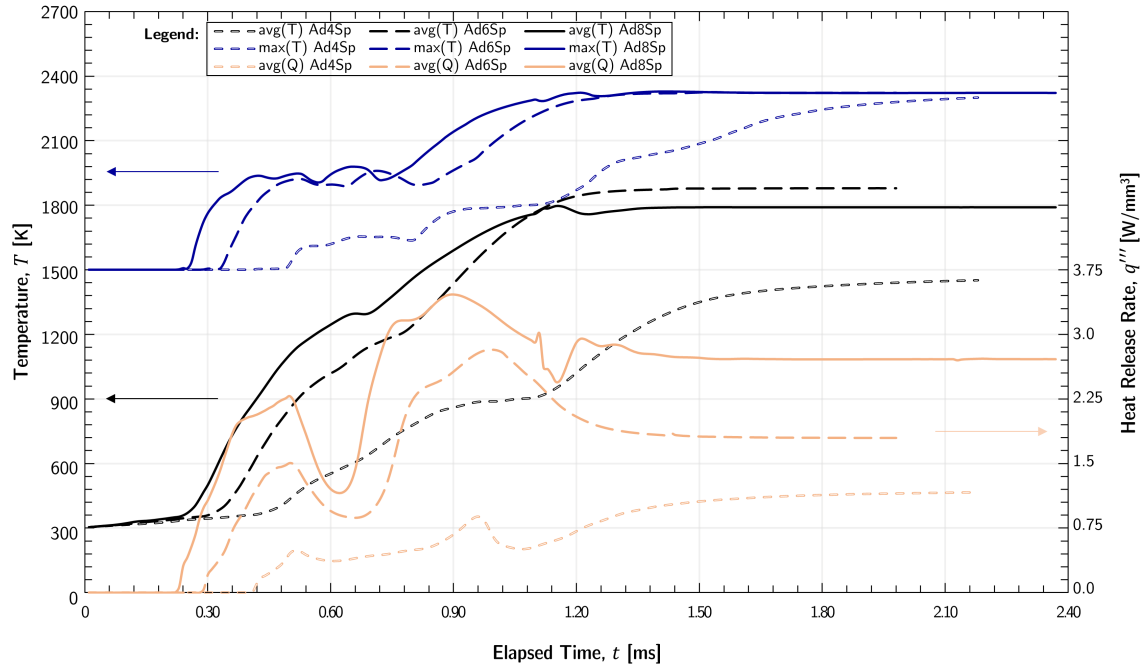


Figure 5.6: Temporal evolution of T_{avg} , T_{max} and q'''_{avg} for the the adiabatic stable cases.

As the flame is anchored later in the microchannel, in the 2nd convex zone for Ad4Sp, it's easily explained why T_{avg} for this case is a lot lower than for the other two, and since there's not heat loss, it's understandable why T_{max} is similar for all cases. What might initially seem strange however is why $T_{max@Ad6Sp} > T_{max@Ad8Sp}$ and $q'''_{avg,max@Ad6Sp} < q'''_{avg,max@Ad8Sp}$, since, in the context of

combustion, this seems counterintuitive given the typical behavior of combustion reactions, which tend to release heat and raise temperatures.

Nevertheless, a longer flame and larger combustion zone mean that the reactants spend more time within the combustion region. This extended residence time can lead to larger region of lower temperature before complete combustion of H_2 occurs. For deeper insights, focusing on the front of the flame, as evidenced by the distribution of hydroxide radical mass fractions (depicted in Figure 5.7), sheds light on this behavior⁽⁸⁾.

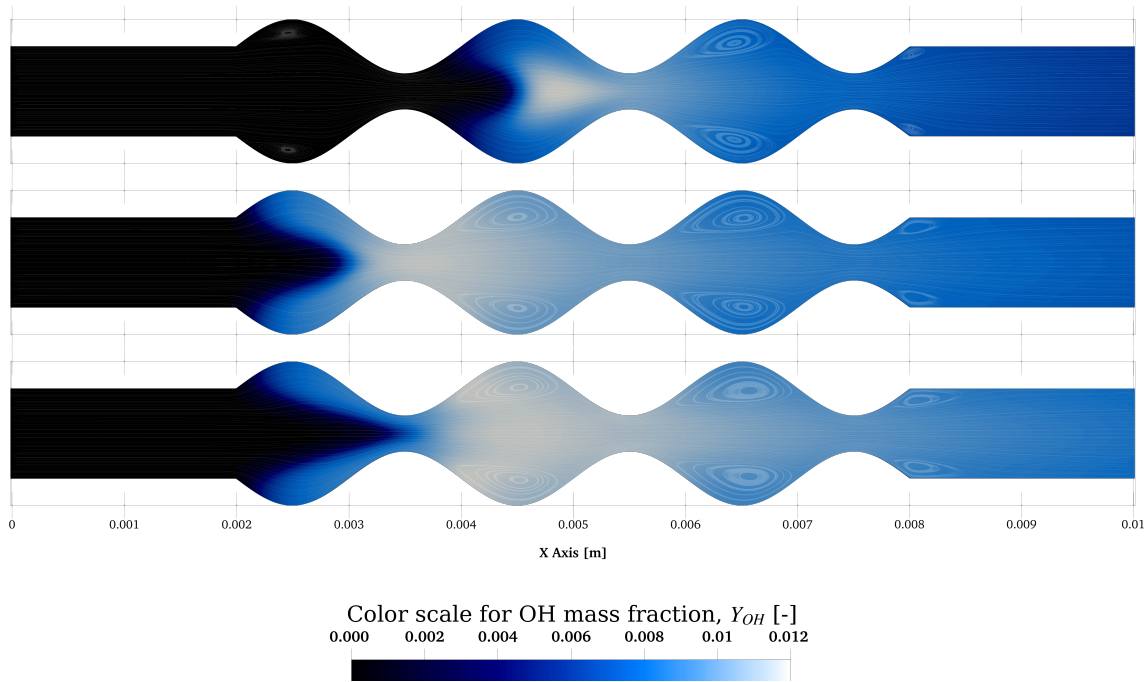


Figure 5.7: Streamlines of the flow field and distribution of OH mass fraction for stable cases (Ad4Sp on the top, Ad6Sp on the middle and Ad8Sp on the bottom).

This analysis showcases that the flame's delay in Ad8Sp compared to Ad6Sp aligns well with our underlying hypothesis (specifically by looking into the 2nd convex zone, where it's clear that $Y_{OH@Ad6Sp} > Y_{OH@Ad8Sp}$), thereby establishing a robust foundation for our understanding.

Moreover, the analysis of velocity streamlines (shown both in Figure 5.3, 5.4 and 5.7) affords the opportunity to discern zones of vorticity arising from escalated velocity gradients. Nonetheless, within the convex domain housing the combustion front, a distinct phenomenon ensues. Herein, the chemical reactions transpiring at the flame's leading edge prompt a fluid expansion, inducing a coercive redirection of flow along the adjacent wall. Consequently, the conducive circumstances for vortex genesis are effectively nullified within this locale.

Finally, the reason why Ad4Sp anchors on the 2nd convex zone is evident when examining Figure 5.8, showing T profiles at the spark's end ($t = 0.5$ [m/s]). The flame anchors in contraction zones due to the wavy geometry, as seen in previous research [112, 113, 140]. Failing to anchor in prior zones, the flame struggles to return without wall conduction, often resulting in blow-by,

⁽⁸⁾This is due to the detailed kinetic mechanism used in the simulations, which allows to obtain different types of combustion reaction

caused by insufficient thermal energy. If temperature is too low in one convex zone, a blow-by ensues, and the flame moves to the subsequent zone. If combustion extends excessively and temperature drops, a complete blow-by leads to extinction. In the case of Ad4Sp, the flame is smaller and cooler compared to Ad8Sp, hindering initial 1st zone anchoring. However, its higher temperature and combustion rate eventually enable later anchoring.

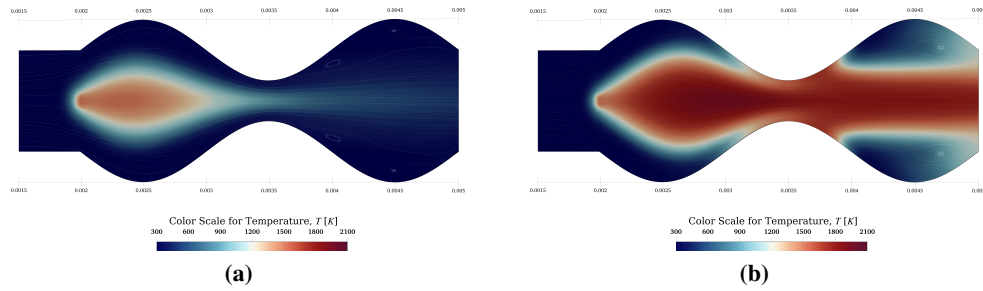


Figure 5.8: Temperature profiles at the end of spark ($t = 0.5$ [m/s]) for: a) Ad4Sp; b) Ad8Sp.

The distribution of mass fractions for the primary species in the three scenarios along the central axis of the burner are depicted in Figure 5.9.

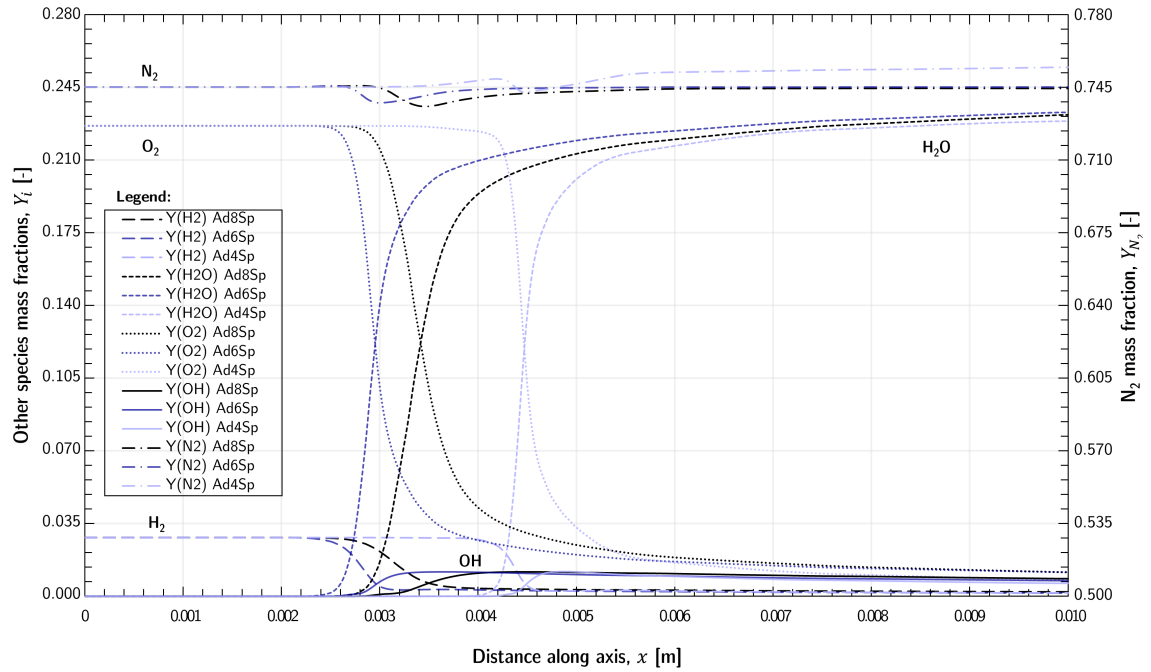


Figure 5.9: Comparison between the cases Ad4Sp (light blue lines), Ad6Sp (dark blue lines) and Ad8Sp (black lines) of the main species mass fractions in axial direction along the centerline.

5.3.2.2 Pulsatory flame burst dynamics

As seen in the preceding analysis and visualized the stability map in Figure 5.2, in instances where the inlet velocity U_{in} is elevated, such as the Ad10Sp, and Ad12Sp scenarios, an intricate dynamic combustion phenomenon referred to as the pulsatory flame burst phenomenon (PFB) becomes evident. Analogous to the stable case, an intricate interplay between fluid dynamics and combustion reactions persists. However, with the escalation of inlet velocity, the complexity of this phenomenon intensifies, leading to the emergence of overlapping flames.

Figures 5.10 and 5.11 illustrate heat release rate contours and flow field streamlines, capturing the flame structure dynamics in a single PFB cycle. Examining various inlet velocities (10 to 12 m/s) with 0.015 ms intervals. It is evident that in both cases, the flame initiates by burning in the 2nd convex zone, and is carried along until the end of the microchannel. However, prior to extinguishing, a new flame emerges again in the 2nd convex zone. As a result, a complete flame extinction never occurs here, since $q''' \neq 0$.

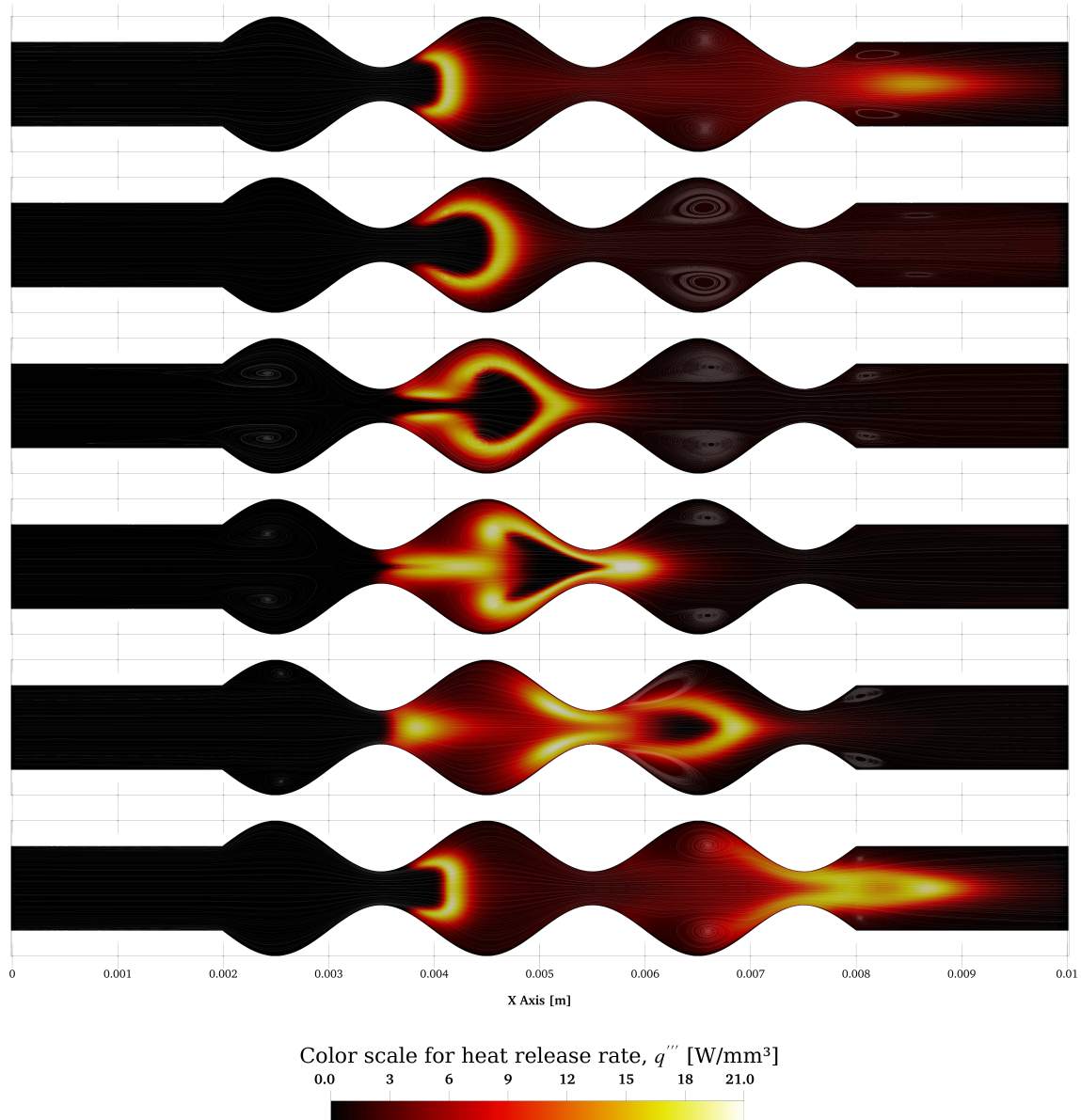


Figure 5.10: Streamlines of the flow field and distribution of heat release rate for Ad10Sp, in 15 μ s intervals.

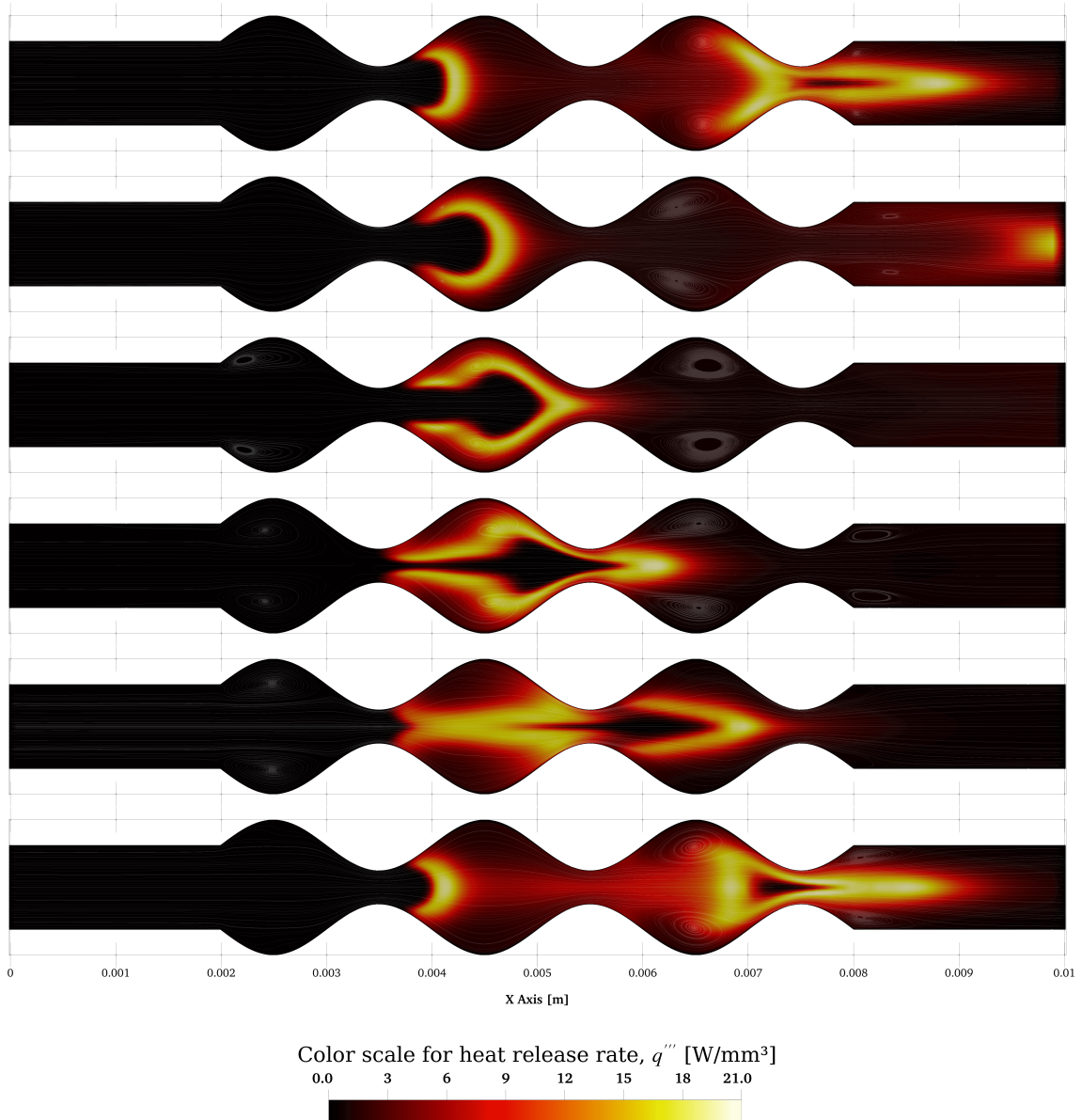


Figure 5.11: Streamlines of the flow field and distribution of heat release rate for Ad12Sp, in 15 [μ s] intervals.

In these figures, we can see that the flame engages with the flow, notably within the curved regions. This interaction arises from vortex generation due to the intricate, non-linear design of the burner. The dynamic behavior of the flame induces oscillations in the values of $q'''_{\max}$ and q'''_{avg} , consequently giving rise to temperature fluctuations. This phenomenon becomes evident when examining the first and last timesteps in both figures, where it is evident that higher velocities delays flame extinction (flame goes out occurs at a greater distance from its point of ignition), intensifying the flame on the brink of leaving the microchannel. Actually, under these conditions, the extinction stage of the PFB shows a closer resemblance to flow-assisted extinction or flame exit. This is due to the fact that the flame continues to display a significant heat release rate at the outlet, as the microchannel's length is insufficient for the full consumption of H_2 . It's anticipated (and confirmed in Macedo [112] and Resende et al. [113]) that in different scenarios, lower U_{in} where PFB occurs, result in complete extinction, even within the confines of the microchannel.

Across both cases, the findings, as presented in Table 5.5, indicate that higher values U_{in} lead to higher values of q''' , suggesting a more robust flame overall as U_{in} increases.

Table 5.5: Maximum and average heat release rate values for the adiabatic PFB cases

Simulation	$\min q'''_{tot}$ [W]	$\max q'''_{tot}$ [W]	$\text{avg } q'''_{tot}$ [W]	$\text{avg } q'''_{avg}$ [W/mm ³]	$\text{avg } q'''_{max}$ [W/mm ³]	$\max q'''_{max}$ [W/mm ³]
Ad10Sp	0.618	1.435	0.975	2.978	20.141	24.354
Ad12Sp	0.652	1.810	1.086	3.144	20.187	25.699

At the same time, as seen before, higher U_{in} also lead to more dispersed flames, which contributes to increased incomplete combustion (higher Y_{H_2} left unburned) and therefore the T_{max} and T_{avg} for the scenarios should decrease, which can be seen in Table 5.6. The extended residence time and larger lower temperature before complete combustion occurs as seen previously will drop the temperatures.

Table 5.6: Maximum and average temperature values for the adiabatic PFB cases

Simulation	$\min T_{avg}$ [K]	$\max T_{avg}$ [K]	$\text{avg } T_{avg}$ [K]	$\min T_{max}$ [K]	$\max T_{max}$ [K]	$\text{avg } T_{max}$ [K]
Ad10Sp	1208.61	1330.81	1280.31	2129.77	2262.25	2212.91
Ad12Sp	1103.72	1302.51	1213.39	2074.98	2254.33	2179.40

The PFB phenomenon is segmented into five distinct phases, as indicated by the progression of images in Figures 5.10 and 5.11: propagation, ignition, burst, bifurcation, and extinction (or flow-assisted extinction, as previously mentioned), as shown in Figure 5.12. The concept of this subdivision was initially introduced by Resende et al. [113], and we have subsequently built upon and enhanced it in our own research.

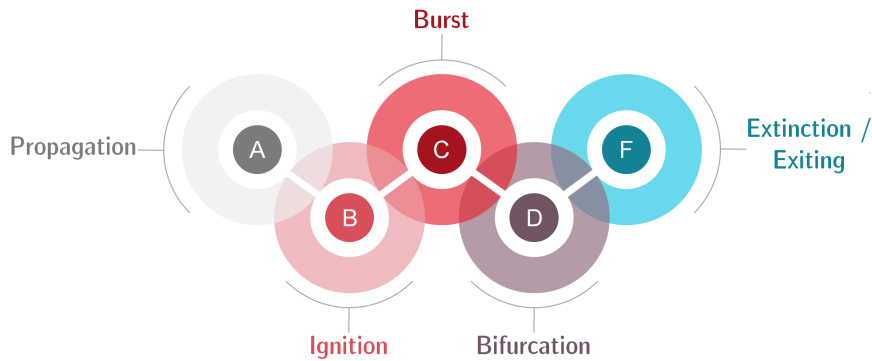


Figure 5.12: Five stages of Pulsatory Flame Burst.

As mentioned earlier, Figures 5.10 and 5.11 were recorded at intervals of 15 $[\mu s]$, spanning from 0 $[\mu s]$ to 75 $[\mu s]$. For these situations, we captured the evolutions of q''' and T along the central axis of the microchannel for each timestep, which are shown in Figure 5.13 and 5.14 (i.e., for every previously displayed time-step, we will now demonstrate the graphical progression alongside with the central x-axis line).

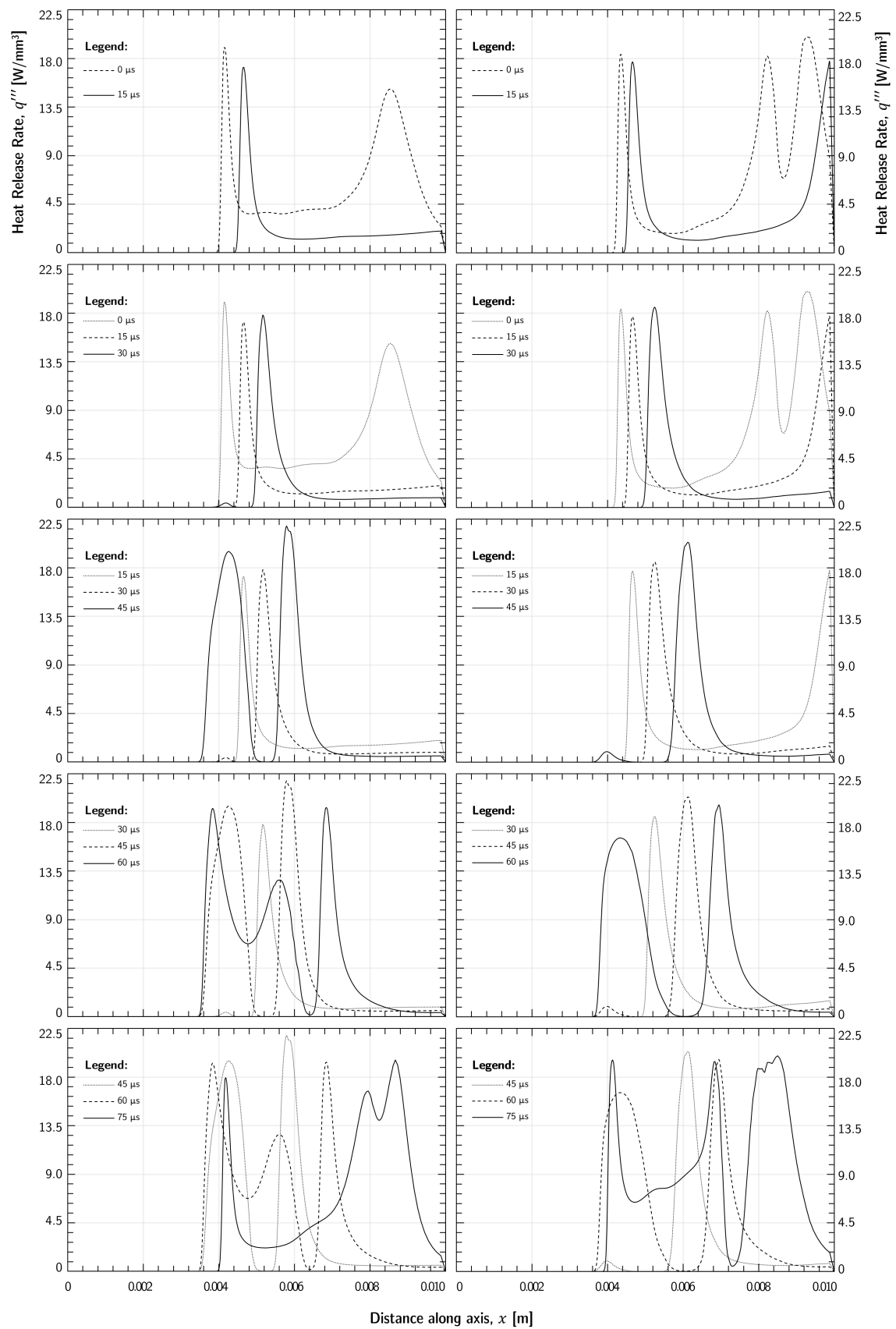


Figure 5.13: Heat release rate profiles along the x axis (centerline) for Ad10Sp (left) and Ad12Sp (right).

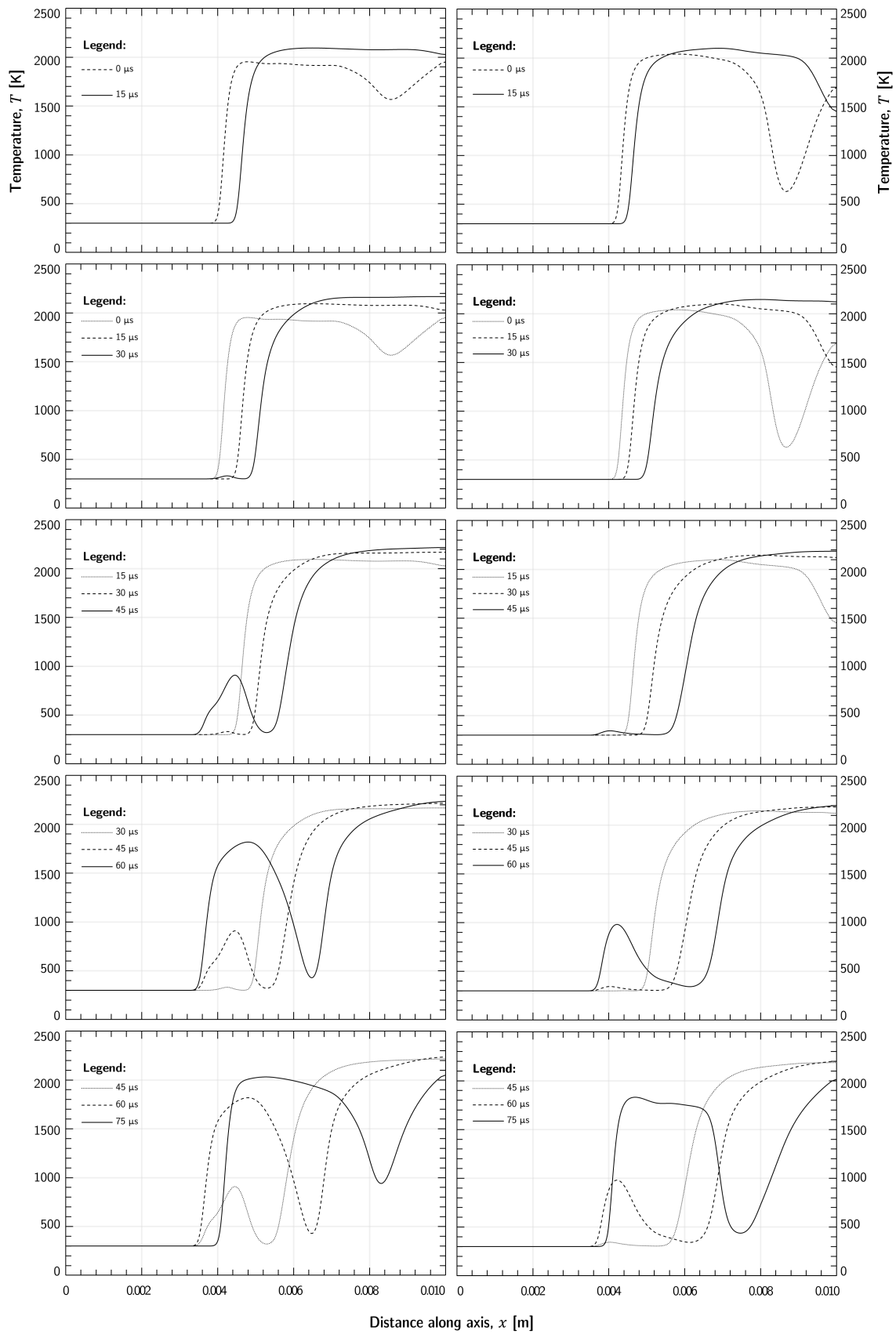


Figure 5.14: Temperature profiles along the x axis (centerline) for Ad10Sp (left) and Ad12Sp (right).

Heat release *versus* distance along axis

1st stage: Propagation

(Ad10Sp: [0, 30] μs and Ad12Sp: [0, 45] μs)

During this phase, a sharp peak of q''' is immediately noticeable in the second convex zone, [4, 5] [mm], which is visually illustrated as a C-shaped flame front⁽⁹⁾. Over the course of time, this flame front is progressively carried downstream and grows larger (this growth doesn't lead to an increase in q''' at the centerline, but does correspond to an obvious rise in the total q'''_{tot} for the convex region). In the end, the flame front takes on the appearance of an arrow-like structure, and the C-shape begins to sharpen, resembling a V-shape.

We assumed that in both cases, this phase initiates at $t = 0$ [μs], implying an overlap of phases (which will be explained shortly). This decision was made because, for certain scenarios, without such flexibility, some phases might not even "exist", which is not accurate. As seen above, this phase lasts slightly longer in the Ad12Sp case, but since capturing the precise start of each phenomenon is challenging, this alone doesn't indicate whether this phase is faster or slower.

2nd stage: Ignition

(Ad10Sp: 45 μs and Ad12Sp: 60 μs)

The regions of vortices induced by velocity promote the retrograde flow of energy (energy moving upstream). This phenomenon causes the arrow-like structure to fold inwards, paving the way for the ignition and growth of the new flame. This outcome is corroborated by the existence of dual peaks in heat release rate along the burner axis at the same time interval. Furthermore, the graphical illustrations reveal that these peaks gradually separate as the inlet velocity increases. This observation indicates that the advancement of the C-shaped flame is accelerated at higher velocities and eventually transforms into a complete V-shape after traversing the contraction zone.

3rd stage: Burst

(Ad10Sp: 60 μs and Ad12Sp: [60, 75] μs)

Following the ignition phase, the flames that evolve within the vortices intermingle with the emerging flame, resulting in an intensified energy reaction zone. At this point, a visual observation reveals two distinct flame fronts. One is exceedingly brief, located in the second convex zone, while the other extends extensively, forming a sharp V-shape in the third convex zone. This configuration is attributed to the passage through the constriction, giving rise to the "burst" phenomenon characterized by a substantial increase in velocity within this region. Consequently, the flame in the third convex zone will from now on experience increased acceleration.

These flames are visibly interconnected, albeit the constriction zone prompts the emergence of three peaks in q''' , with the second peak manifesting roughly around the constriction area (which cause a sharper peak relative to most of 2nd convex zone). Between this second peak and the third peak, where $q''' = 0$, it becomes apparent that the H_2 in this zone (centerline) has not yet been consumed.

The time gap noted between the ignition phase and the burst across the two scenarios stems from the delay in vortex formation. This delay subsequently lessens the upstream energy transfer necessary for the ignition of the new flame⁽¹⁰⁾.

⁽⁹⁾Throughout this explanation, when we mention "visually," we are referring to Figures 5.10 and 5.11, and when we say "graphically," we are referring to Figures 5.13 and 5.14

⁽¹⁰⁾And as seen in Resende et al. [113], for low velocities and PFB, the ignition of the new flame and merging of flames can occur instantaneously

4th stage: Bifurcation(Ad10Sp: 75 μ s and Ad12Sp: [75, 0] μ s)

The bifurcation phase arises as a portion of the heat release rate moves upstream into the contraction zone while the remainder moves downstream. During this phase, the flame advancing downstream merges with the preceding V-shaped flame prior to extinguishing, thereby resulting in an escalation of the peak q''' (leading to the merging of the second peak observed in the burst with the downstream peak). Moreover, it's evident that elevated U_{in} leads to a more dispersed energy distribution along the burner due to the heightened inlet velocity, which causes that the separation of the flames becomes more pronounced at lower U_{in} , where the q''' between the flames is notably lower compared to higher velocities.

5th stage: Extinction(Ad10Sp: 0 μ s and Ad12Sp: [0, 15] μ s)

The flame initially moving upstream will continue to propagate downstream. However, due to the finite length available in the straight part of the microchannel, the flame exits it without completely consuming all the H_2 present, and $q''' >> 0$. Consequently, this phenomenon can be classified as a flow-assisted extinction. It's worth noting, as demonstrated in Resende et al. [113], that lower velocities can lead to complete consumption and hence full extinction before the flame exits the channel. Simultaneously, we can observe the initial progression of the propagation phases, characterized by an overlap of these two stages in both scenarios.

Temperature versus distance along axis

To provide a deeper insight into the temperature evolution during a PFB cycle, we present Figures 5.15 and 5.16, which illustrate the temperature contours and flow streamlines for the same PFB cycle in Ad10Sp and Ad12Sp scenarios, respectively. Notably, the higher U_{in} at [60, 75] μ s for Ad10Sp and at [75, 0] μ s for Ad12Sp results in a discernible gap between the flames.

This effect is also discernible in the temperature profiles along the centerline of the burner across all cases, as depicted in Figure 5.14. Following the emergence of the new flame (indicated by the initial peak within the mentioned intervals), the temperature experiences a decline before rising downstream to attain peak values around 2250, K. Nevertheless, the distance between the first peak and the temperature plateau ($T \approx 2250$, K) expands as U_{in} increases. In the case of Ad10Sp, the gap between the flames measures around 4.0, mm and escalates to nearly 5.0, mm for Ad12Sp.

As a result, the reduced temperature between the flames contributes to a decrease in the transfer of heat flux between them. This reduction in heat transfer hampers the increase in temperature within the gap where the fuel mixture is present. Therefore, this serves as an additional explanation for why the distinctions in T_{avg} are more noticeable than in T_{max} . On the other hand, it is observed that as the inlet velocity increases, the profile becomes non-monotonic. As we've seen, with higher velocity, the energy flow through the vortices accelerates. Prior to the flame extinguishing, another flame is already emerging at a position upstream of the microchannel and this impacts specifically on how quickly the new flame develops.

Furthermore, the delay in the ignition phase, indicated by the emergence of the new flame at the entrance of the convex zone, becomes evident from the less pronounced temperature increase

observed at $45, \mu\text{s}$ for Ad10Sp and within the interval $[45, 60], \mu\text{s}$ for Ad12Sp. This delay is attributed to the lower heat release rate resulting from the vortices effects.

Additionally, it's worth noting, as observed in Macedo [112], that it can be concluded that, in most cases, adiabatic conditions show smaller temperature amplitudes than in cases with a heated burner wall. This is reasonable because, in the heated wall scenario, there's an inherent input of thermal energy due to the wall heating. Therefore, it is expected that the phenomenon alters significantly in this aspect during the simulations in which we will be using finite walls.

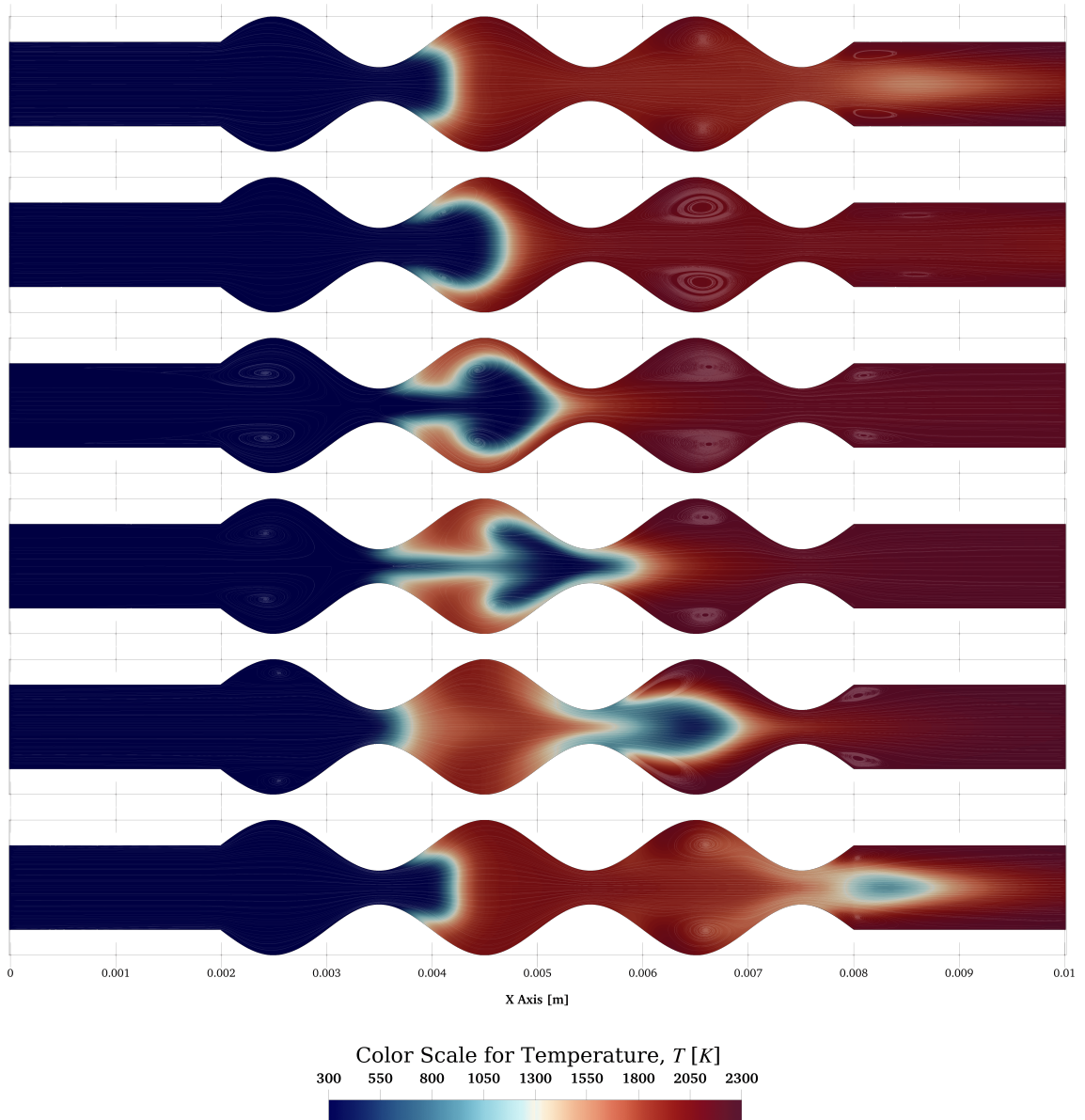


Figure 5.15: Streamlines of the flow field and distribution of Temperature for Ad10Sp, in 15 $[\mu\text{s}]$ intervals.

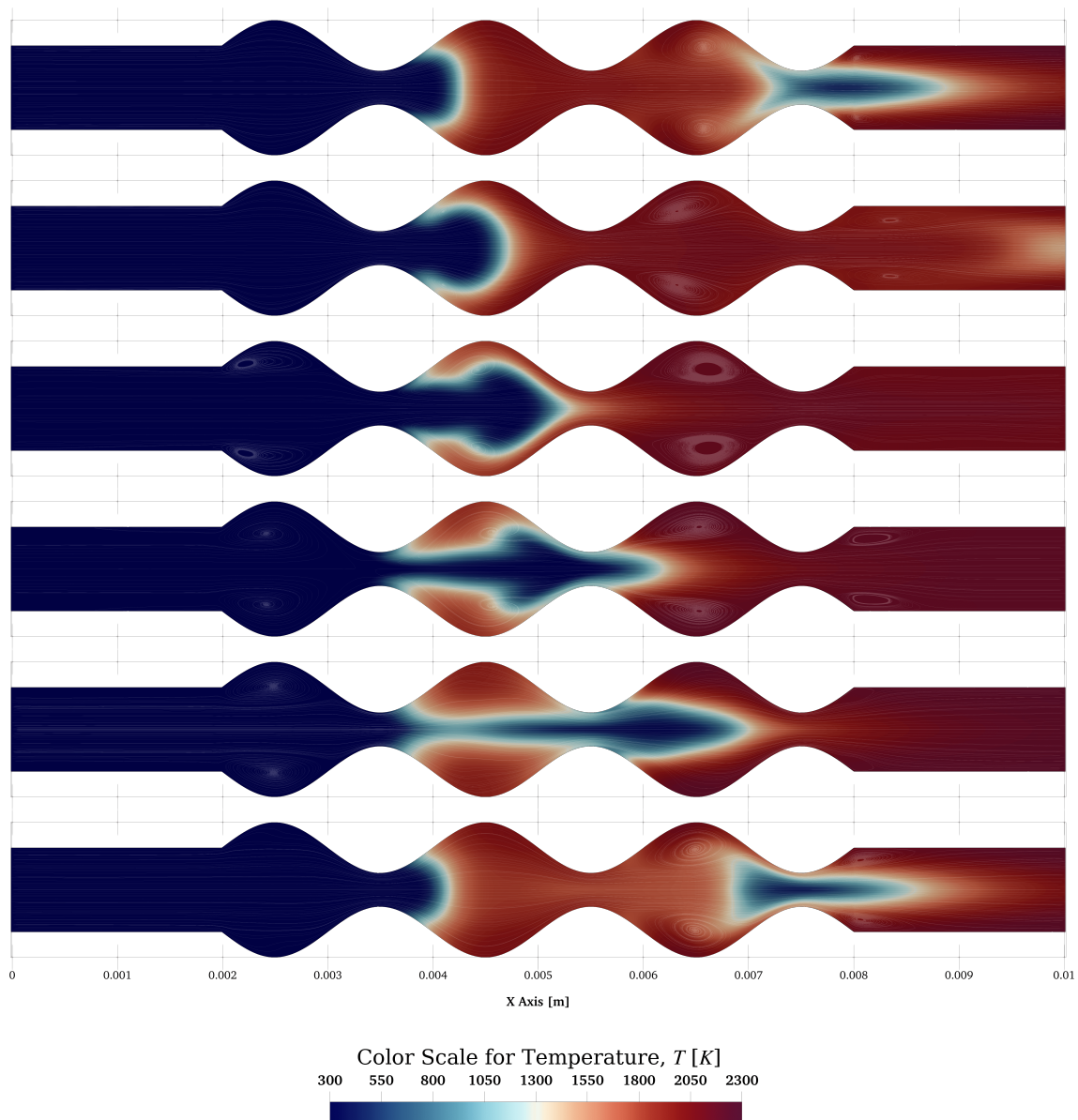


Figure 5.16: Streamlines of the flow field and distribution of Temperature for Ad12Sp, in 15 $[\mu\text{s}]$ intervals.

Let's now shift our approach to studying the non-stationary behavior of the flame, delving into the periodicity and amplitude of the cycles in detail. To achieve this, we conducted a dynamic analysis of the maximum temperature and the maximum heat released by the combustion reaction.

In Figures 5.17 and 5.18, it's presented the highest and mean measurements of q''' and T , respectively, illustrating data for more or less 5 PFB cycles. These figures specifically cover the time interval $[2.000, 2.400]$ ms, which corresponds to a distinct phase in the evolution of the system. Further insight into the evolution during the full simulation, $[0.000, 2.800]$ ms, is presented through Figure 5.19, showcasing the maximum and average values.

As talked about before, we can see that throughout the simulation, before extinction occurs, a new flame emerges, which is shown by the evolution of the maximum values of heat release rate and temperature along time, inside the burner.

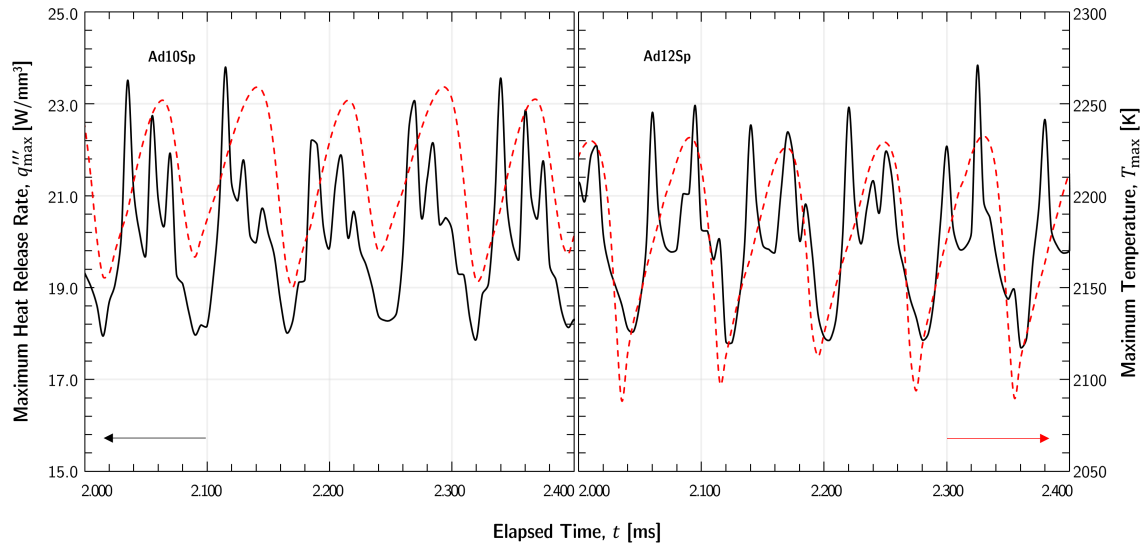


Figure 5.17: Evolution of the maximum values of the heat release rate and temperature along time, inside of the burner, for Ad10Sp (left) and Ad12Sp (right), zoomed in for $t = [2.000, 2.400]$ ms.

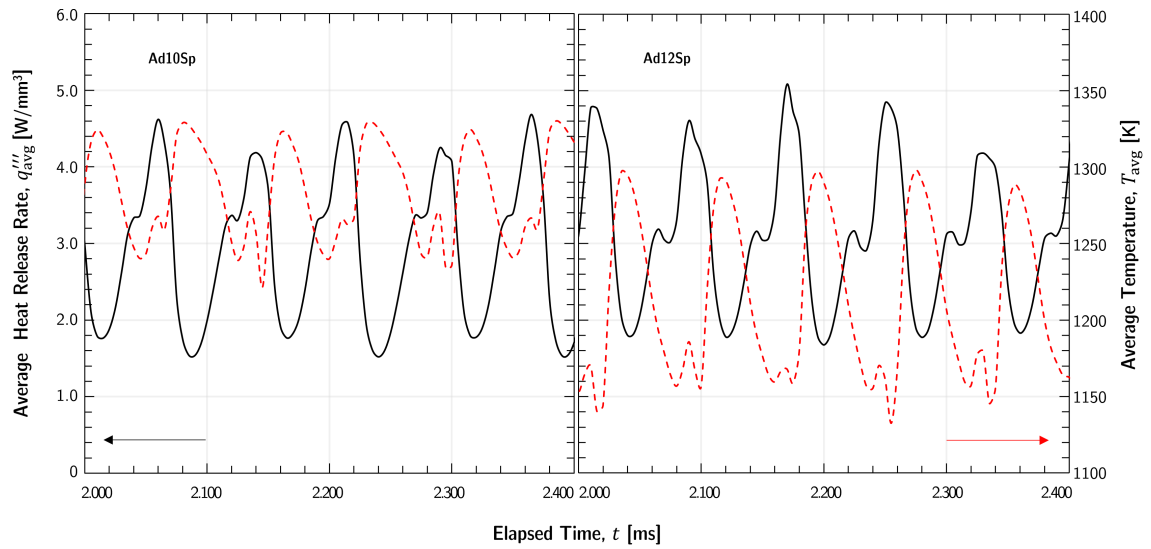


Figure 5.18: Evolution of the average values of the heat release rate and temperature along time, inside of the burner, for Ad10Sp (left) and Ad12Sp (right), zoomed in for $t = [2.000, 2.400]$ ms.

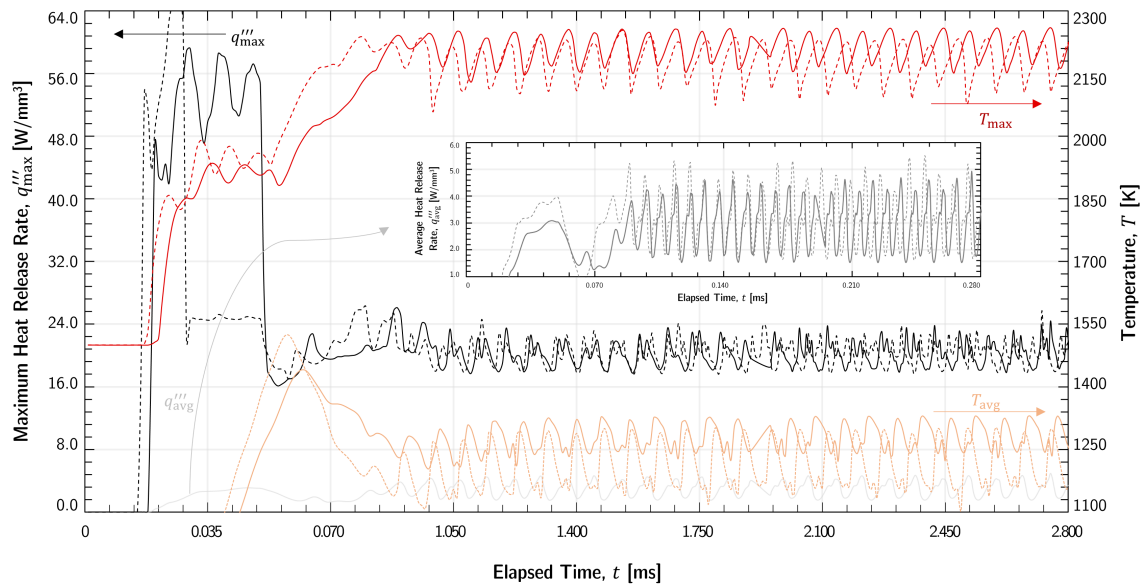


Figure 5.19: Evolution of the maximum and average values of the heat release rate and temperature along time, inside of the burner, for Ad10Sp (solid lines) and Ad12Sp (dashed lines).

Clearly, the behavior in both scenarios exhibits significant chaos during the spark ignition phase (when external heat is introduced to the mixture due to the spark). Subsequent to this stage, it initiates evolution marked by minor oscillations during the consolidation phase, progressing toward the periodic oscillations observed in the primary PFB stage.

During the spark phase ($t = [0, 0.05]$ [ms]), we also note the highest peak values of $q'''_{\max}$ (which is reasonable considering the additional heat release from the 1500 K spark), while in the consolidation phase, T_{avg} reaches its highest peak (possibly due to PFB anchoring in the 2nd convex zone, but throughout much of the consolidation phase, combustion persists even in the 1st convex zone, which, as observed previously, notably influences the average values). After this phase, the behavior of variables T and q''' gradually adopts a more periodic nature and q'''_{avg} and $T_{\max}$ reach the peak values. Nevertheless, as discussed in Subsection 2.3.6.2, the recurring oscillations and the varying frequency and amplitude observed throughout the simulation affirm the existence of a non-steady, quasi-periodic behavior in both instances. Now, it's also more evidently noticeable that T significantly decreases with U_{in} , while the values of q''' remain similar.

Given the non-steady nature of PFB, exhibiting dynamic and repetitive behavior, a spectral analysis of the observed signals in various cases was performed. This investigation was conducted utilizing MATLAB R2023 software, employing FFT analysis (Fast Fourier Transform). FFT is an algorithm used to efficiently compute the Discrete Fourier Transform (DFT) of a sequence or signal [201]. The DFT is a mathematical operation that transforms a time-domain signal into its frequency-domain representation, showing the different frequency components present in the signal. As such, using FFT we can analyze the frequency content of a signal and compute its power spectrum [201]. The detailed procedure and accompanying code are available in Appendix E.

The signal spectral analysis code facilitated the derivation of maximum amplitude values (A^{var}) and corresponding frequencies (f) within specific time intervals, with **var** signifying the variable under analysis. This analysis was executed between $t = 2.000$, ms and $t = 2.800$, ms, since during this time, there's visible periodicity. In this process, we introduced in the software the designated time intervals alongside their corresponding temperature and released heat values. The results of spectral signal analysis using FFT are shown in Table 5.7.

We observe an increase of released heat amplitude with U_{in} can be readily elucidated from a physical perspective. As the velocity of the mixture increases, the flow rate also increases, given that the cross-sectional area remains constant over time. Consequently, within the same time interval, a greater quantity of gases, specifically fuel, reaches the reaction zone. The presence of larger quantities of H_2 downstream of the burner results in a more intense ignition, leading to a higher heat release. Consequently, the peaks of released heat increase in their absolute value, thereby amplifying the magnitude of their signal. Subsequently, one can anticipate a corresponding modulation in the values of maximum temperature. With an increased heat release, the energy per unit length rises, consequently elevating the peaks of maximum temperature observed within the burner. The identical variation supporting this assertion is also evident in Macedo's research, as reported in the study by Macedo [112], where it was observed that the equivalence ratio of the mixture also induces an augmentation in the amplitude of maximum temperature, as during the ignition phase, larger quantities of fuel are present, thereby giving rise to higher flame temperatures.

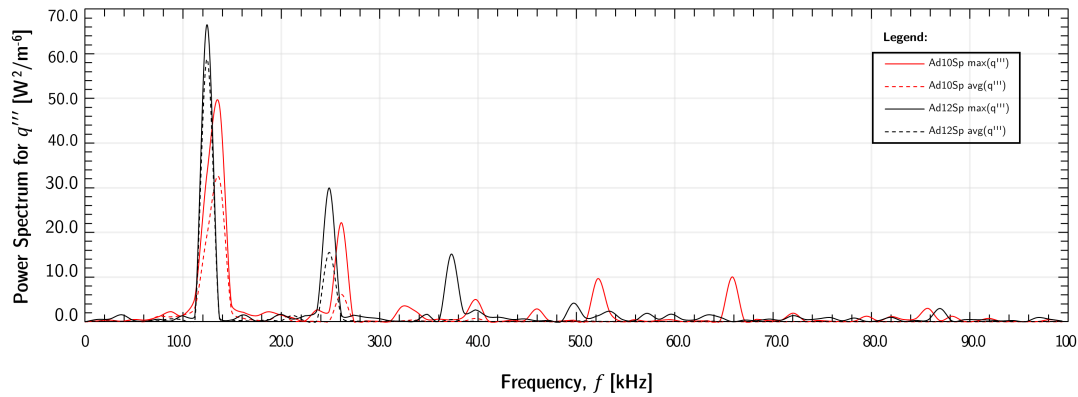
Table 5.7: Signal spectral analysis results for frequency, f and maximum amplitude values, A^{var} , for the simulations Ad10Sp and Ad12Sp

Simulation	f [Hz]	$A^{T_{\text{avg}}}$ [K]	$A^{T_{\text{max}}}$ [K]	$A^{q'''_{\text{tot}}}$ [W/mm ³]	$A^{q'''_{\text{avg}}}$ [W/mm ³]	$A^{q'''_{\text{max}}}$ [W/mm ³]
Ad10Sp	13665	109.24	110.37	0.817	3.405	6.523
Ad12Sp	12422	198.79	161.74	1.157	3.891	7.995

The frequency denoted as f corresponds to what is known as the “peak frequency”. This term signifies the specific frequency within a signal’s power spectrum where there is a significant surge in power or energy. In the realm of signal analysis and Fourier transformation, the power spectrum is visualized as a graphical depiction that reveals how power or energy is distributed among the diverse frequency components present within a given signal [201]. Essentially, the power spectrum provides insights into the dispersion of energy content across the spectrum of frequencies inherent to the signal [201].

We see that higher velocities correlate with lower frequencies and higher amplitudes, especially for $T^{(11)}$, across the signals. As the inlet velocity increases, the heat release rate transmitted through the vortices decreases and a delay in ignition occurs, as evidenced by a decrease in the pulsatory burst frequency and an increase in the maximum value of the heat release rate. Also, there is a synchronization in all signals which points to a clear link between the intensity of the combustion process, seen in heat release, and the resulting thermal effects, as captured by temperature measurements.

As depicted in Appendix E, our procedure involved computing the power spectral density, extracting frequency-power pairs, and subsequently saving this data in the "fft_sinal.dat" file. With the information from this file, we conducted an examination of the power spectrum pertaining to q''' within each distinct scenario. This analysis is visually presented in Figure 5.20.

**Figure 5.20:** Power Spectrum (q''') versus frequency (f) for Ad10Sp and Ad12Sp.

Upon observation, the Ad10Sp signal’s peaks display notably higher frequencies throughout the entire power spectrum when contrasted with the Ad12Sp signal. Furthermore, while the distributions of $(-)\text{max}$ and $(-)\text{avg}$ appear similar in both cases, the $(-)\text{avg}$ signals manifest fewer secondary peaks. These secondary peaks exhibit smaller amplitudes, occur less frequently, and

⁽¹¹⁾More H_2 downstream intensifies ignition, increasing heat release and its peaks. This drives higher maximum temperatures as well, due to increased energy per length unit.

this trend is consistent in Figures 5.17 and 5.18, showing that $(-)\text{avg}$ demonstrates diminished recurrence and higher periodicity. Moreover, the Ad12Sp signal demonstrates elevated amplitudes, signifying that these signals possess relatively lower amplitudes at those frequencies in comparison to the Ad10Sp. This discrepancy suggests a weakened signal strength in the context of the Ad10Sp case.

Furthermore, we analyzed a Ad10Sp PFB cycle for the same time instants used in Figures 5.10, 5.13, and 5.14. We compared the evolution of the average and maximum values of q''' and T with the previously mentioned PFB stage cycles (Figure 5.12), the results of which are presented in the subsequent Figures 5.21a and 5.21b for q''' and T , respectively.

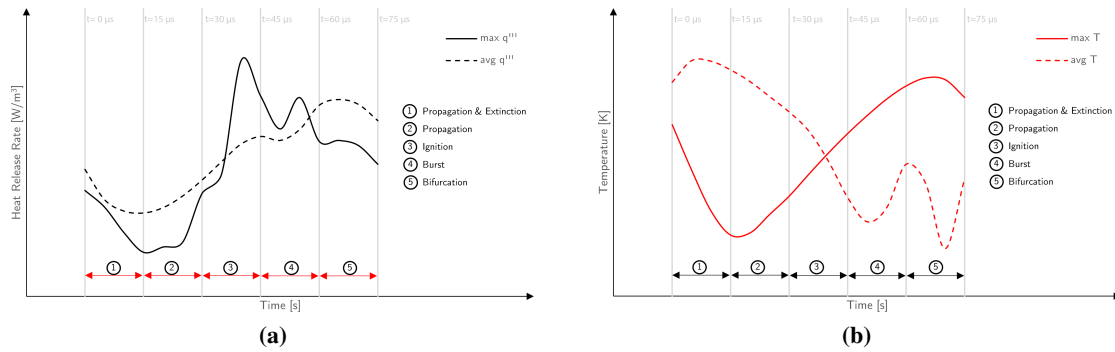


Figure 5.21: A Single PFB Cycle Illustrated in 5 Stages: (a) q''' ; (b) T .

Observing $q'''_{\max}$, we note its peak during ignition and a second peak during the burst phase. These instances correspond to the most intense combustion reactions (flame reaching continuously upstream, transferring energy to ignite a new flame), yielding higher maximum values. As the flame diminishes, these values gradually decline, reaching their nadir in the final propagation phase.

Similarly, q'''_{avg} exhibits a parallel trend but with inverted peaks. The peak maximum aligns a bit later, during the bifurcation phase, characterized by extensive flame occupancy within the reactor, resulting in elevated average values spanning the reactor length.

Shifting focus to $T_{\max}$, it follows a comparable evolution to $q'''_{\max}$ but lacks peaks, displaying a more harmonious progression. Conversely, T_{avg} demonstrates an opposing trend. It exhibits peak values during the initial propagation phase (prior to extinction), with the lowest values occurring during the burst-bifurcation phases. This might be attributed to the presence of a smaller region of cooler, unburned H_2 as depicted in Figure 5.14, contributing to an overall higher temperature.

5.4 Dynamics of amorphous materials

We are about to begin exploring the initial set of substances, which are amorphous materials. These include an examination of Fused Silica (in simulations FS4Sp to FS12Sp) and Borosilicate Glass (in simulations BG4Sp to Bg12Sp). Given that the λ_s of these materials is relatively low, it is anticipated that the outcomes will not deviate significantly from what has been observed previously for an ideally adiabatic material.

5.4.1 Stability map

The stability map depicting various velocities and the two materials is provided in the subsequent Figure 5.22. However, adopting the pseudo-stationary approach of equating combustion and conduction times leads to notable numerical instabilities, particularly for thermal conductivity values below a threshold of $\lambda_s \leq 1$. In these instances, due to Fourier Law, Equation (4.4)), for the same heat flux that's going into the wall, the ∇T becomes very large and even slight heat flux variations between the upper and lower walls result in considerable divergences in wall temperatures, creating unrealistic asymmetries. This phenomenon, as elaborated upon and better explained later on in this work, prompts us to treat the scenarios for Borosilicate glass (BO4...12Sp) as equal to those of Fused Silica. This ensures that in the worst-case scenario, the outcomes are the same, and in the best case, they mirror the adiabatic instances.

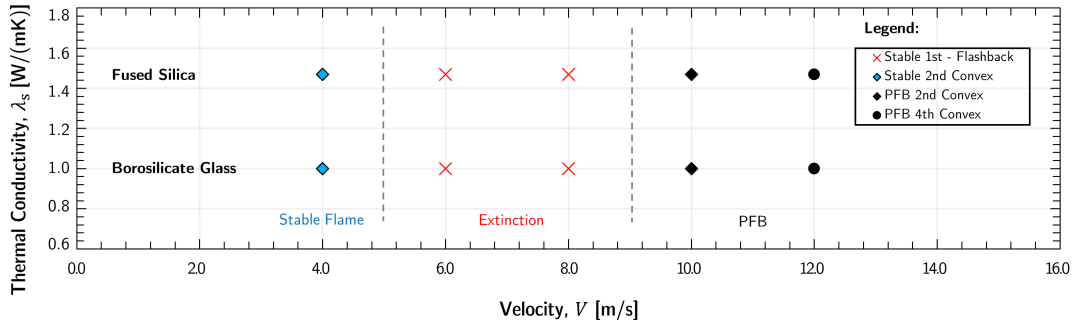


Figure 5.22: Stability map for the various simulations using a spark conducted with amorphous materials.

5.4.2 Stable flame and transitional Pulsatory Flame Burst (tPFB) dynamics

Let's begin by examining the simulations where a stable flame was achieved within the secondary convex zone at a flow rate of $U_{in} = 4$ [m/s]. To illustrate this, we present Figures 5.23 and 5.24, which showcase temperature distribution and a visualization of the heat release rate distribution and heat flux in the solid domain, q'' , respectively:

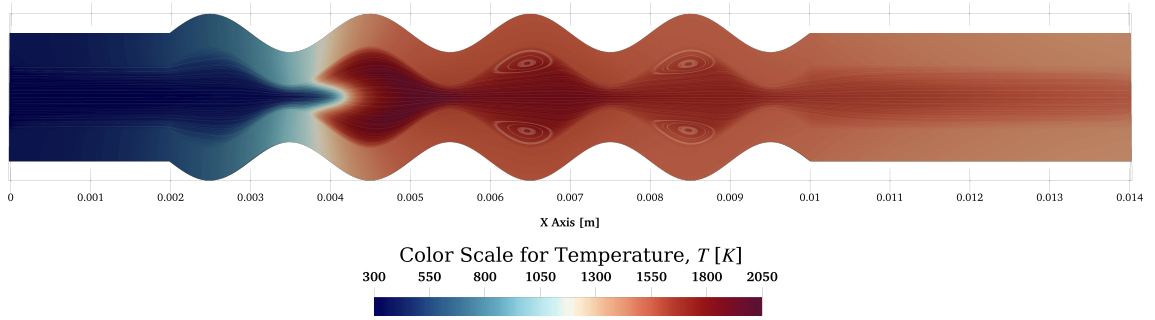


Figure 5.23: Streamlines of the flow field and distribution of temperature for FS4Sp (FluidRegion and SolidRegion's).

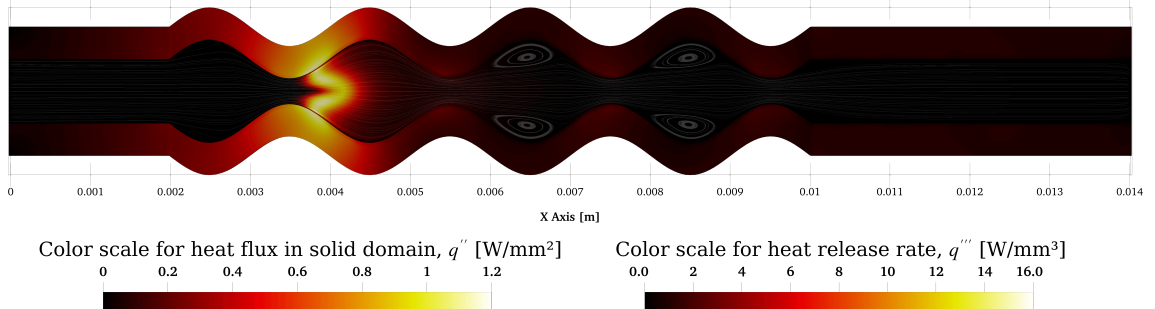


Figure 5.24: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for FS4Sp.

Table 5.8 presents the outcomes for T and q''' at the concluding time step, marked by the complete stabilization of the flame.

Table 5.8: Maximum and average values for temperature and heat release rate for FS4Sp and Ad4Sp (for comparison)

Scenario	ℓ_{fl} [mm]	T_{avg} [K]	T_{max} [K]	q'''_{avg} [W/mm ³]	q'''_{max} [W/mm ³]	q_{tot} [W]
Ad4Sp	0.5	1451.25	2299.96	1.164	19.094	0.423
FS4Sp	0.3	1364.47	1962.38	0.793	16.023	0.342

In comparison to Ad4Sp, this leads to a relative change (denoted as $\Delta X/X(\%)$, where X represents the change variable) of $\Delta\ell_{fl}/\ell_{fl} = -40\%$, $\Delta T_{avg}/T_{avg} = -6.0\%$, $\Delta T_{max}/T_{max} = -14.7\%$, $\Delta q'''_{avg}/q'''_{avg} = -31.9\%$, $\Delta q'''_{max}/q'''_{max} = -16.1\%$, $\Delta q_{tot}/q_{tot} = -19.1\%$. The temporal evolution of these variables is visually depicted throughout the simulation time in Figure 5.25.

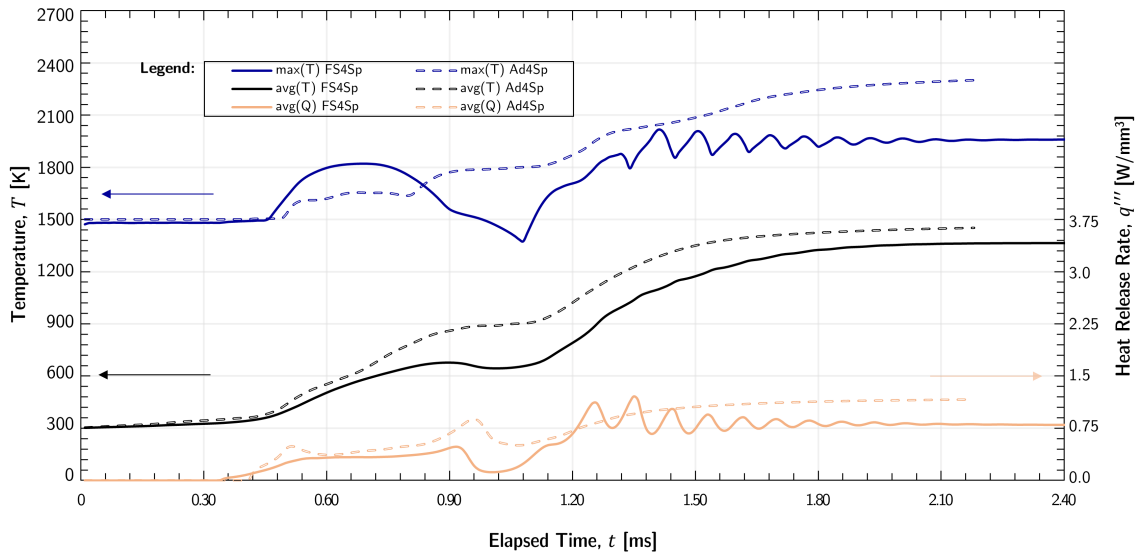


Figure 5.25: Temporal evolution of maximum and average values of heat release rate and temperature for FS4Sp and Ad4Sp (for comparison).

This unequivocally demonstrates that the inclusion of a finite amorphous wall, which allows heat dissipation, results in a noteworthy reduction across all variables. This reduction is indicative of a less robust flame and diminished chemical reaction, leading to the release of lesser heat. This phenomenon arises from the dissipation of heat through the combustor walls, triggering a decline in average temperatures and subsequently leading to a decrease in the overall energy level. Conversely, due to the relatively small value of λ_s , the disparity turns out to be less pronounced compared to what might be observed with other materials.

Significantly, a notable divergence from any stable state observed under adiabatic conditions is the emergence of a minor transitional PFB phenomenon within the second convex zone during the flame's advancement, occurring approximately between $t = [1.2, 2.2]$ [ms]. Intriguingly, this phenomenon rapidly dissipates, leading to the cessation of oscillations in conjunction with the flame stabilizing to a consistent configuration. To facilitate a clearer comprehension of what we

term the “transitional Pulsatory Flame Burst” (tPFB), we now present Figures 5.26 and 5.27. These figures depict the temporal evolution of maximum and average values of T and q''' during the mentioned interval ($t = [1.2, 2.2]$ [ms]).

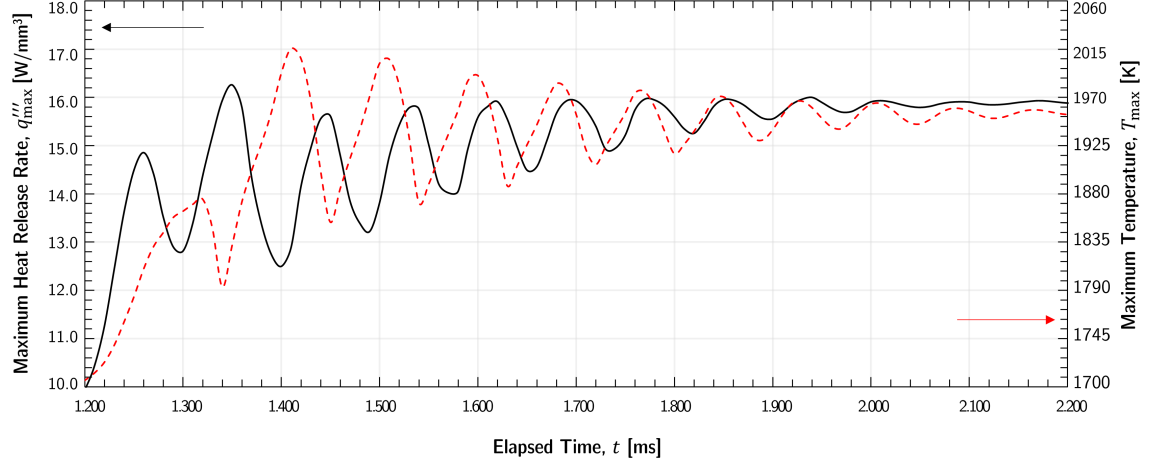


Figure 5.26: Temporal evolution of maximum values of heat release rate and temperature for FS4Sp (zoomed into tPFB).

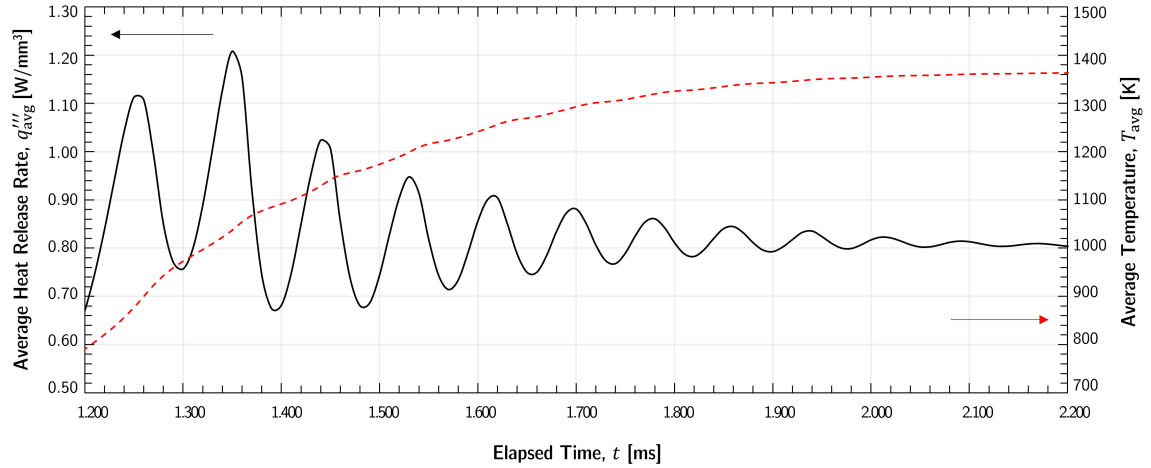


Figure 5.27: Temporal evolution of average values of heat release rate and temperature for FS4Sp (zoomed into tPFB).

Conducting a spectral analysis on the signal revealed that the dominant frequency component of the variable’s signal was approximately $f = 11,628$ [kHz]. An evident feature is the progressive reduction in amplitude. For instance, it commenced (e.g. $q'''_{\max}$) with an amplitude of $A_{q'''_{\max}} = 3.765$ [W/mm³], which gradually diminished to $\approx$ zero by the end of tPFB. Figures 5.28 and 5.29 illustrate the progression of the heat release rate and the heat flux in the solid material, correspondingly, for the case of FS4Sp.

The graphical progression of tPFB bears resemblance to the phenomenon of PFB at low velocities, where T profiles are imposed, which has been observed in other studies, most notably in the works of Macedo [112] and Resende et al. [113]. In this case (FS4Sp), the development of the unburned H₂ pocket, which takes on an arrow-like structure, is of a considerably shorter length until extinguishment. This distinct behavior, possibly characteristic of tPFB, renders the unburned pocket almost needle-like, which diverges from findings in other research, since there

it kept the longer heart like tip. Notably, all the stages of PFB witnessed earlier occur within the 2nd convex zone, a significant departure from PFB in Ad10Sp and Ad12Sp. This distinction is primarily influenced by the lower inlet velocity ($U_{in} = 4$ [m/s]).

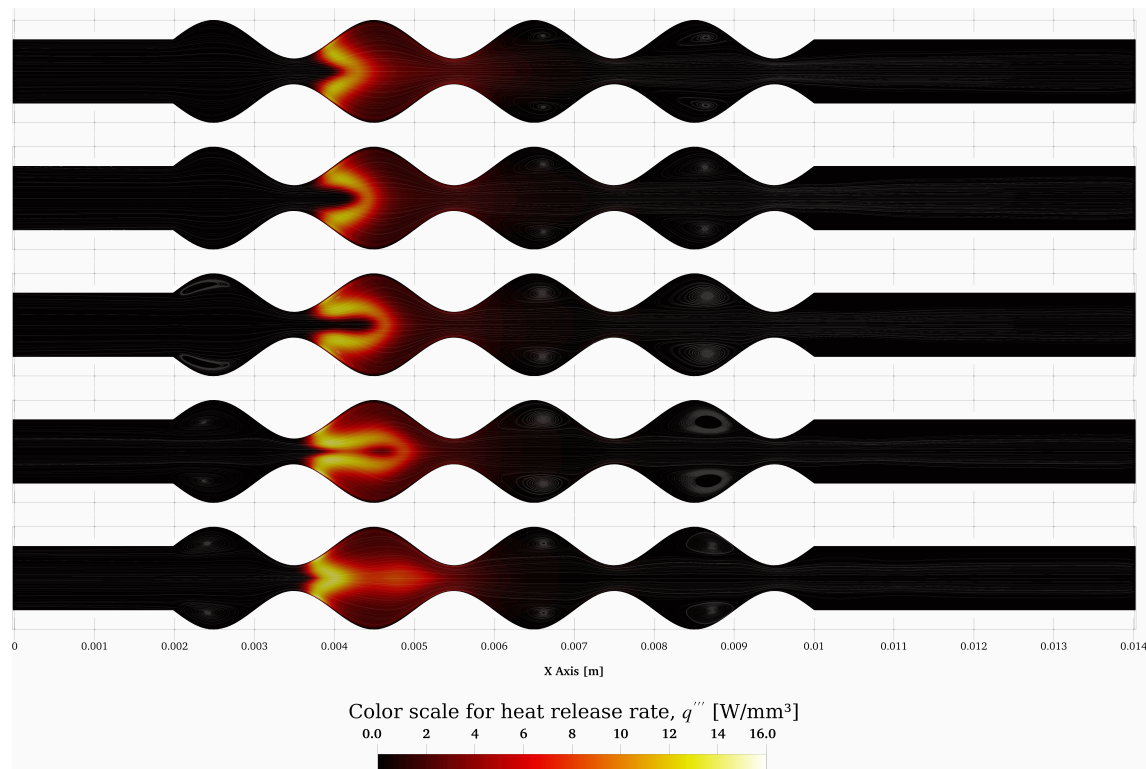


Figure 5.28: Streamlines of the flow field and distribution of heat release rate for FS4Sp, in 20 μ s intervals, over 1 cycle tPFB.

Regarding the distribution of wall heat flux, minimal differences are observed compared to the scenario where the flame is fully stabilized, as the wall heat flux (q''_s) remains largely unchanged.

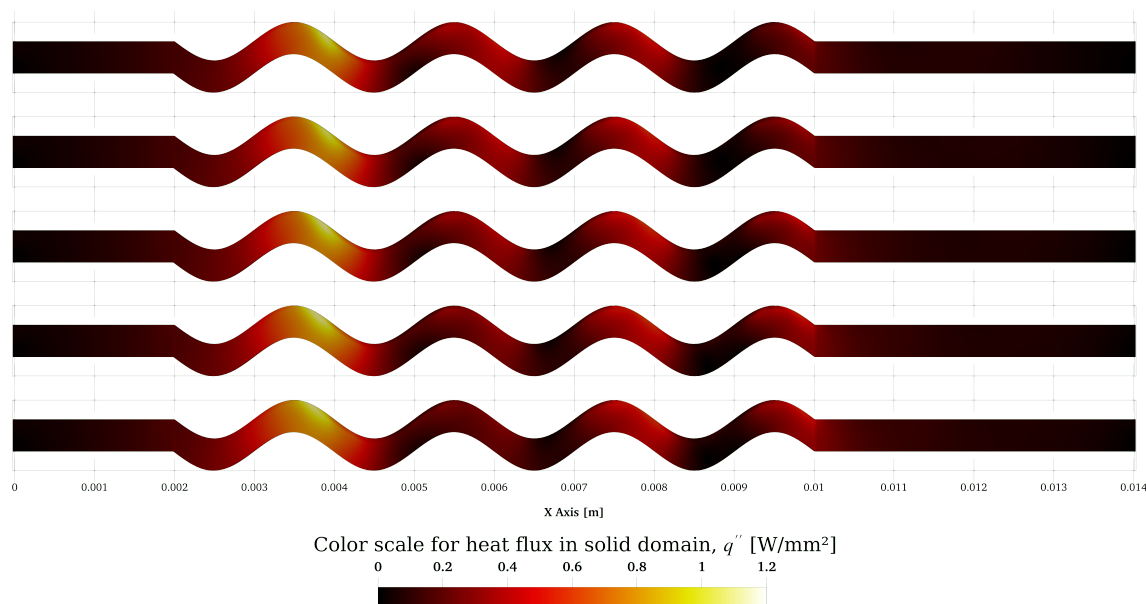


Figure 5.29: Distribution of wall heat flux for FS4Sp, in 20 μ s intervals, over 1 cycle tPFB.

In Figure 5.30, we will examine the variations of T and q''' along the x-axis (centerline) over one cycle.

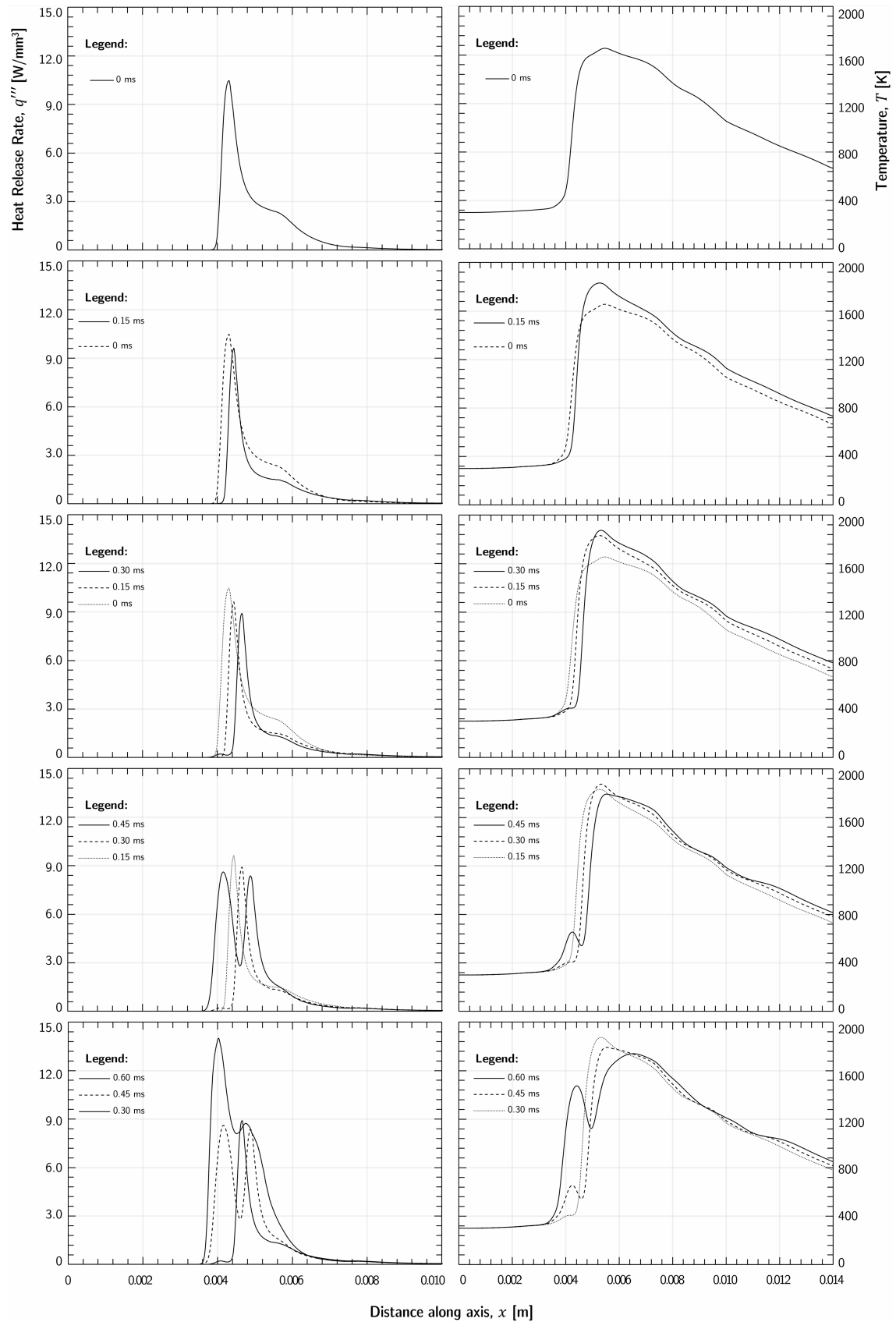


Figure 5.30: Heat release rate (left) and Temperature (right) profiles along the x axis (centerline) for FS4Sp.

As observed earlier, q''' is limited to the convex region. Ignition takes place near the contraction zone ($x \approx 4$ [mm]), followed by flame extinction. Prior to extinction, a new flame emerges. This is depicted in Figure 5.30 through the temporal evolution of maximum heat release rate and temperature values within the burner. However, a significant contrast from the previous analysis is that in this case, the flame extinction becomes apparent in the last timestep, $t=60$ [μ s], and is fully accomplished by approximately $t=15$ [μ s], without requiring flow-assisted extinguishment⁽¹²⁾. Additionally, it's worth noting that at approximately $t \approx 45$ [μ s], the ignition of the new flame and the merging of flames take place instantaneously.

In contrast to the adiabatic simulations, heat loss leads to a noticeable temperature decrease over time. This difference becomes evident when comparing with the adiabatic scenario. In Figure 5.31, temperature and heat flux (FS4Sp and Ad4Sp) profiles are presented along the microchannel's x-axis. Notably, beyond the 2nd convex zone, the adiabatic case displays a continuous temperature rise, reaching levels near T_{af} . However, in the presence of heat loss, Fused Silica exhibits a slight temperature decline along the microchannel's x-axis.

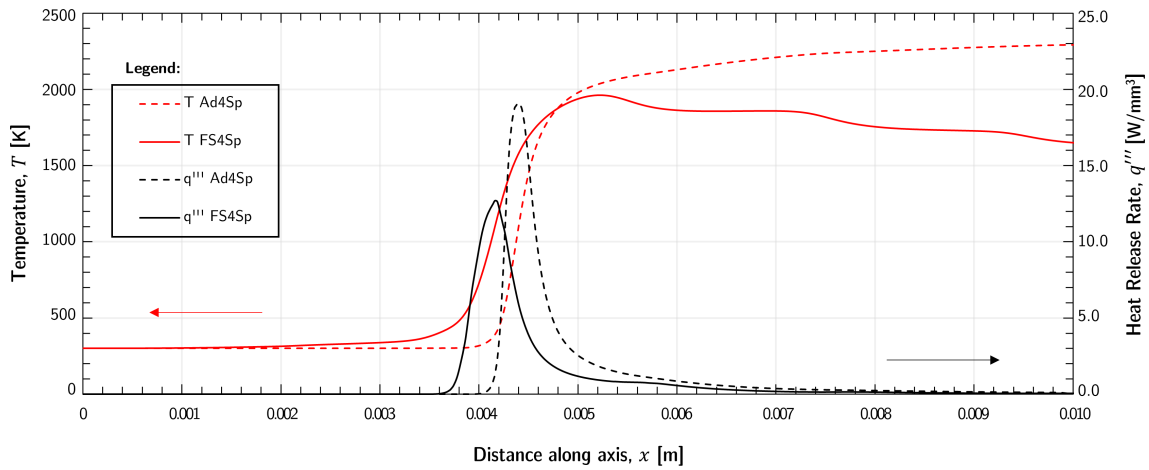


Figure 5.31: Evolution of temperature and heat release rate profiles along the x axis (centerline) for the FS4Sp and comparison with Ad4Sp.

Concerning the dynamics of the wall (heat retention attributes within Fused Silica), we recorded averages for heat transfer across the x-direction and y-direction planes of $q''_{s,x} = -0.137$ [W/m^2] and $q''_{s,y} = 0.065$ [W/m^2] respectively. Notably, maximum values are observed as $q''_{s,x,max} = -1.121$ [W/m^2] and $q''_{s,y,max} = 0.263$ [W/m^2]. These results show the remarkable heat insulating characteristics of Fused Silica, leading to minimal thermal loss to the surrounding environment.

The evolution of all parameters was shown in Figure 5.32. It is observable that the heat fluxes in the y (and maximum values in x) direction exhibit oscillations concurrent with the time steps of the tPFB. Additionally, as anticipated, the magnitude of the heat flux was predominant in the x direction, since there is a steeper temperature gradient in the x-direction, leading to a larger heat flux in that direction compared to the y-direction (see Figure 5.23).

It's interesting to note that, in the y-direction, the heat flux remained consistently ≥ 0 , while in the x-direction, ≤ 0 . This was expected due to the absence of heat from the surroundings, with the system's interior being much hotter than the exterior, and, after the flame has stabilized, the temperature gradient became less steep in the forward direction as wall temperatures increased significantly (see Figure 5.23). However, during the consolidation phase, a temporary positive

⁽¹²⁾The flame extinguishes solely through the complete combustion of H_2 .

flux was observed in the x -direction. This was because, in the initial simulation stages, downstream wall temperatures were still low, and heat was primarily conducted forward in heating this microchannel section.

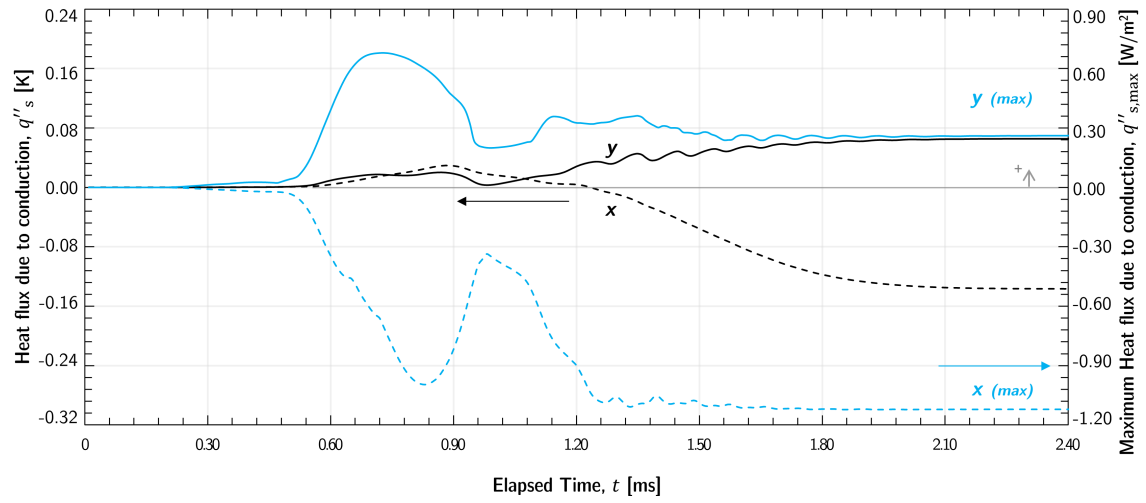


Figure 5.32: Variation of average and maximum heat flux in the solid (conduction) along the x and y directions.

In order to get a clearer picture of how much heat is being lost to the outside, we used Equation (4.3) to calculate the heat flux escaping to the surrounding environment, which we've labeled as q'_{out} . The changes in q'_{out} at the final time step of the FS4Sp simulation are visualized in Figure 5.33, giving us a better understanding of its fluctuations along the outer wall of the microchannel. Furthermore, Figure 5.34 illustrates the dynamic alterations in total Heat Fluxes emitted to the surrounding environment over the course of the simulation (and contributions of radiation and convection). These changes are presented in conjunction with the variations observed in both the average and maximum temperature of the solid wall.

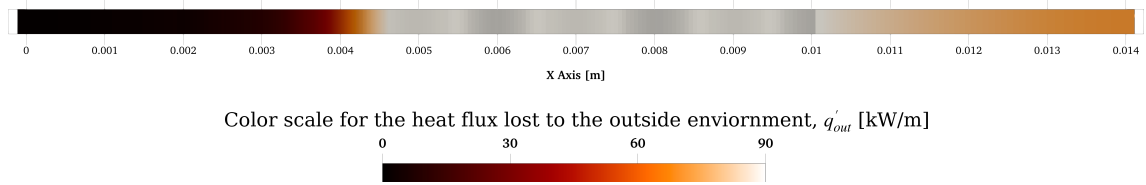


Figure 5.33: Variation of the heat flux to the outside, q'_{out} , at the outer wall of *solidRegion2* (just one cell in z direction).

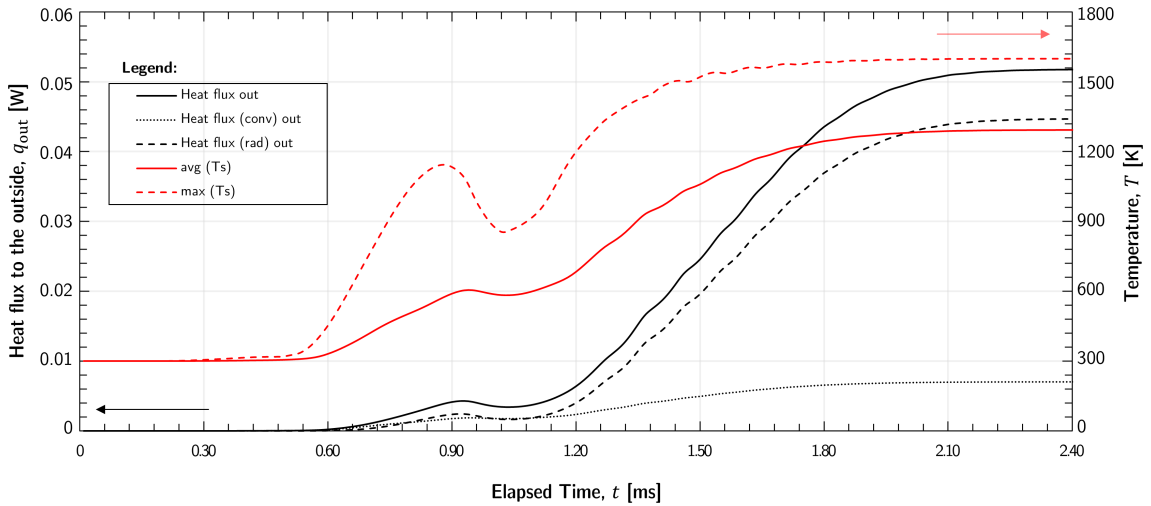


Figure 5.34: Changes in Total, Convection, and Radiation Heat Fluxes to the surrounding environment throughout the simulation, alongside fluctuations in average and maximum Temperature of the solid wall.

During the last time step, the heat fluxes were as follows: $q_{\text{out}} = 0.052$ [W], $q_{\text{out,conv}} = 0.007$ [W], and $q_{\text{out,rad}} = 0.045$ [W]. As anticipated, given our consideration of natural convection, it's worth noting that radiation typically plays a more substantial role in contributing to the overall heat loss of a thermal system. In this instance, radiation accounted for 86.4% of the total thermal loss⁽¹³⁾. To gain a more profound understanding of the energy dissipation, we computed the cumulative heat loss over the course of the simulation⁽¹⁴⁾. Tables 5.9 and 5.10 present the E_{out} values for 10 equidistant timesteps within the simulation.

Table 5.9: Cumulative E_{out} for FS4Sp (Part 1)

t [s]	0.50	1.00	1.45	1.90	2.35
E_{out} [J]	0.00	5.78×10^{-7}	3.38×10^{-6}	1.67×10^{-5}	5.18×10^{-5}

Table 5.10: Cumulative E_{out} for FS4Sp (Part 2)

t [s]	2.80	3.25	3.70	4.15	4.50
E_{out} [J]	6.21×10^{-5}	8.55×10^{-5}	1.09×10^{-4}	1.32×10^{-4}	1.55×10^{-4}

As observed, the evolution of total dissipated heat (energy) exhibits an initial phase of exponential growth, transitioning into the stable phase characterized by a linear trend, as anticipated.

5.4.3 Stable to Flashback Dynamics

As we observed earlier, both in Ad6Sp and Ad8Sp, the flame stabilized within the first convex zone (no conduction in x axis). Similarly, in FS6Sp and FS8Sp, this behavior persists. However, a significant distinction arises: rather than maintaining stability, the flames are gradually pushed further inwards due to wall horizontal (x axis) conduction. Eventually, this leads to flashback occurring at the inlet. The wall conduction results in an increase in temperature throughout the microchannel. The walls become sufficiently hot, facilitating the initiation of chemical combustion reactions further inward. This escalating heat facilitates the movement of the flame front. This phenomenon did not manifest in FS4Sp, primarily due to the sinusoidal geometry of the microchannel. The undulating shape poses a challenge for the walls in the region behind the flame front to reach the requisite temperature to initiate this mechanism. Furthermore, the relatively smaller height of the convex zone, in comparison to the diameter at the end of the inlet straight tube, also contributes to this behavior. It does so by facilitating and aiding the concentration of heat outwards. Essentially, this convex zone acts as a barrier, preventing the inward movement of heat.

The phenomenon is illustrated in Figure 5.35. The wall temperature at the region behind the flame front becomes sufficiently high, influenced by solid conduction, causing the flame front

⁽¹³⁾These values are entirely contingent on the T_{wall} , which is intricately linked to the complex interplay of dynamics within the microchannel. Nonetheless, it's worth noting that as ϵ_{rad} increases, the contribution of $q_{\text{out,rad}}$ to the overall heat loss will obviously also increase.

⁽¹⁴⁾This process entails summing the heat loss values at various time intervals to ascertain the overall energy dissipated throughout the entire duration. This computation was executed using MATLAB; additional details can be located in Appendix E, Section E.2

to progressively move inward. Eventually, this movement extends to the mixture inlet and, in practical scenarios, result in flame extinction⁽¹⁵⁾.

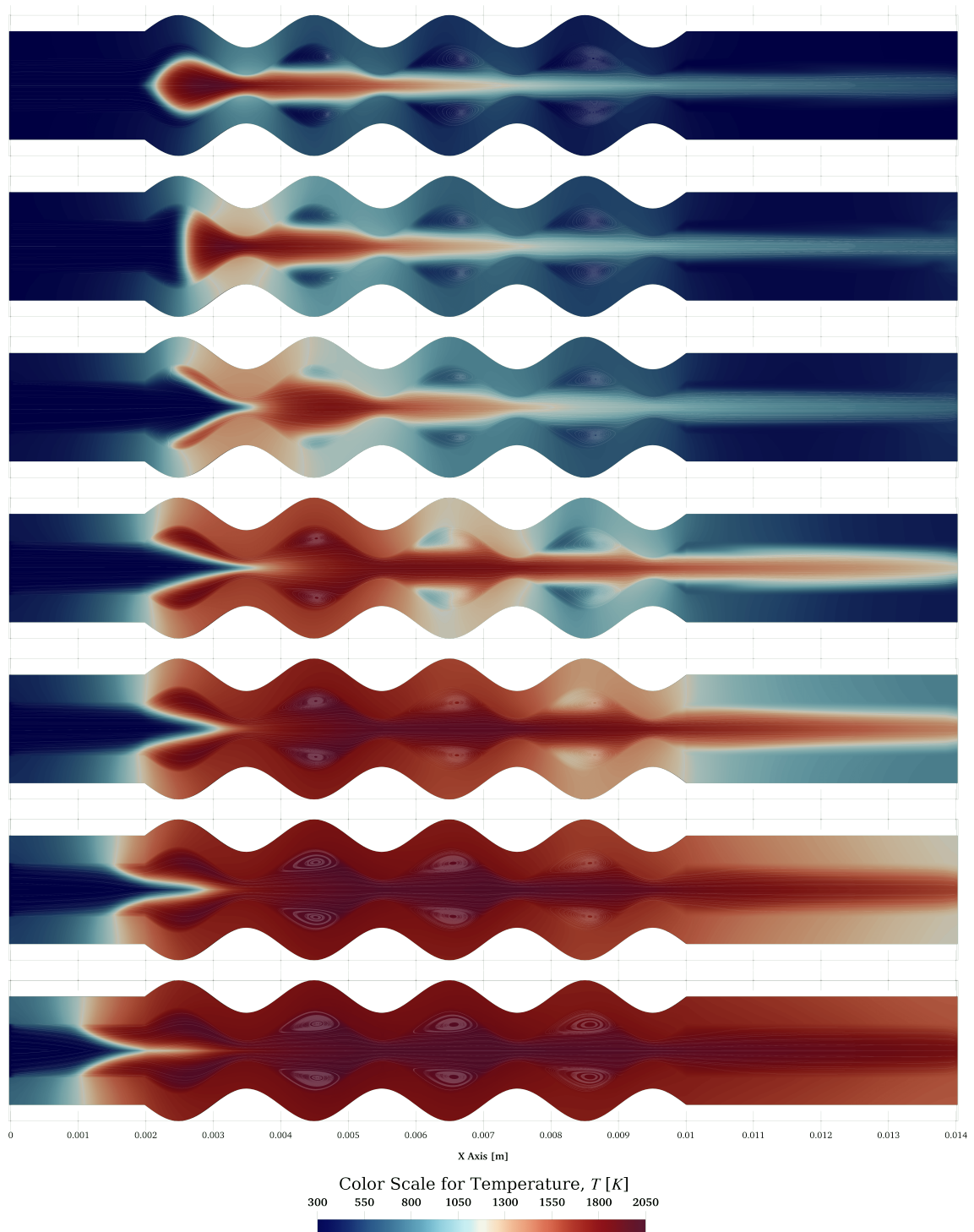


Figure 5.35: Streamlines of the flow field and distribution of heat release rate for FS6Sp, in 20 μs intervals.

⁽¹⁵⁾However, it remains uncertain whether the flame would continue to move inward or not if the straight zone were infinitely extended. Such a scenario would unequivocally confirm flashback, irrespective of the geometry.

The reason for this mechanism causing flashback is straightforward. When the flame front nears the fuel inlet, it risks consuming available fuel before fresh fuel can enter the combustion zone. This can lead to flame extinction, sudden loss of combustion and heat. Moreover, it can cause combustion instabilities, like flickering, pulsation, and flashback, where the flame travels back into the fuel inlet. Hence, we will categorize all simulations displaying this behavior as flashback.

Considering that this phenomenon occurred in a material characterized by very low thermal conductivity, the issue becomes increasingly exacerbated as λ_s is heightened. Consequently, an urgent requirement emerges for a geometry adjustment, garnering attention as a prime focus for future research works. Clearly, a substantial portion of the microchannel essentially mirrors an extended straight zone, given that the effective minimum length for flame stabilization lies within the 1st contraction zone. On the contrary, a viable solution emerges through the inversion of the sinusoidal geometry, as depicted in Figure 5.36.

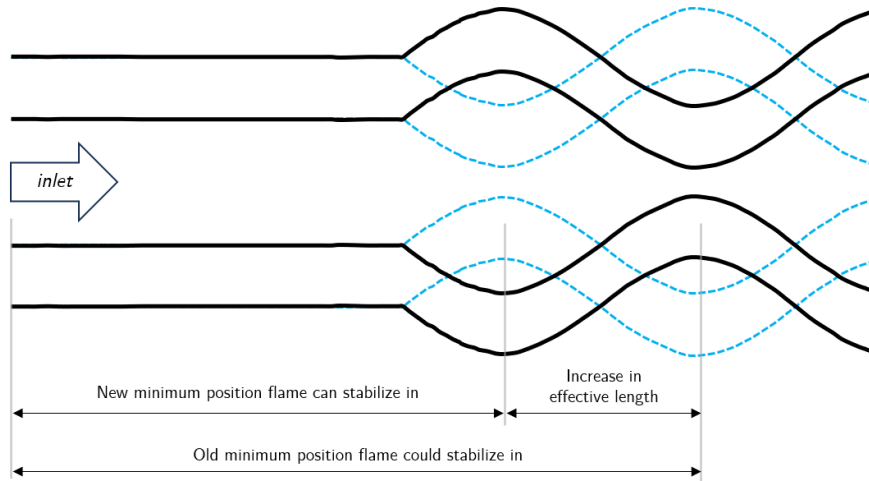


Figure 5.36: The existing microchannel geometry and the suggested modification to mitigate flashback within the 1st convex zone.

By adopting this approach, a fresh minimum point for flame stabilization can be established, while upholding the length of the microchannel's straight segment. This alteration results in a noticeable enhancement in effective length.

5.4.4 Pulsatory flame burst dynamics

In simulations FS10Sp and FS12Sp, PFB emerged, maintaining stable oscillations throughout the entire simulations. Our initial emphasis will be on examining the flow dynamics of PFB in situations involving gas-solid phases, and to do so, we present Figures 5.37 and 5.39, which provide a visual representation of PFB, depicting heat release rate distribution and temperature contours, respectively, as well as flow field streamlines, which collectively capture the dynamic flame structure within a single PFB cycle. Figure 5.38 depicts the temporal evolution of heat release rate and temperature within the microchannel over the interval $t = [3.000, 3.800]$ ms, including maximum and average values.

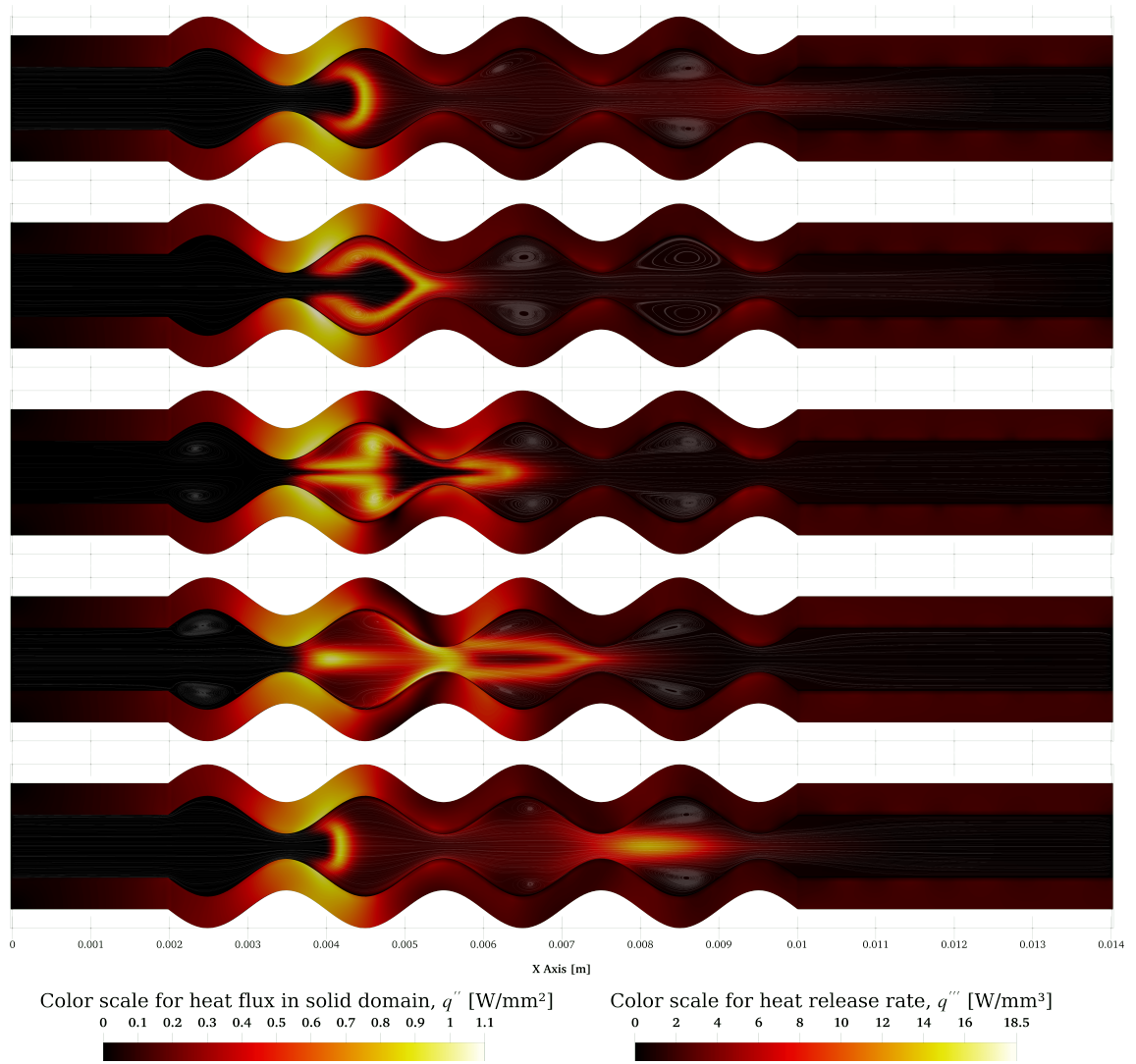


Figure 5.37: Streamlines of the flow field and distribution of heat release rate for *fluidRegion* and the heat flux due to conduction for *solidRegion*'s for FS10Sp.

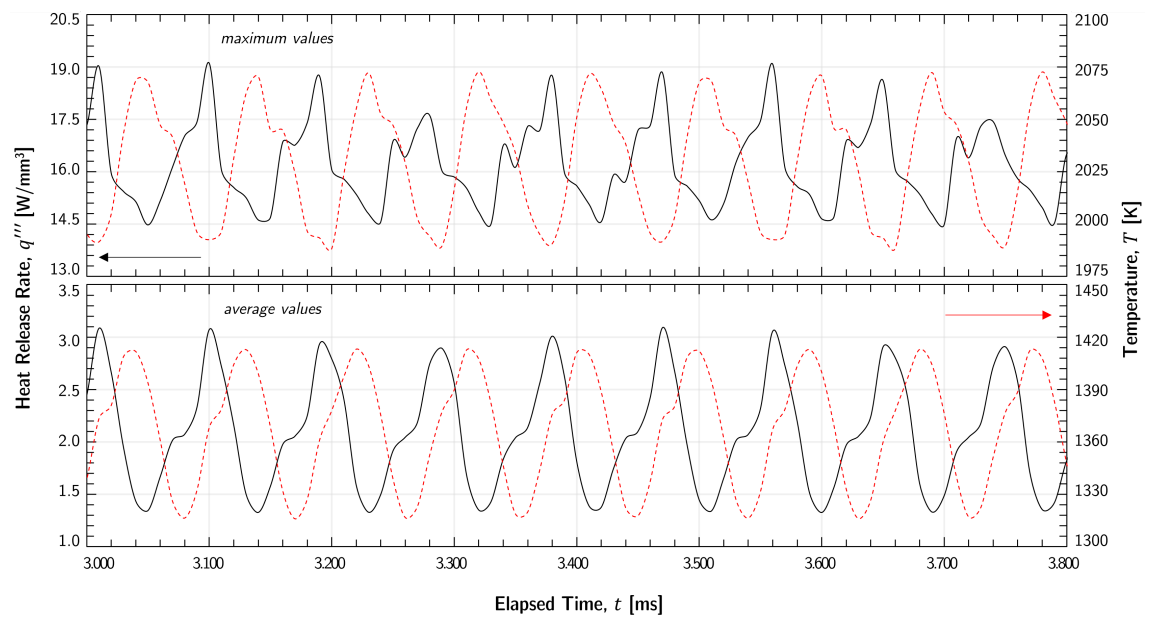


Figure 5.38: Evolution of the maximum (top) and average (bottom) values of the heat release rate and temperature along time, inside of the microchannel, for FS10Sp, zoomed in at $t = [3.000, 3.800]$ ms.

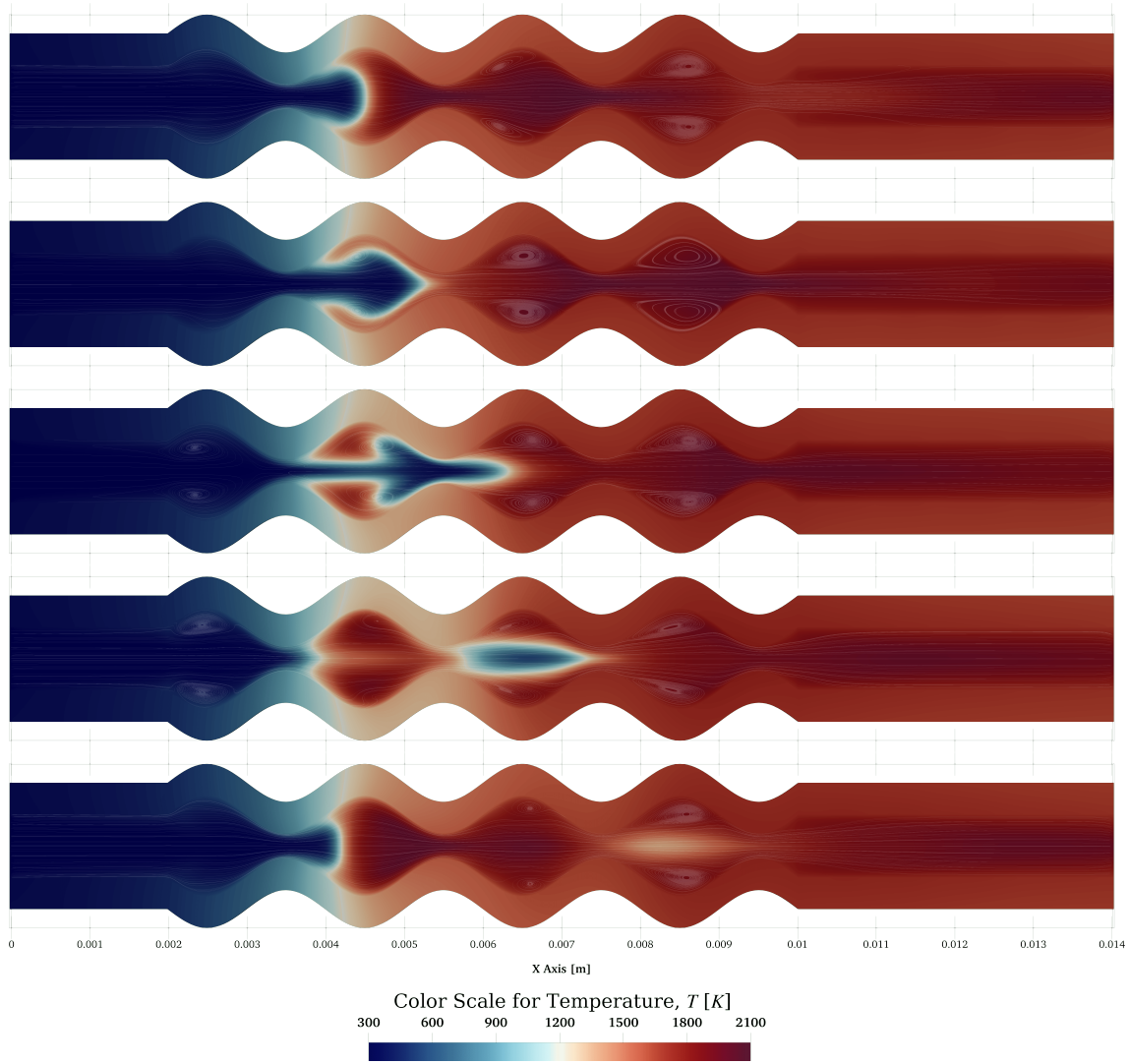


Figure 5.39: Streamlines of the flow field and distribution of temperature for FS10Sp (*FluidRegion* and *SolidRegion*'s).

In these Figures, we observe that the way the flame interacts with the flow exhibits remarkable similarity to its adiabatic counterpart. This implies that the fundamental dynamics of PFB maintain their overall characteristics. Noteworthy distinctions can be observed, as depicted in Figure 5.38, where there is a noticeable reduction in the recurrence of oscillations in both $q'''_{\max}$ and T_{avg} . All signals demonstrate a more harmonious progression in contrast to Ad10Sp, as illustrated in Figures 5.17 and 5.18⁽¹⁶⁾. This phenomenon is clearly linked to the presence of heat flux along the walls. It supports the claim that the inclusion of prescribed or natural wall heat flux aids in harmonizing the signals by preventing excessive heat accumulation within the vortex region of the microchannel, thereby reducing the likelihood of heat recirculation flux formation in these areas, ultimately resulting in lower signal recurrence.

The impact of thermal inertia becomes more noticeable, clarifying the reason for the time lag in the fluid temperature signals compared to the heat release rate signals. This phenomenon also occurs in the Ad10Sp scenario because there is a certain amount of time required for the

⁽¹⁶⁾ Similar findings were noted when employing imposed temperature profiles that enforce a consistent heat flux from the wall, as utilized in Maecedo [112] and Resende et al. [113].

temperature to rise after energy is introduced into the system through combustion. Nonetheless, the absence of recurrence and the presence of heat loss both contribute to a more pronounced explanation of the delay in the response of $T_{\max}$ when compared to q'' .

Equally noteworthy, the increased length of the microchannel resulted in the complete extinguishment of the emerging flame, as clearly illustrated in Figure 5.37. This is in stark contrast to the scenario depicted in Figure 5.10, concerning Ad10Sp, where such extinguishment did not occur. This observation further reinforces the argument that an extended microchannel was indeed necessary, particularly due to the presence of heat loss⁽¹⁷⁾.

As depicted in Table 5.11, it is evident that the existence of heat loss indeed results in weaker flames. This is evident as all the T maximum values are notably lower, with reductions ranging from 6% to 9%. The longer microchannel in FS10Sp contributes to the skewed nature of the average values. Otherwise, there is no apparent reason for them not being lower than Ad10Sp.

Table 5.11: Maximum and average temperature values for the fluid domain for FS10Sp and comparison with Ad10Sp

Simulation	avg T_{avg} [K]	min T_{avg} [K]	max T_{avg} [K]	avg T_{max} [K]	min T_{max} [K]	max T_{max} [K]
Ad10Sp	1280.314	1208.61	1330.81	2212.91	2129.77	2262.25
FS10Sp	1367.052	1316.01	1420.92	2029.55	1988.24	2072.62
$\Delta X/X$	6.8%	8.9%	6.8%	-8.3%	-6.6%	-8.4%

Table 5.12 reveals that the flame is noticeably more robust, displaying higher heat release rates across all parameters. The presence of heat loss results in lower temperatures because the microchannel consistently loses heat. This, in turn, establishes an overall cooler environment within the microchannel, leading to a less energetic and less explosive chemical reaction.

Also, the total heat generated by the chemical reaction, denoted as q_{tot} , exhibits a smaller disparity between cases. This is primarily attributed to the previously mentioned fact that in Ad10Sp, H_2 is not completely consumed, leading to a skewed representation.

Table 5.12: Maximum and average heat release rate values for the fluid domain for FS10Sp and comparison with Ad10Sp

Simulation	avg q_{tot} [W]	min q_{tot} [W]	max q_{tot} [W]	avg q'''_{avg} [W/mm ³]	max q'''_{avg} [W/mm ³]	avg q'''_{max} [W/mm ³]	max q'''_{max} [W/mm ³]
Ad10Sp	0.975	0.618	1.435	2.978	4.926	20.141	24.354
FS10Sp	0.933	0.662	1.247	2.080	3.092	16.222	19.104
$\Delta X/X$	-4.4%	7.0%	-13.1%	-30.1%	-37.2%	-19.5%	-21.6%

On the following page, Figure 5.40 presents the temporal progression of heat flux within the solid wall, specifically in the x and y directions ($q''x^{(18)}$ and $q''y$), the total heat flux dissipated to the surroundings (q_{out}), and the average temperature of the solid wall (T_s) during the time

⁽¹⁷⁾Heat loss leads to weaker flames and lower temperatures, causing hydrogen (H_2) to require more time for complete consumption.

⁽¹⁸⁾Using absolute values, since has seen before, $q''x$ is negative since there's a predominant heat flux upstream.

interval $t = [3.000, 3.800]$ ms, during which PFB is exhibiting consistent oscillations. Meanwhile, Figure 5.41 illustrates the temporal temperature profiles, covering T_{wall} (which is the temperature of the surface facing the outside), T_s , T_{int} (which is the temperature of the surface on the *fluid-solid* interface), and peak temperatures across the entire wall during the same interval. Given that both graphs share the same x -axis, it is feasible to simultaneously compare these 7 variables.

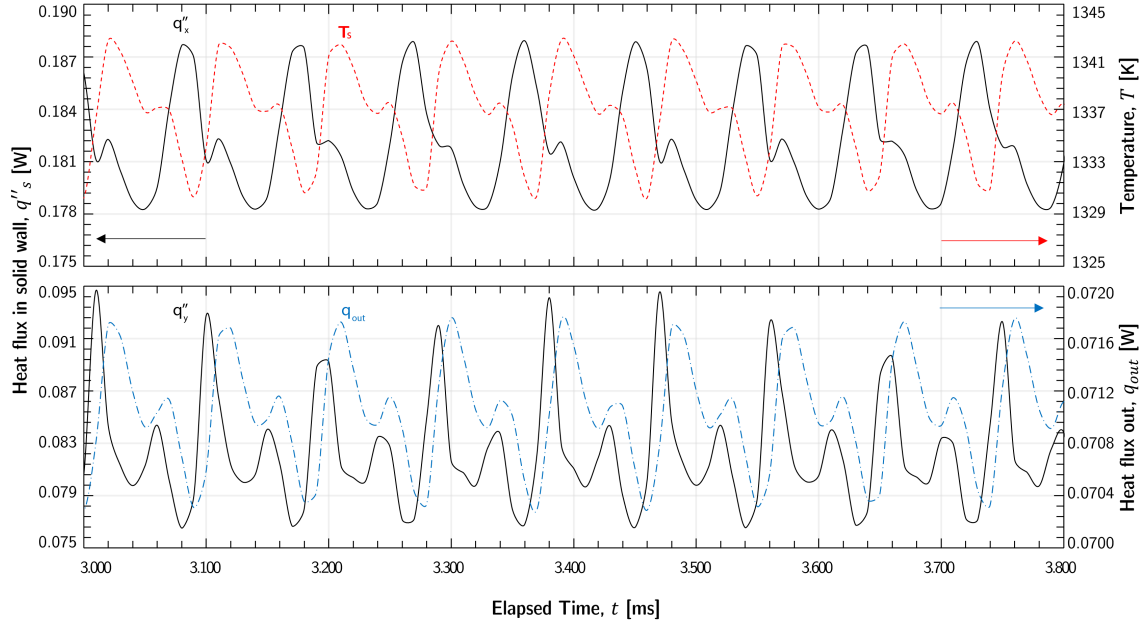


Figure 5.40: Temporal evolution of heat flux in solid wall (in the x and y directions (q''_x and q''_y), total heat flux lost to the surroundings (q_{out}), and average solid wall temperature (T_s) throughout the time interval $t = [3.000, 3.800]$ ms in the FS10Sp scenario.

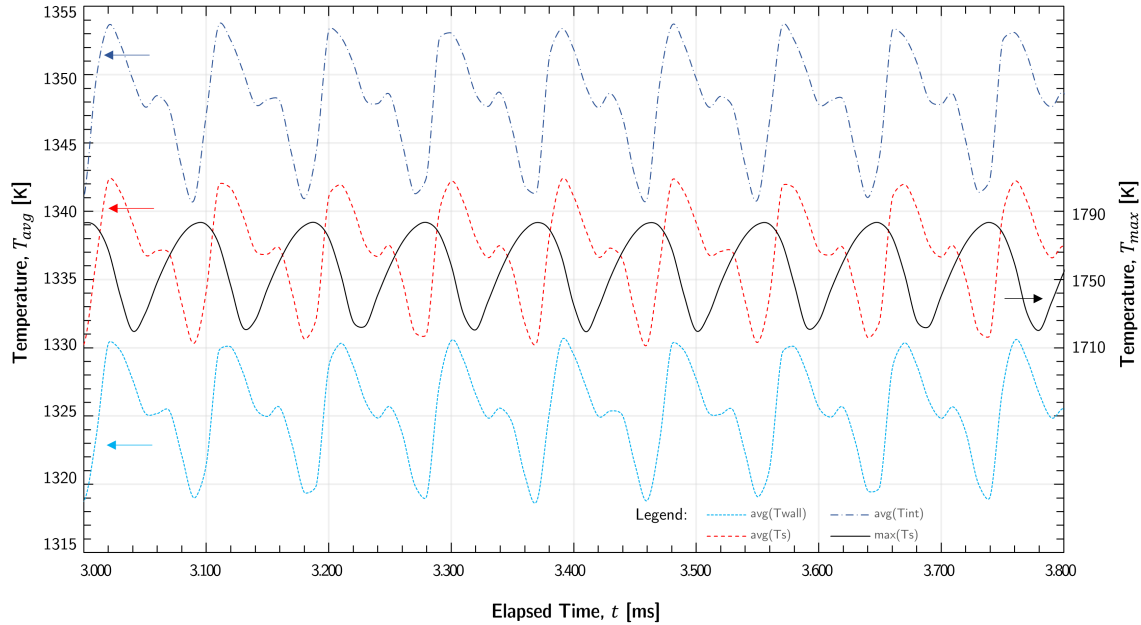


Figure 5.41: Temporal evolution of temperature profiles: average values of T_{wall} (outer surface), T_s (solid), and T_{int} (solid-fluid interface), along with peak temperatures across the entire wall during the time interval $t = [3.000, 3.800]$ ms for the FS10Sp scenario.

Just as in previous cases, we observe that $|q''_x|$ is greater than $|q''_y|$, indicating that PFB does not negate this trend ⁽¹⁹⁾. Additionally, we notice that the average wall temperatures, both T_s and the fluid-solid and solid-exterior interface temperatures, are perfectly synchronized, exhibiting similar profiles and frequencies without any noticeable delay or rush in relation to each other. Thanks to the adoption of a pseudo-stationary approach where the timescales of chemical reactions and heat transfer are equated ($S_0 = 0$), the temperature signals are synchronized with a very minimal delay relative to the fluid temperatures, as one would anticipate.

Furthermore, a desynchronization emerges between the maximum temperatures observed in the solid wall, $T_{s,max}$, and all other temperatures, whether fluid or solid. Given the intricate nature of PFB, the dynamics of heat transfer and conduction and the influence of wall thermal inertia, numerous factors can contribute to this phenomenon, making it challenging to identify a specific cause. Tables 5.13 and 5.14 display key temperature and heat flux values for the solid wall.

Table 5.13: Maximum and average temperature values for the solid domain for FS10Sp

Simulation	avg T_{int} [K]	avg T_{wall} [K]	avg T_s [K]	max T_s [K]	avg $T_{s,max}$ [K]	max $T_{s,max}$ [K]
FS10Sp	1348.47	1325.75	1337.46	1349.2	1757.74	1788.29

Table 5.14: Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for FS10Sp

Simulation	avg q''_x [W/mm ²]	avg $q''_{x,max}$ [W/mm ²]	avg q''_y [W/mm ²]	avg $q''_{y,max}$ [W/mm ²]	avg q_{out} [W]	min q_{out} [W]	max q_{out} [W]
FS10Sp	0.182	0.998	0.082	0.313	0.07109	0.07029	0.07250

As we have done previously, we performed a spectral analysis on the temperature and heat release signals within the fluid domain and compared them to the values of Ad10Sp. However, a problem arises concerning the interpretability of the results, since, despite the flame anchoring in the same position within the microchannel, there are substantial differences between the average values of T and q''' . To address this, we normalized the amplitude by calculating a ratio of the amplitude relative to the average value:

$$A_{\sim}^{var} (\%) = \frac{A^{var}}{\text{avg}(var)} \cdot 100 \quad (5.2)$$

and this ratio can then be used as a scaled amplitude value, which reflects the significance of amplitude concerning the average value. The results can be found in Table 5.15 and 5.16

As evident, the inclusion of a solid wall results in a notable decrease in the peak frequency of PFB. This phenomenon highlights the role of heat loss in expediting flame extinction, which, as previously discussed, leads to less signal recurrence in q''' . When a signal lacks frequent oscillations or variations, it inherently exhibits a lower frequency, a concept supported by Cooley's work on signal analysis [201].

⁽¹⁹⁾A comparison with stable flame, FS4Sp, will be conducted later when a generalized analysis of Fused Silica is performed.

Table 5.15: Signal spectral analysis results for frequency, f , and maximum amplitude values, A^{var} , for the simulations FS10Sp and Ad10Sp

Simulation	f [Hz]	$A^{T_{\text{avg}}}$ [K]	$A^{T_{\text{max}}}$ [K]	$A^{q_{\text{tot}}}$ [W]	$A^{q_{\text{avg}}'''}_{\text{avg}}$ [W/mm ³]	$A^{q_{\text{max}}'''}_{\text{max}}$ [W/mm ³]
Ad10Sp	13665	109.24	110.37	0.817	3.405	6.523
FS10Sp	10972	101.57	84.38	0.559	1.777	4.754
$\Delta X/X$ (%)	-19.7%	-7.0%	-23.5%	-31.6%	-47.8%	-27.1%

Table 5.16: Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the simulations FS10Sp and Ad10Sp

Simulation	$A_{\sim}^{T_{\text{avg}}}$ [—]	$A_{\sim}^{T_{\text{max}}}$ [—]	$A_{\sim}^{q_{\text{tot}}}$ [—]	$A_{\sim}^{q_{\text{avg}}'''}_{\text{avg}}$ [—]	$A_{\sim}^{q_{\text{max}}'''}_{\text{max}}$ [—]
Ad10Sp	8.53%	4.99%	83.7%	114.3%	32.4%
FS10Sp	7.43%	4.16%	59.9%	85.4%	29.3%
ΔX	-1.1%	-0.8%	-23.8%	-28.9%	-3.1%

Additionally, we note a reduction in the scaled amplitudes of released heat compared to the adiabatic simulation. This decrease can be explained from a physical standpoint, by drawing a parallel with the concept of a less intense and less explosive flame due to heat loss.

In conclusion, we conducted an analysis of how the heat flux within the solid-fluid interface evolves during PFB, in comparison with the heat release rates. As depicted in Figure 5.42, there are no significant variations in the heat release rate evolution when compared to the adiabatic counterpart illustrated in Figure 5.13. The key distinction lies in the fact that in this case, the flame is completely extinguished, as opposed to flow-assisted extinction as previously mentioned. We observe that $q''_{s,x}$ exhibits a clear upstream conduction trend during PFB, with $q''_{s,x} \lesssim 0, \forall x$. In the regions far from the flame front, these values tend to approach approximately zero due to smaller ∇T_s . However, during the ignition to burst phases, two distinct peaks emerge, coinciding with the peaks in the heat release rate. This indicates a greater tendency for heat to be transported upstream in these regions of the microchannel.

These same peaks also appear in $q''_{s,y}$, where during the periods of PFB containing the flame front, the highest values of $q''_{s,y}$ are found in these regions. The notable difference is the existence of areas where $q''_{s,y} < 0$ is evident. However, due to the low thermal conductivity of this material, the values in these areas are comparatively lower than the rest of the wall. These zones persist throughout almost the entire cycle. The most significant one is in the 2nd convex region, where combustion has not yet occurred, and temperatures of the fluid are around 300 [K], lower than those in the wall. In this region, heat flows from the wall into the fluid. The following zone primarily occurs in the 2nd contraction and only during the burst and bifurcation phases when the flame covers this area more extensively does $q''_{s,y} > 0$.

In general, due to the low value of λ_s (thermal conductivity), there is no significant flame flashback observed. However, it is reasonable to anticipate the possibility of flashback occurring as we increase the material's thermal conductivity.

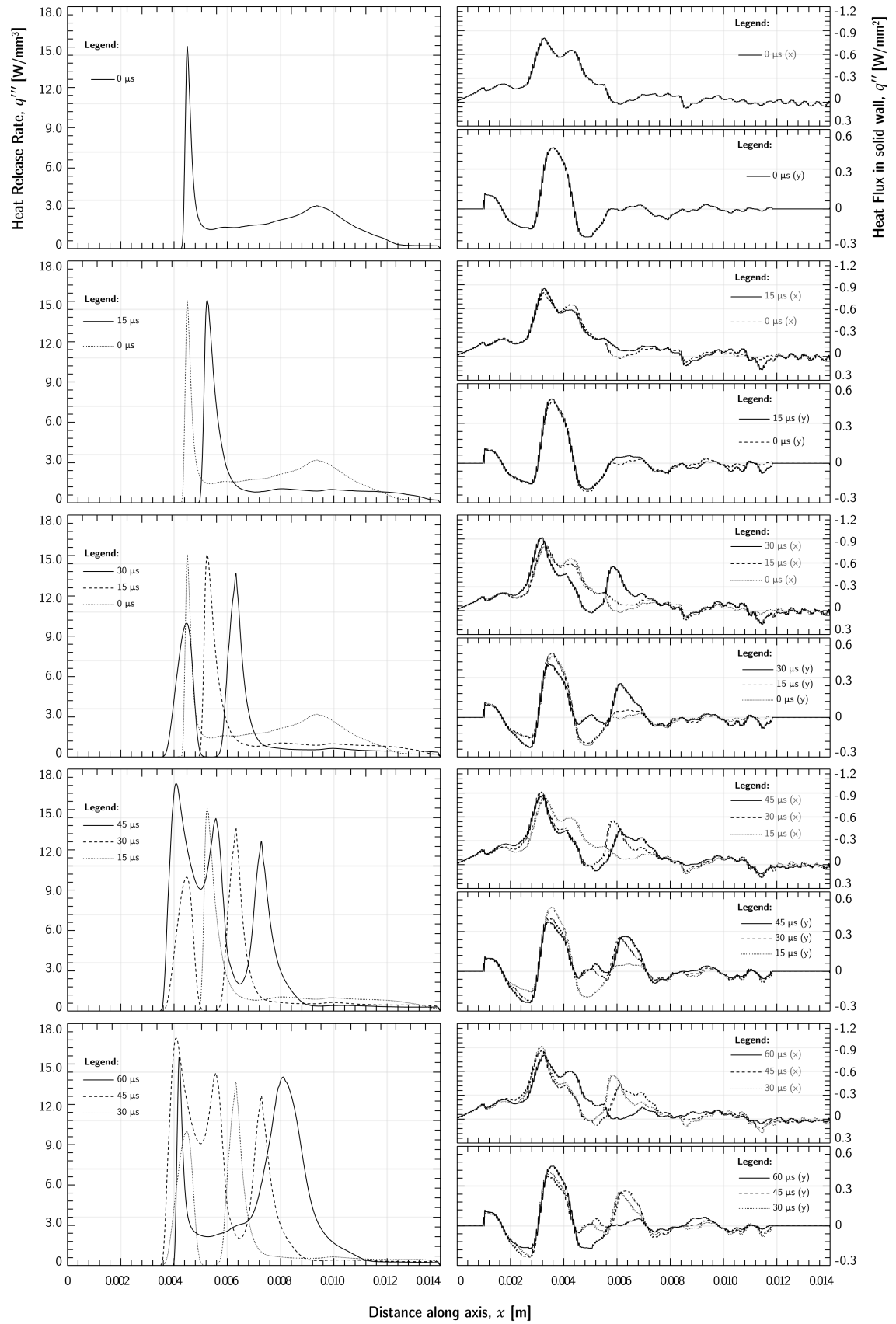


Figure 5.42: Heat release rate (left) and heat flux in the x (top right for each column) and y directions (bottom right) profiles along the x axis (centerline) for FS10Sp during one PFB cycle.

5.4.5 Migrating Pulsatory Flame Burst (mPFB)

Concluding the Fused Silica simulations now, the last one, FS12Sp, also ended up exhibiting the PFB phenomenon, just like FS10Sp, but it occurred in the last (4th) convex zone. The significant difference is the emergence of a new phenomenon, migratory Pulsatory Flame Burst, or mPFB. This phenomenon essentially exhibits the same dynamics as those previously examined for PFB but entails a propagation from its initial location downstream of the microchannel. This occurs between convex zones, as these zones are typically where the flame front stabilizes.

As depicted in Figure 5.43, this mPFB takes place twice. The first instance occurs when the flame migrates from the 2nd to the 3rd convex zone, roughly within the range of [1.300, 1.600] [ms]. The second instance occurs during the time interval of [2.800, 3.200] [ms], wherein there is a migration of PFB from the 3rd to the 4th convex zone. During moments of mPFB, a clear deviation from periodicity in fluctuations of T and q''' is visible. Furthermore, the position of the flame front downstream after each mPFB significantly affects the evolution of T_{avg} , lowering after each migration, because as the flame front is positioned further downstream, a larger region of lower temperature exists.

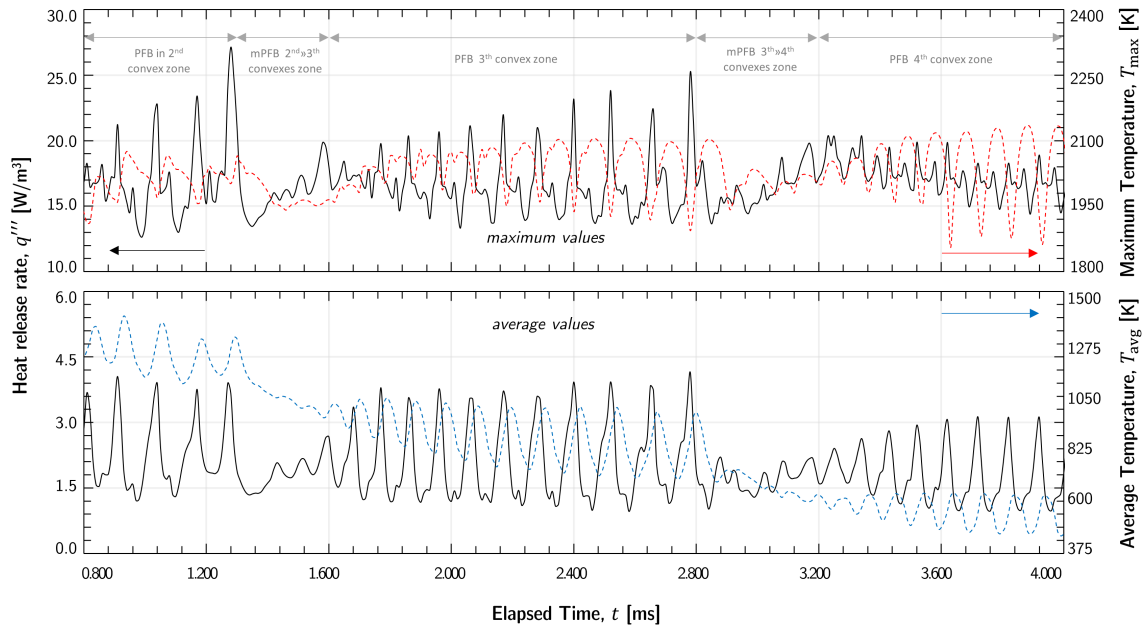


Figure 5.43: Evolution of maximum and average values of heat release rate and temperature in the fluid for FS12Sp, over time $t = [0.800, 4.000]$ [ms].

We also observe a transitional PFB (tPFB) following each PFB cycle. However, in contrast to FS4Sp, this time it leads to a gradual increase in signal amplitude until it stabilizes. While it stabilizes as a PFB, we also notice a slight increase in signal frequency. However, instead of achieving permanent stability, the high velocity causes τ_{res} , the flow residence time, to dominate over the characteristic combustion time, τ_c , gradually resulting in less complete combustion in the current convex zone, as discussed in section 2.3.3. In the last few cycles of PFB before mPFB, we observe a decrease in the minimum values of T_{max} and T_{avg} . This suggests that, given the increased frequency, the region of lower temperature after PFB flame extinction becomes more substantial,

leading to a loss of thermal energy in the walls and fluid in the convex zone. This increasing incomplete combustion is expected to result in lower temperatures, favoring a longer period of flame extinction.

To verify this, we selected a midpoint within the convex zone and another within the solid wall, both located at a position of $x = 6.5$ [mm]. We then generated plots during the final stages of PFB within the third convex zone, illustrating the mass fractions of H_2 , the heat flux in the y direction in the solid, and the temperatures within both the solid and fluid domains. These plots are depicted in Figure 5.44. We observe that both temperatures are consistently decreasing, and the Y_{H_2} is increasing (indicating less H_2 burned in this zone). Furthermore, the temperature gradient at the surface (∇T_s) decrease. Consequently, we observe more pronounced and longer-lasting minima in the heat flux in the y direction ($q''_{s,y}$), which is a strong indicator of significant thermal energy loss in the wall, based on what we've discussed so far.

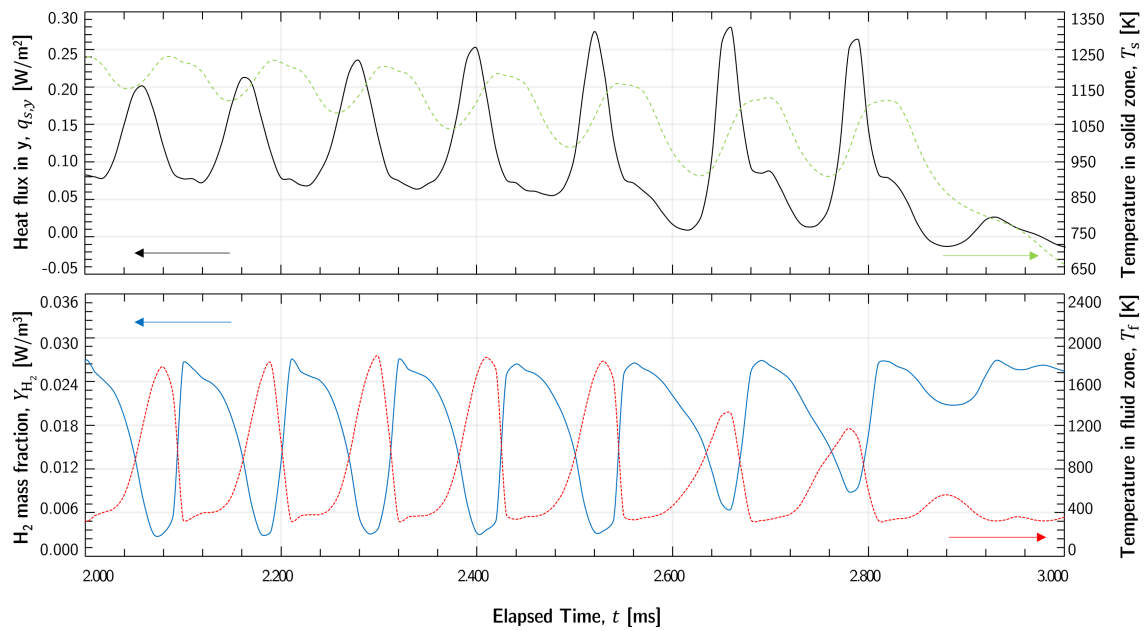


Figure 5.44: Evolution of various characteristics over time, specifically at the center of the convex zone (bottom: H_2 mass fraction and fluid temperature) and at the center of the solid wall (top: heat flux in the y direction and solid temperature), located approximately at $x \approx 6.5$ [mm] for the FS12Sp scenario, within the time range $t = [2.000, 3.000]$ [ms].

To better visualize mPFB, Figure 5.45 illustrates the evolution of the temperature distribution within the microchannel at intervals of 20 [μs]. Additionally, it provides insight into the interaction between the fluid flow and the combustion reaction by displaying the streamlines of the flow field. We can clearly see that the temperatures at the wall are insufficient to maintain the flame front in this area. Additionally, the heat generated by the chemical reaction in this zone dissipates rapidly towards the wall due to the significant temperature gradient (∇T) between the fluid and solid phases. Consequently, following the final burst, there is no re-ignition of a new flame, leading to the transition of PFB to the subsequent convex zone.

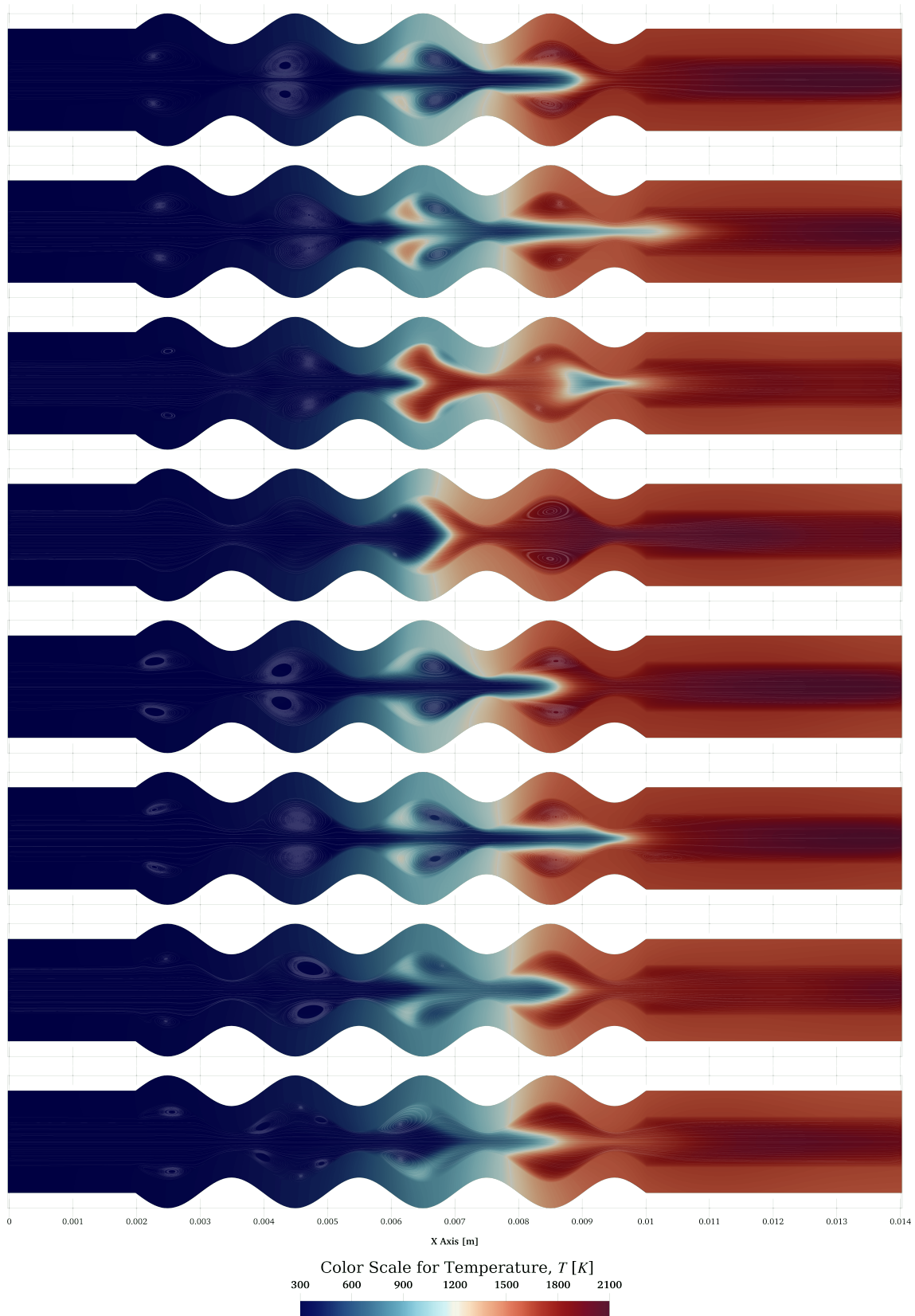


Figure 5.45: Visualizing the culmination of mPFB: streamlines of the flow field and temperature distribution in the microchannel for FS12Sp, captured at 20 μs intervals.

5.4.6 Overview of Fused Silica

Let us now examine the three simulations which didn't result in extinction in Fused Silica. The preceding sections have delved extensively into Fused Silica, so we will provide a general analysis here. In summary of our findings, we have come to comprehend that the introduction of heat loss ultimately yields flames of reduced strength and intensity. This is primarily because a greater proportion of heat dissipates to the external environment, resulting in lower temperatures and, consequently, diminished heat release rates

Additionally, when PFB occurs, we notice reduced signal recurrence in q''' and T , which, when compared to the adiabatic simulations, results in lower frequencies (see Figure 5.47, which illustrates this as explained before). You can observe this phenomenon in Figure 5.46, where we examine a single FS10Sp PFB cycle at the identical time points as those utilized in Figures 5.37 and 5.39. Here, especially in comparison to the adiabatic counterpart illustrated in Figure 5.21, we see that q''' and T signals are more harmonic, with less peaks, due to less heat accumulation.

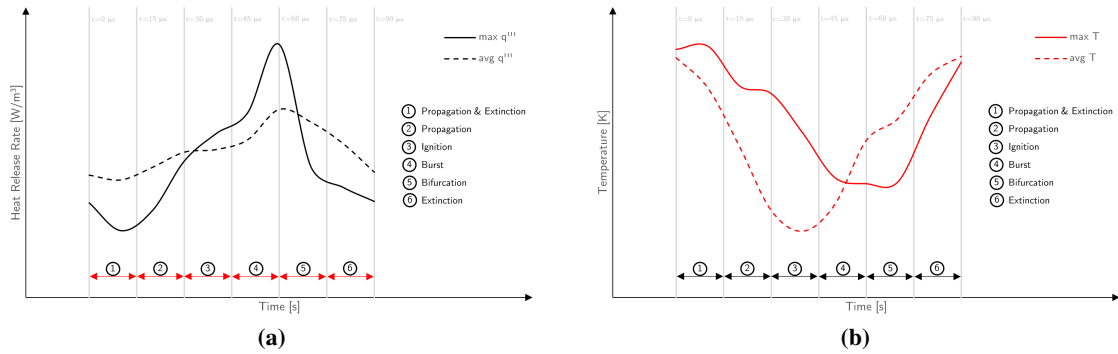


Figure 5.46: A single PFB cycle with heat loss present in the microchannel illustrated in 5 stages: (a) Heat Release Rate; (b) Temperature.

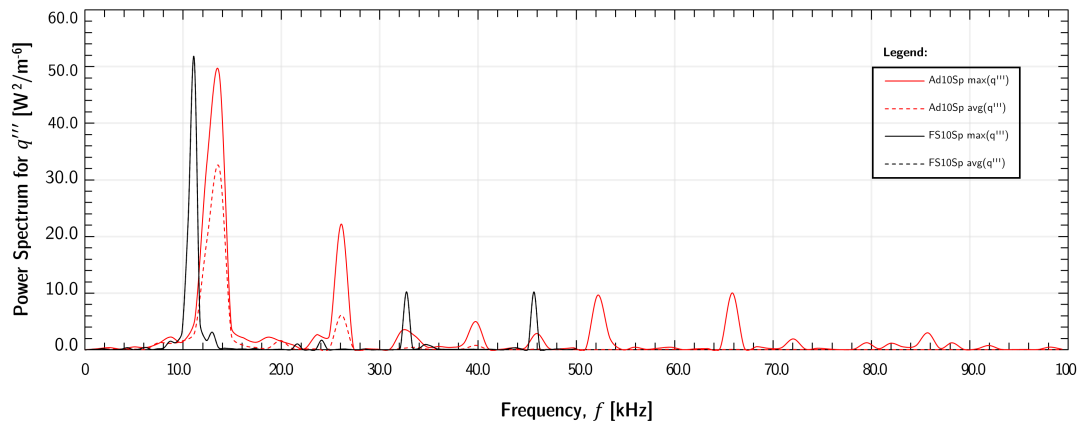


Figure 5.47: Power Spectrum (q''') versus frequency (f) for Ad10Sp and FS10Sp.

As mentioned previously, there is a noticeable delay in the $T_{\max}$ signal here, when in comparison to the adiabatic scenario. It becomes clearer when you consider that Figure 5.46b represents a cycle that immediately follows the one shown in Figure 5.46a. Temperature fluctuations are influenced by several factors, including the heat release rate, reactant flow-rate, and heat transfer mechanisms at play. Consequently, it's reasonable to expect that accounting for heat transfer phenomena can impact the system. What we observe is the lack of the heat transfer in the solid, which we can observe in adiabatic conditions, results in smaller delay (faster thermal response).

When concentrating solely on the Fused Silica simulations, Tables 5.17 and 5.18 exhibit key insights. These tables present the average, maximum, and minimum values for certain temperature and heat release rate parameters in the *fluidRegion* domain. It becomes evident that the anticipated consequence of increased velocity holds true: stronger and more intense flames result, mirroring the trends observed in the adiabatic simulations⁽²⁰⁾.

Table 5.17: Maximum and average temperature values for the fluid domain for the Fused Silica simulations

Simulation	avg T_{avg} [K]	min T_{avg} [K]	max T_{avg} [K]	avg T_{max} [K]	min T_{max} [K]	max T_{max} [K]
FS4Sp	1364.47	1364.47	1364.47	1962.38	1962.38	1962.38
FS10Sp	1367.05	1316.01	1420.92	2029.55	1988.24	2072.62
FS12Sp	734.35	650.21	808.27	2044.89	1834.68	2148.79

Table 5.18: Maximum and average heat release rate values for the fluid domain for the Fused Silica simulations

Simulation	avg q_{tot} [W]	min q_{tot} [W]	max q_{tot} [W]	avg q'''_{avg} [W/mm ³]	max q'''_{avg} [W/mm ³]	avg q'''_{max} [W/mm ³]	max q'''_{max} [W/mm ³]
FS4Sp	0.342	0.342	0.342	0.793	0.793	16.023	16.023
FS10Sp	0.933	0.662	1.247	2.080	3.092	16.222	19.104
FS12Sp	1.006	0.579	1.855	1.718	3.130	16.887	19.868

It was anticipated that within the solid domain, the peak temperatures of the *solidRegion*'s denoted as $T_{\text{s,max}}$, would rise in tandem with the intensification of the flame's strength and intensity. Surprisingly, while this pattern is discernible from FS4Sp to FS10Sp, it does not hold from FS10Sp to FS12Sp, as seen in Table 5.48. This prompts a straightforward question: “How can the maximum temperatures in the solid domain be lower when the flame is more intense?”

Based on our previous discussions, we understand that it requires time for temperatures to stabilize, both within the fluid and the solid components. In stable flames, temperatures gradually approach specific values, while in the case of PFB, they end up exhibiting oscillations between more consistent values. However, given that both simulations have reached steady-state conditions, this cannot explain why $T_{\text{s,max@FS10Sp}}$ is greater than $T_{\text{s,max@FS12Sp}}$.

On the other hand, we have yet to explore how the temperature varies within the solid. With the interior of the microchannel consistently hotter than the exterior, it's evident that the maximum temperatures in the solid will occur at the solid-fluid interface, meaning $T_{\text{s,max}} = T_{\text{int,max}}$. Consequently, we conducted a temperature variation analysis along the solid-fluid interface of *solidRegion1*, and the results are illustrated in Figure 5.48 for both FS10Sp and FS12Sp.

Both curves exhibit a remarkable similarity, with FS12Sp displaying a noticeable rightward shift compared to FS10Sp, due to the fact that in the former case, the flame anchors in the 4th convex zone, while in the latter, it anchors in the 2nd convex zone. In FS10Sp, during the ignition and burst phase of the PFB cycle, 30 ~ 45 [μs], there is a distinct downward oscillation in the temperature (T_{int}) near the flame front, occurring within the range of $x \approx [4.0, 6.0]$ [mm]. The same happens in FS12Sp, but at around $x \approx [9.0, 11.0]$ [mm]⁽²¹⁾. As the flame progresses into the bifurcation stage, there is a subsequent upward oscillation once more.

⁽²⁰⁾And as seen before, some of the average values, especially T_{avg} , are not comparable due to the flames anchoring at different positions, making maximum values a better indicator, as we've seen before

⁽²¹⁾This phenomenon arises because, during these stages, a higher percentage of unburned mixture is present, leading to overall lower average temperatures in the fluid in the region, and as such, smaller heat flux transferred to the solid.

Furthermore, we observe that in FS10Sp, it requires until approximately $x \approx 11$ [mm] to reach the location of the maximum temperature, at a considerable distance from the flame front. However, in FS12Sp, since the microchannel has a length of only 14 [mm], there isn't sufficient distance to allow for the temperatures to increase to the maximum value possible. This can primarily be attributed to the fluid temperatures being higher than the solid temperatures throughout the microchannel. As such, there is a greater heat flux from the fluid to the solid compared to the heat loss to the external environment. Additionally, within the solid material, there is a flow of heat towards the cooler regions of the microchannel walls at the inlet.

Notably, it is important to elucidate the existence of the buffer zones that cause the temperature to increase more in certain areas. One as mentioned, occurs at $x \approx 11$ [mm] (at the start of the final straight zone of the microchannel), and a second minor peak at $x \approx 8.5$ [mm] (4th convex zone). These buffer zones were similarly observed in the fluid temperature profiles in Resende et al. [113]. They can be attributed to a reduction in external heat losses due to the flow dynamics caused by the presence of the vortices in the convex zone, which also occur in the latter part of the microchannel, resulting in heat accumulation.

In contrast, this pattern is not seen in the fluid temperature, since the maximum temperature values are usually found adjacent to the flame front, and here a more intense flame correlates with higher maximum temperatures. Also, just like in the adiabatic scenario, we also observe an increase of f and $A_{\sim}^{\text{var}}$ with higher values of U_{in} , as seen in Table 5.21, showing that this trend remains consistent even in the presence of heat loss.

Table 5.19: Maximum and average temperature values for the solid domain for the Fused Silica simulations

Simulation	avg T_{int} [K]	avg T_{wall} [K]	avg $T_{\text{s,avg}}$ [K]	max $T_{\text{s,avg}}$ [K]	avg $T_{\text{s,max}}$ [K]	max $T_{\text{s,max}}$ [K]
FS4Sp	1296.96	1284.12	1293.35	1293.35	1598.74	1598.74
FS10Sp	1348.47	1325.75	1337.46	1349.20	1757.74	1788.29
FS12Sp	771.26	763.91	767.82	794.11	1673.99	1693.21

Table 5.20: Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for the Fused Silica simulations

Simulation	avg $q''_{\text{x,max}}$ [W/mm ²]	avg $q''_{\text{y,max}}$ [W/mm ²]	avg q_{out} [W/mm ²]	min q_{out} [W]	max q_{out} [W]
FS4Sp	-1.121	0.263	5.18×10^{-2}	5.18×10^{-2}	5.18×10^{-2}
FS10Sp	-0.998	0.313	7.11×10^{-2}	7.03×10^{-2}	7.25×10^{-2}
FS12Sp	-0.956	0.276	3.32×10^{-5}	2.95×10^{-5}	3.59×10^{-5}

Table 5.21: Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the Fused Silica that resulted in PFB

Simulation	f [Hz]	$A_{\sim}^{T_{\text{avg}}}$ [—]	$A_{\sim}^{T_{\text{max}}}$ [—]	$A_{\sim}^{q_{\text{tot}}}$ [—]	$A_{\sim}^{q''_{\text{avg}}}$ [—]	$A_{\sim}^{q''_{\text{max}}}$ [—]
FS10Sp	10972	7.4%	4.2%	59.9%	85.4%	29.3%
FS12Sp	9910	21.5%	15.4%	126.9%	125.6%	33.0%

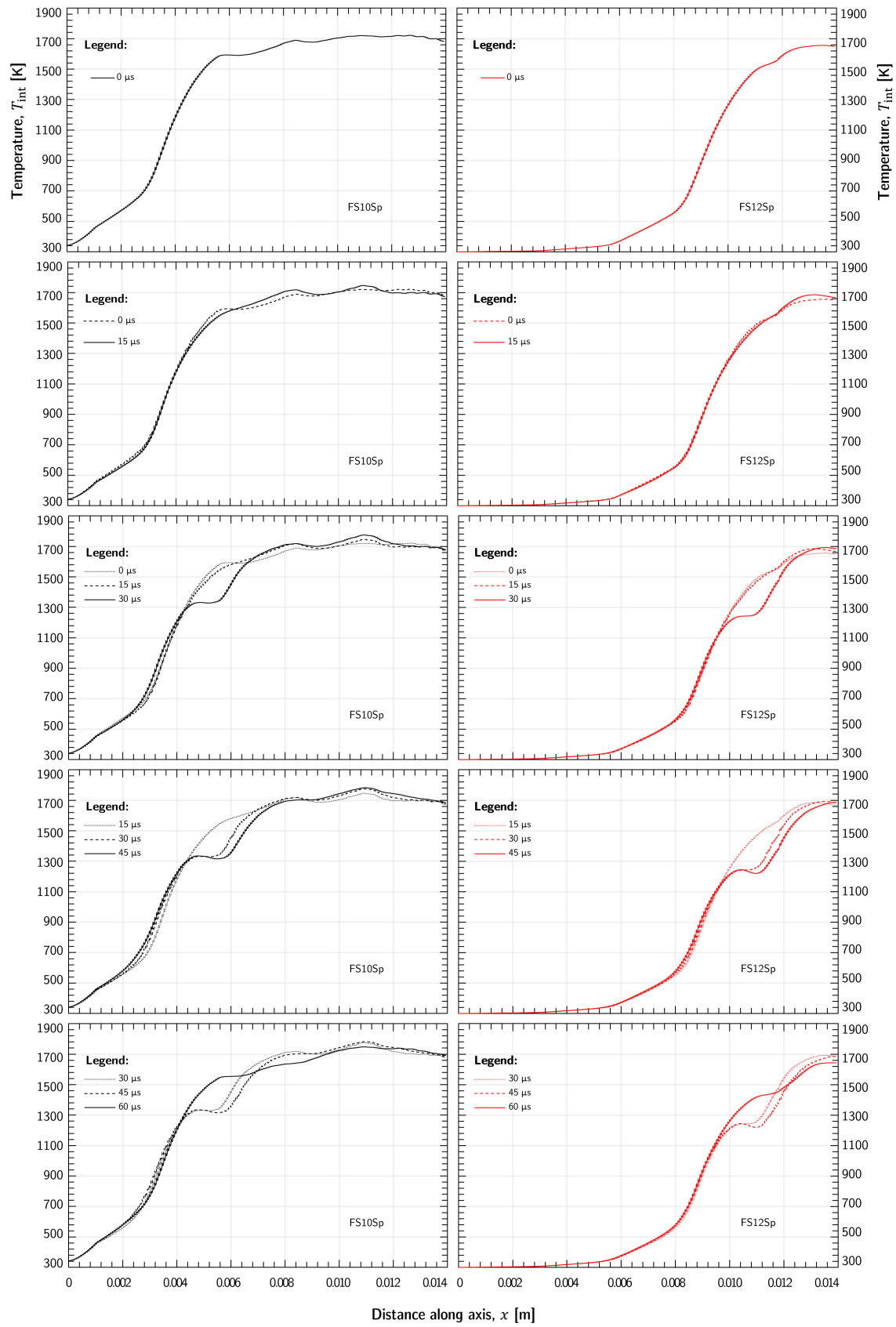


Figure 5.48: Temperature profiles in *solidRegion1* along the microchannel length in the fluid-solid interface, T_{int} , for FS10Sp (left) and FS12Sp (right).

5.5 Dynamics of ceramics materials

We will now start an exploration of ceramic materials, specifically Co-fired ceramics. These are monolithic⁽²²⁾ ceramic microelectronic devices in which the entire ceramic support structure, along with any conductive, resistive, and dielectric⁽²³⁾ materials, is fired in a kiln⁽²⁴⁾ simultaneously [202]. Co-fired ceramics can be broadly categorized into two groups: low-temperature co-fired ceramics (LTCC) and high-temperature co-fired ceramics (HTCC). In our study, we will investigate one example from each category, represented by simulations HT4Sp to HT12Sp for HTCC and LT4Sp to LT12Sp for LTCC.

The thermal conductivity of LTCC ($\lambda_{s,LTCC} = 2.8 \text{ [W/(mK)]}$) is low, comparable to amorphous materials. Consequently, it is expected that the outcomes will not significantly deviate from what has been observed previously for amorphous materials. In contrast, the thermal diffusivity of LTCC ($\alpha_{T,LTCC} = 1.34 \times 10^{-6} \text{ [m}^2/\text{s}]$) is nearly one order of magnitude larger than that of Fused Silica ($\alpha_{T,FS} = 9.97 \times 10^{-7} \text{ [m}^2/\text{s}]$). This significant difference results in LTCC being more effective at heat transfer, minimizing temperature gradients within the solid, and making its thermal responsiveness much faster.

Conversely, HTCC has a much higher thermal conductivity ($\lambda_{s,HTCC} = 20 \text{ [W/(mK)]}$), comparable to the values seen in stainless steels. This means there will be a significant higher amount of heat transfer in the walls due to conduction which will result in higher heat flux to the outside.

5.5.1 Stability map for ceramic materials

The stability map depicting various velocities and the two materials is provided in the subsequent Figure 5.49.

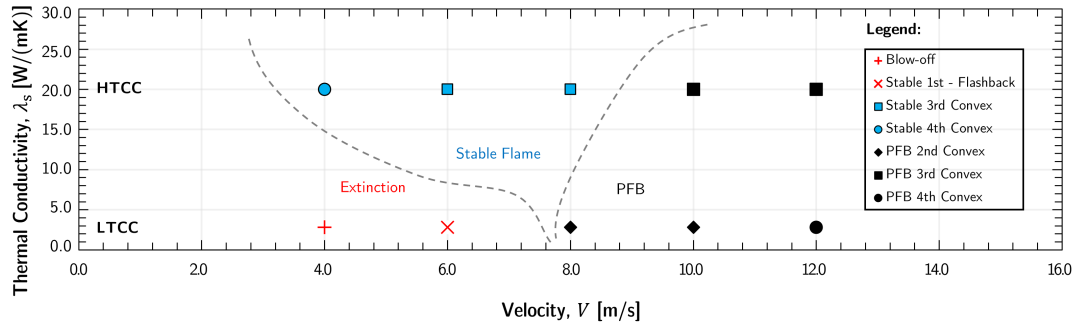


Figure 5.49: Stability map for the various simulations using a spark conducted with ceramic materials.

A new phenomenon was observed in the LTCC when the inlet velocity, denoted as U_{in} , was set to 4.0 [m/s] , characterized by flame extinction, and will be thoroughly examined in the subsequent subsection. The simulation LT6Sp exhibited a similar behavior to that observed in FS6sp and FS8Sp: the flame initially stabilized within the first convex zone. However, due to the specific burner geometry and heat conduction within the chamber walls, it eventually experienced a flashback to the inlet, leading to the extinguishment of the flame. In three simulations, the flame

⁽²²⁾Meaning the different materials used in the ceramic device are combined into a single, solid structure → There are no separate layers or components (it's a unified whole).

⁽²³⁾Insulator materials that store electrical energy in the form of an electric field.

⁽²⁴⁾Firing in a kiln is a process of heating the materials at high temperatures to achieve specific properties like hardness, durability, and desired electrical characteristics

exhibited characteristics of PFB. In Figures 5.50 and 5.51, we present the profiles of q''' and the H_2 mass fractions during the ignition phase of PFB, respectively.

In the cases of LT8Sp and LT10Sp, PFB was observed in a manner akin to FS10Sp, without any manifestation of mPFB. However, in simulation LT12Sp, just like FS12Sp, PFB manifested differently, commencing within the second convex zone and subsequently migrating, driven by the mPFB mechanism, to the 4th convex zone, due to the increased U_{in} .

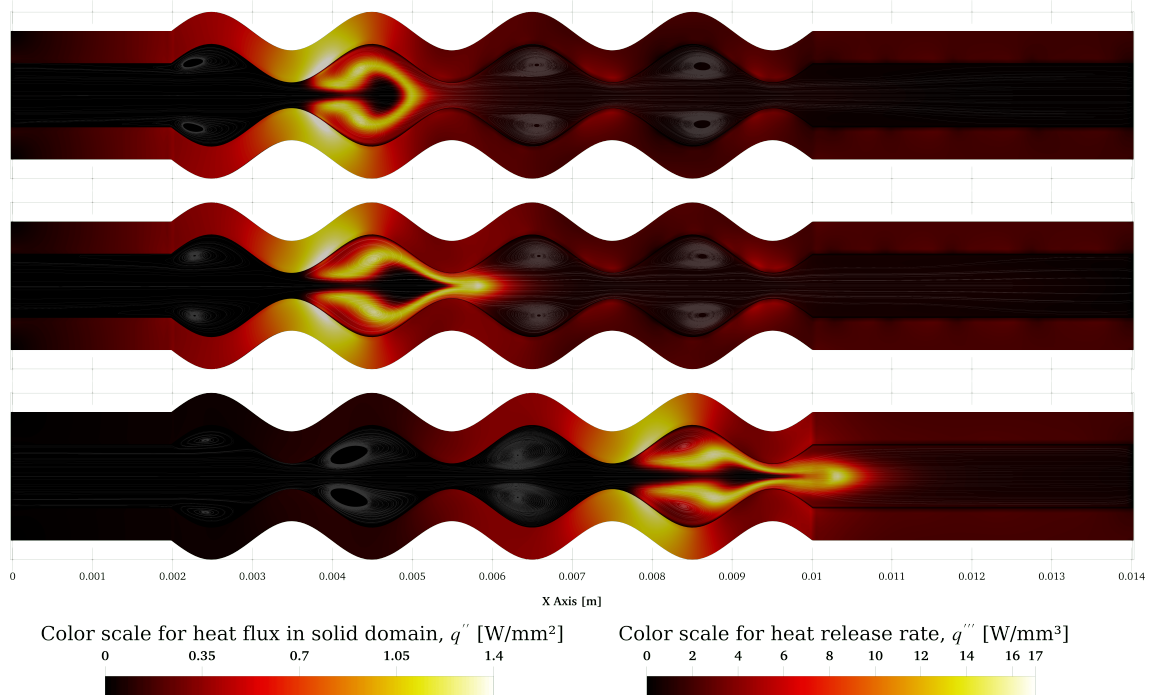


Figure 5.50: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for LT8Sp, LT10Sp and LT12Sp, from top to bottom respectively.

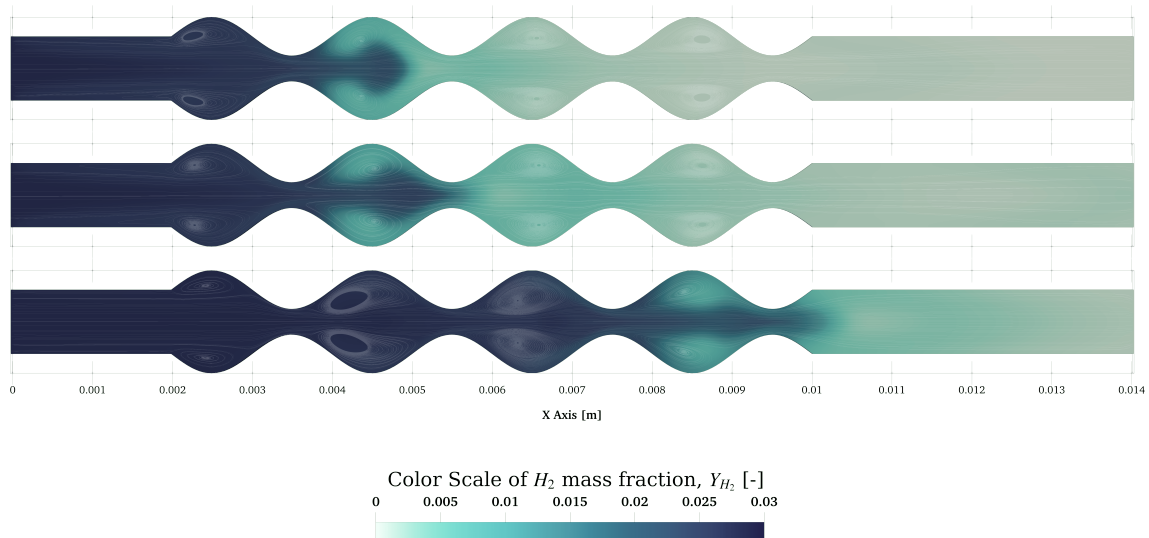


Figure 5.51: Streamlines of the flow field and distribution of the H_2 mass fraction for LT8Sp, LT10Sp and LT12Sp, from top to bottom respectively.

In the simulations using HTCC, for $U_{in} < 10$ [m/s], stable flames were obtained in all three simulations. One stable flame anchored in the fourth convex zone for HT4Sp (as shown in Figure 5.52), another in the third convex zone for HT6Sp (Figure 5.53), and also the third convex zone

for HT8Sp (Figure 5.54). As expected, and in line with previous observations, higher velocities led to stable flames with larger flame lengths (ℓ_f), which is visually evident from the contours of mass fraction of OH, and also a sharper configuration. In contrast, flames at lower velocities exhibited a shorter, more rounded appearance.

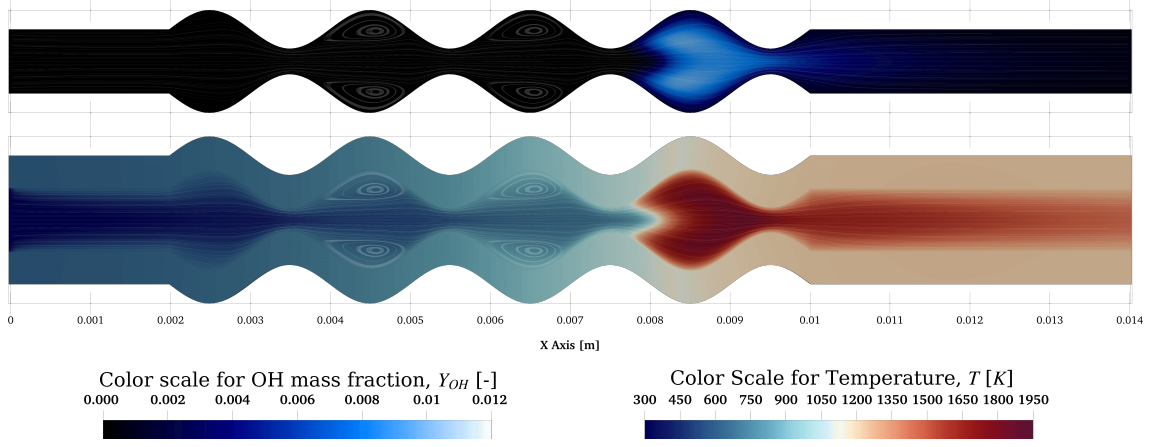


Figure 5.52: Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for HT4Sp (*FluidRegion* and *SolidRegion*'s).

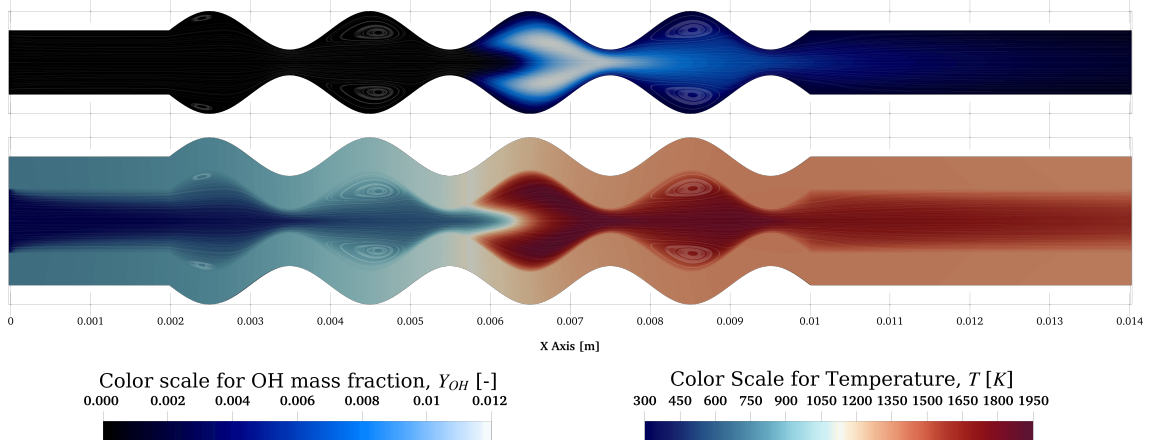


Figure 5.53: Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for HT6Sp (*FluidRegion* and *SolidRegion*'s).

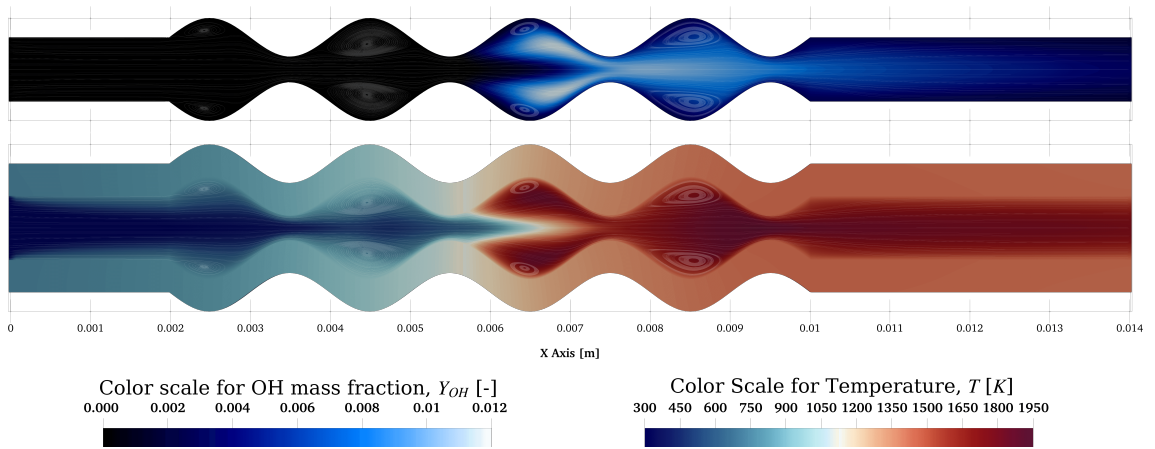


Figure 5.54: Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for HT8Sp (*FluidRegion* and *SolidRegion*'s).

Additionally, it was observed that wall and fluid temperatures were higher in simulations with higher inlet velocities. This was a consequence of the more intense and explosive flame resulting from the higher mass flow rate of the fuel. Finally, the fact that flames with higher U_{in} anchored further upstream made sense for the same reasons discussed in the previous subsections: higher velocities during the ignition phase led to a greater accumulation of thermal energy, which, in turn, contributed to flame stabilizing at a more upstream location along the microchannel.

As we raise the value of U_{in} , the flame starts to display PFB oscillations, anchoring itself in the 3rd convex zone⁽²⁵⁾ for both HT10Sp and HT12Sp, as illustrated in Figure 5.55. The influence of higher thermal conductivity is readily discernible when examining the heat flux, which is not only more elevated than before, but also exhibits a more extensive distribution across the microchannel wall compared to the preceding materials.

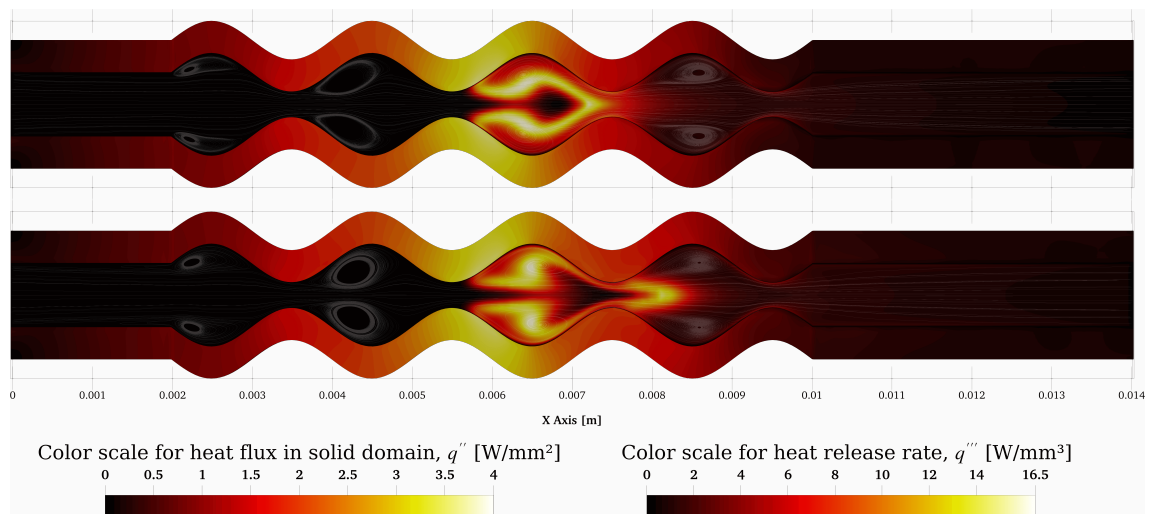


Figure 5.55: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for HT10Sp and LT12Sp.

5.5.2 Blow-off due to heat loss to the wall

In the LT4Sp simulation, no flame was obtained, as the initial flame from the spark was extinguished in the early moments of the simulation after the spark. This extinction occurred due to a phenomenon similar to blowoff. However, it is important to immediately distinguish it from the phenomenon typically associated with blowoff: in those scenarios, the reactants supply velocity of the mixture is higher than the flame speed (how fast the flame burns). This causes the flame, which initially anchors at a specific position, to start being carried by the high velocity downstream of the reactor. A clear example previously observed in this dissertation is cases of mPFB downstream, where although there is no extinction (and therefore cannot be classified as blowoff), the supply velocity of the mixture is higher than the flame velocity, resulting in migration towards one of the downstream convex zones of the microchannel.

In the simulations conducted, we introduce a spark for a duration of 0.5 [ms], which provides the necessary temperature to initiate the combustion process. Consequently, as the inflow velocity U_{in} increases, a larger amount of fuel comes into contact with the heat source, leading to a higher final temperature of the fluid and an increased amount of thermal energy within the microchannel

⁽²⁵⁾Just like before, it starts on the 2nd convex zone and due to mPFB migrates to the 3rd.

at the end of this phase⁽²⁶⁾. Simultaneously, we must consider that the walls of the microchannel start at a temperature of 300 [K]. Thus, until these walls heat up, there exists a significant temperature gradient between the solid walls and the fluid, resulting in a higher heat flux being transferred to the exterior.

Hence, if there's insufficient thermal energy generated during this phase or if excessive heat is lost, especially in the vicinity of the flame anchoring point, there is a risk of flame extinction. As visible in Figure 5.56, where we compare the temperature profiles of LT4Sp with HT4Sp FS4Sp, where the flame stabilizes in the 2nd convex zone, between time intervals $t \in [0.9, 1.1]$ [ms] with 0.01 [ms] intervals, it's evident that at the last time instant, the temperatures in LT4Sp have already dropped below 1000 [K], and combustion is becoming less intense, ultimately leading to the extinction of the flame.

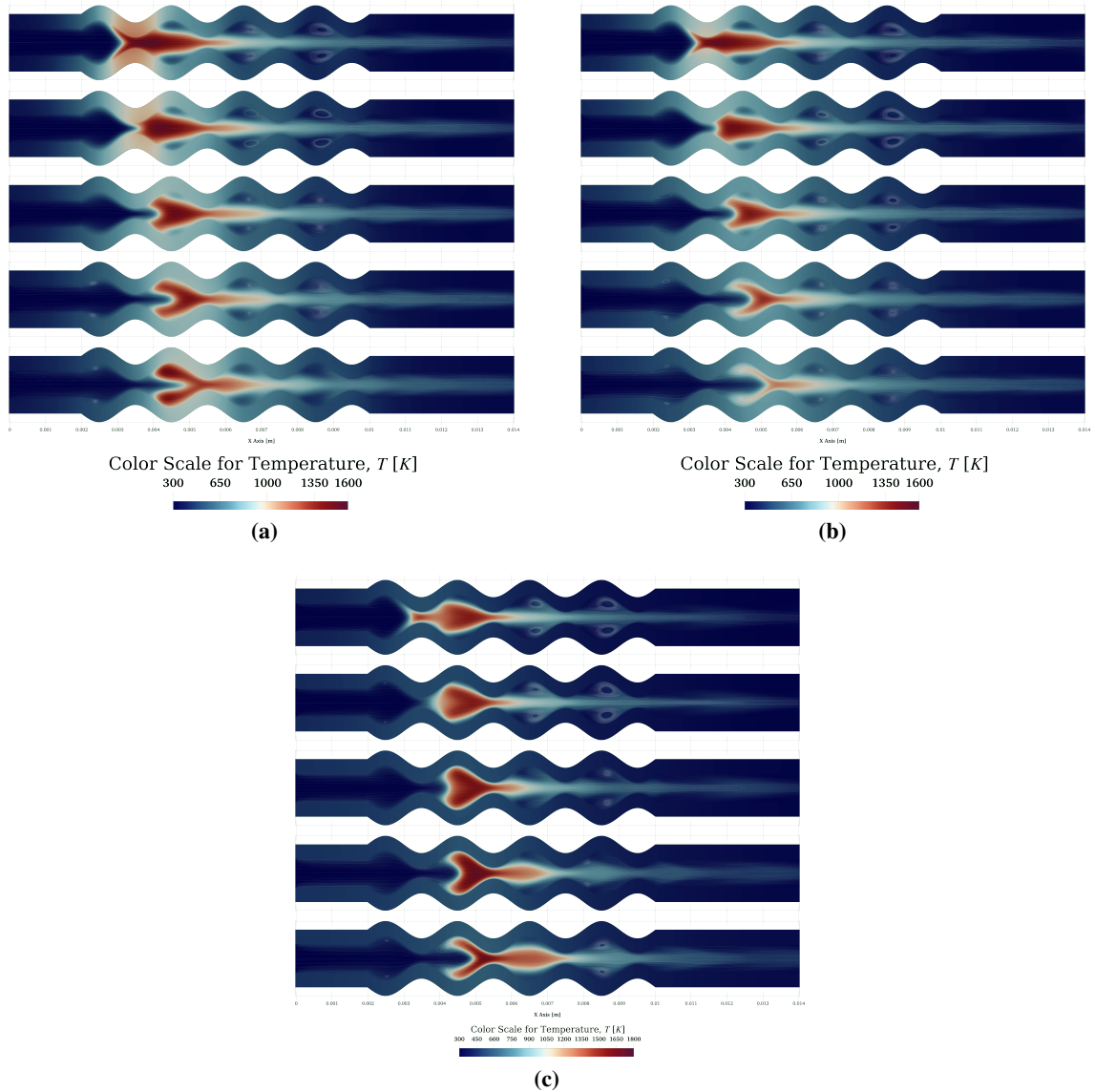


Figure 5.56: Streamlines of the flow field and distribution of temperature (FluidRegion and SolidRegion's), in 50 μ s starting from $t = 0.90$ [ms] for: (a) FS4Sp; (b) LT4Sp; (c) HT4Sp.

⁽²⁶⁾This implies that when $U_{in} = 4$ [m/s], we will witness the simulation with the least initial production of thermal energy.

Initially, one might assume that the higher thermal conductivity (λ_s) of LTCC leads to more heat loss, and, as such, lower wall and fluid temperatures. However, a pertinent question arises: “Why doesn’t this phenomenon occur with HTCC, which has a much higher λ_s ?” The answer lies in the fact that simply examining thermal conductivity is insufficient and that we are examining the initial stages of the simulation.

First, one must also consider other material properties, particularly thermal diffusivity. LTCC, as mentioned previously, possesses a higher thermal diffusivity (α_T) compared to Fused Silica. Thermal diffusivity quantifies a material’s capacity to conduct heat compared to its heat storage per unit volume. A high thermal diffusivity indicates rapid heat transfer because heat conduction outpaces heat retention within the material, which is illustrated in Figure 5.57. Consequently, LTCC, with a higher α_T facilitates the rapid dispersion of heat, lower heat retention in the solid, and combined with the higher λ_s , leads to cooler wall temperatures of the microchannel in the vicinity of the flame front.

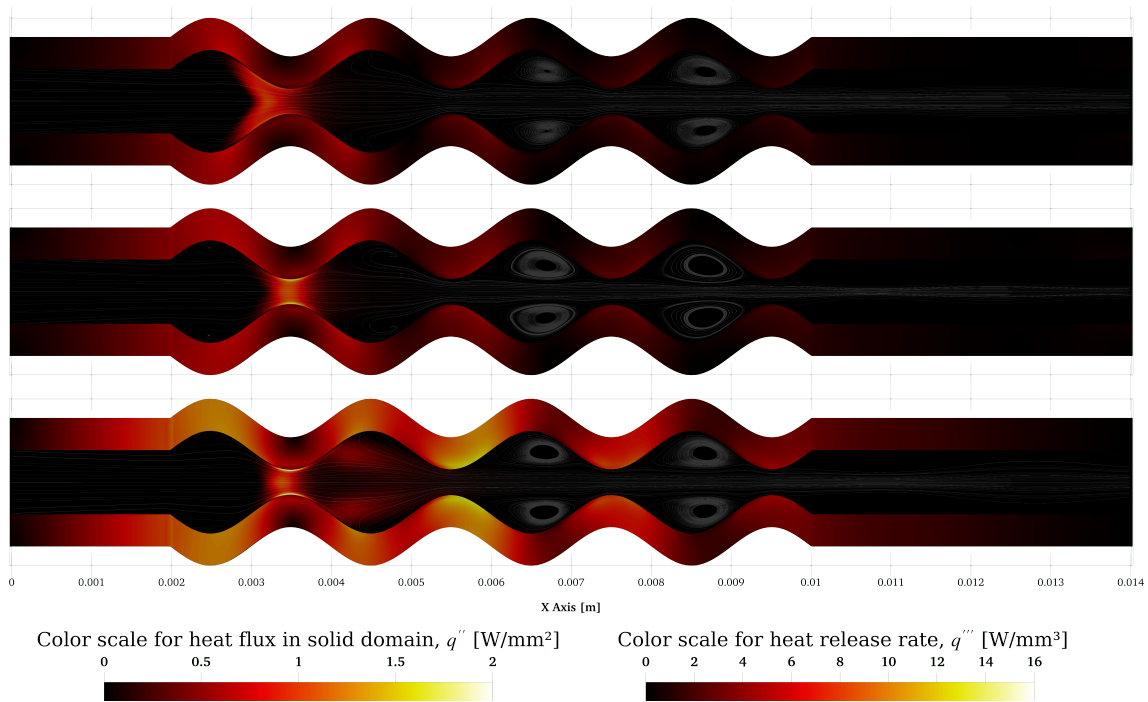


Figure 5.57: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for FS4Sp (top), LT4Sp (middle) and HT4Sp (bottom).

On the other hand, HTCC, a material with higher thermal diffusivity and conductivity, it becomes evident that it undergoes an extended phase during which the flame remains at a higher temperature. Our observations in this specific microchannel under the tested conditions reveal that as we augment thermal diffusivity, the thermal resistance in the microchannel walls also decreases, and there is a diminished heat retention at the interface between the solid and fluid, with the majority of the heat flow encountering minimal resistance as it dissipates outward. Consequently, during these early stages, the fluid retains more energy, facilitating chemical reactions within the microchannel. As a result, this prolonged period of elevated temperatures on the fluid domain provides the combustion reaction with an extended window for progression, even as it advances further along the microchannel without anchoring.

While this dissertation has highlighted the intricate nature of kinetics and flow dynamics, it is evident that variations in other material properties, such as specific heat capacity (C_p) and density (ρ), significantly impact these dynamics. Nevertheless, it is reasonable to assert that the lower thermal diffusivity (α_T) of Fused Silica enhances their ability to retain heat in the vicinity of the flame, facilitating efficient heat distribution. In contrast, LTCC, with its higher thermal diffusivity, may lead to a more dispersed temperature distribution in the wall, with less heat accumulation in the vicinity of the flame front, and as such, leading to a less stable flame.

5.5.3 Overview of ceramics materials

In the prior section, we presented a thorough examination of simulations involving Fused Silica, both in terms of their internal comparisons and their contrast with adiabatic counterparts when considering heat transfer. We are presented with a distinct opportunity to compare two similar ceramic materials, both of which involve heat transfer phenomena within their walls. However, owing to the distinctive properties of each material (HTCC boasting higher values of λ_s , ρ , and C_p), they will exhibit distinct behaviors. For this purpose, we present in Tables 5.22 and 5.23 the maximum and average values of temperature in the fluid domain, as well as the heat release rate values in the flame, for every simulation involving LTCC and HTCC (that yielded a flame).

Table 5.22: Maximum and average temperature values for the fluid domain for the LTCC and HTCC simulations

Simulation	avg T_{avg} [K]	min T_{avg} [K]	max T_{avg} [K]	avg T_{max} [K]	min T_{max} [K]	max T_{max} [K]
LT8Sp	1356.66	1321.44	1384.80	1988.80	1917.18	2046.47
LT10Sp	1320.21	1273.70	1363.81	1988.01	1907.74	2048.94
LT12Sp	764.03	680.46	801.88	2025.32	1907.08	2091.85
HT4Sp	943.74	943.74	943.74	1857.20	1857.20	1857.20
HT6Sp	1182.82	1182.81	1182.82	1907.23	1907.22	1907.23
HT8Sp	1195.59	1195.59	1195.59	1932.02	1932.02	1932.02
HT10Sp	1161.79	1124.90	1184.64	1939.51	1903.20	1962.29
HT12Sp	1109.39	1056.58	1161.91	1952.95	1936.75	1974.33

Table 5.23: Maximum and average heat release rate values for the fluid domain for the LTCC and HTCC simulations

Simulation	avg q_{tot} [W]	min q_{tot} [W]	max q_{tot} [W]	avg q'''_{avg} [W/mm ³]	max q'''_{avg} [W/mm ³]	avg q'''_{max} [W/mm ³]	max q'''_{max} [W/mm ³]
LT8Sp	0.780	0.582	1.009	1.767	2.483	16.046	17.245
LT10Sp	0.977	0.736	1.198	2.183	3.009	16.794	20.960
LT12Sp	0.995	0.682	1.598	1.924	2.882	17.723	19.983
HT4Sp	0.327	0.327	0.327	0.734	0.734	17.821	17.821
HT6Sp	0.579	0.579	0.579	1.278	1.278	18.816	18.816
HT8Sp	0.684	0.684	0.684	1.498	1.498	18.049	18.049
HT10Sp	1.017	0.816	1.289	2.262	3.080	16.700	19.444
HT12Sp	1.205	0.893	1.755	2.563	4.195	17.237	23.951

A noticeable trend emerges, particularly when taking in consideration with previous results from the adiabatic and fused silica simulations. It becomes evident that with an increase in wall conduction within the microchannel, there is a corresponding rise in heat flux, leading to greater heat dissipation and consequently lower fluid temperatures. This outcome aligns with expectations, as more of the heat generated by the chemical reaction escapes to the external environment. Furthermore, it's observed that while the trend of rising maximum temperatures with U_{in} remains consistent, certain scenarios, especially those involving PFB, exhibit intricate interactions between combustion kinetics and wall heat transfer. These interactions can lead to variations in the buffer zones, with notable implications on temperatures. This is seen e.g. in scenarios such as LT8Sp and LT10Sp.

As a general principle, it can be observed that both the heat release rate, denoted as q''' , and the integrated heat release rate, denoted as q_{tot} , tend to rise as the inlet velocity U_{in} increases. This behavior arises from higher velocities resulting in a larger quantity of the mixture undergoing combustion.

When examining the evolution of the heat release rate in various scenarios, it's essential to distinguish between the stable cases and those involving PFB. Therefore, let's begin by analyzing HOW IS THE HEAT RELEASE RATE AFFECTED BY THE HEAT DIFFUSIVITY IN STABLE CONFIGURATIONS. As a reminder three of this scenarios resulted in Stable Flame dynamics: HT4Sp, HT6Sp and HT8Sp. In order to do a fair comparison with other materials, let's compare Ad4Sp, FS4Sp, which also resulted in a stable configuration with HT4Sp. We observe that:

$$q_{tot, @Ad4Sp} = 0.432 [W] > q_{tot, @FS4Sp} = 0.342 [W] > q_{tot, @HT4Sp} = 0.327 [W]$$

$$q'''_{avg, @Ad4Sp} = 1.164 [W/mm^3] > q'''_{avg, @FS4Sp} = 0.793 [W/mm^3] > q'''_{avg, @HT4Sp} = 0.734 [W/mm^3]$$

In stable flames, the higher values of α_T and λ_s seen in HTCC seem to result in reduced heat generation from combustion kinetics. This observation aligns with our current understanding of combustion in this microchannel, as it corresponds to diminished H_2 combustion, likely stemming from decreased fluid temperatures due to heat loss. To validate this hypothesis, we employed the *IntegrateVariables* filter in *ParaView* to compute the integrated mass fraction of H_2 . By multiplying this fraction by the outlet area, we determined that in the case of HT4Sp, there remained a total of 18 ppm of unburned H_2 , while in FS4Sp, there were 13 ppm, and in Ad4Sp, there were 10 ppm, thereby confirming our initial hypothesis.

Let's now understand HOW IS THE HEAT RELEASE RATE AFFECTED BY THE HEAT DIFFUSIVITY IN SCENARIOS EXHIBITING PFB DYNAMICS. As we observed earlier in the context of Fused Silica, the heat release rate decreased when heat loss from the walls was introduced, as compared to adiabatic scenarios. However, what becomes apparent is that as we enhance the thermal diffusivity, particularly through increased heat conduction, we begin to observe an upward trend in the heat release rate values.

So we understand that the regions with vortices induced by velocity play a crucial role in facilitating the retrograde flow of energy, where energy moves upstream, ultimately triggering the ignition of new flames. When we introduce heat conduction in the walls, we observe that the more

conductive the material is, the greater the heat flux due to conduction in the solid becomes. Consequently, this further encourages an even more pronounced retrograde flow of energy, leading to faster ignitions. This is perfectly illustrated in Table 5.24, where HTCC shows higher frequencies than both Fused Silica and LTCC, indicating that these cycles occur at an accelerated pace.

Table 5.24: Signal spectral analysis results for amplitude values, A^{var} , for HTCC and LTCC that resulted in PFB

Simulation	f [Hz]	$A^{T_{\text{avg}}}$ [K]	$A^{T_{\text{max}}}$ [K]	$A^{q_{\text{tot}}}$ [W]	$A^{q_{\text{avg}}''''}$ [W/mm ³]	$A^{q_{\text{max}}''''}$ [W/mm ³]
LT8Sp	12109	63.36	129.29	0.427	1.273	2.897
LT10Sp	11032	90.11	141.2	0.462	1.521	5.650
LT12Sp	10937	121.42	184.77	0.916	1.645	4.415
HT10Sp	17187	59.74	59.09	0.4729	1.4158	3.7811
HT12Sp	15625	105.33	37.58	0.8623	2.4793	8.4396

As a result, there is an increased consumption of hydrogen gas (H_2), leading to higher values of q''' and q_{tot} . To verify this, we utilized the *IntegrateVariables* filter within *ParaView* to calculate the integrated mass fraction of H_2 . By then multiplying this fraction by the outlet area, we observed that during the LT10Sp phase, the average molar concentration of unburned H_2 was 141 ppm (oscillating between 108 and 178 ppm). In contrast, for the HT10Sp phase, these values were significantly lower, with an average unburned H_2 concentration of 56 ppm (fluctuating between 52 and 63 ppm).

Additionally, when we calculate the scaled amplitudes (Table 5.25, we observe that, even when accounting for heat transfer within the walls, higher inlet velocities result in a more potent burst, leading to a significant increase in amplitude. This is primarily due to the increased flow velocities, which create more substantial periodic gaps between the flames. When compared to the adiabatic and fused silica cases, there is also a discernible trend of scaled amplitudes growing smaller with the thermal diffusivity increasing. It's challenging to pinpoint the exact reasons for this phenomenon, given the complexities of heat transfer and the kinetics of the reaction. However, it is evidently linked to the higher frequencies of the signals. This is because the cycles unfold at a faster pace, leading to a higher overall combustion intensity within the same time frame. Consequently, both the maximum and minimum values increase.

Table 5.25: Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for HTCC and LTCC that resulted in PFB

Simulation	f [Hz]	$A_{\sim}^{T_{\text{avg}}}$ [—]	$A_{\sim}^{T_{\text{max}}}$ [—]	$A_{\sim}^{q_{\text{tot}}}$ [—]	$A_{\sim}^{q_{\text{avg}}''''}$ [—]	$A_{\sim}^{q_{\text{max}}''''}$ [—]
LT8Sp	12109	4.7%	6.5%	54.8%	72.0%	18.1%
LT10Sp	11032	6.83%	7.10%	47.3%	69.7%	33.6%
LT12Sp	10937	15.89%	9.12%	92.1%	85.5%	24.9%
HT10Sp	17187	5.14%	3.05%	46.5%	62.6%	22.6%
HT12Sp	15625	9.49%	1.92%	71.6%	96.7%	49.0%

Now, when we compare the temperatures of the microchannel walls, we observe in Table 5.26 that as thermal diffusivity increases, there is a corresponding decrease in temperatures. This pattern aligns with our expectations since higher thermal diffusivity implies that heat moves more rapidly, with heat conduction occurring at a faster rate than heat storage within the material. Consequently, more heat is dissipated, resulting in lower temperatures.

Furthermore, when we contrast temperatures at simulations with different velocities, it is evident, as demonstrated throughout this study, that higher velocities tend to generate more heat in the combustion kinetics, due to the higher air/fuel mixture flow rate. Consequently, fluid temperatures rise, leading to an increase in convective heat flux to the solid walls. This, in turn, contributes to an overall elevation in the solid temperatures. However, it's important to note that the location of the flame, as discussed in Section 5.4.6, exerts a substantial influence on the temperature distribution. Additionally, the presence of buffer zones, influenced by vortices within the convex regions, can introduce variations in solid temperatures. Therefore, while this trend holds true for flames anchoring in relatively consistent positions with similar dynamics, the complex heat transfer and flow dynamics of this non-linear geometry can lead to significant deviations.

Table 5.26: Maximum and average temperature values for the solid domain for LTCC and HTCC simulations

Simulation	avg T_{int} [K]	avg T_{wall} [K]	avg T_s [K]	max T_s [K]	avg $T_{s,\text{max}}$ [K]	max $T_{s,\text{max}}$ [K]
LT8Sp	1262.56	1243.52	1253.30	1257.42	1547.23	1555.09
LT10Sp	1247.02	1228.10	1237.83	1241.50	1577.83	1594.94
LT12Sp	779.47	772.69	776.29	807.26	1494.00	1503.11
HT4Sp	929.01	927.98	928.49	928.49	1223.12	1223.12
HT6Sp	1137.35	1135.41	1136.37	1136.37	1373.50	1373.50
HT8Sp	1162.85	1160.70	1161.76	1161.77	1427.33	1427.34
HT10Sp	1165.87	1163.80	1164.85	1167.57	1465.59	1467.95
HT12Sp	1132.71	1130.80	1131.77	1134.64	1473.87	1475.72

Table 5.27: Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for LTCC and HTCC simulations

Simulation	avg $q''_{x,\text{max}}$ [W/mm ²]	avg $q''_{y,\text{max}}$ [W/mm ²]	avg q_{out} [W/mm ²]	min q_{out} [W]	max q_{out} [W]
LT8Sp	-1.403	0.434	6.88×10^{-3}	6.86×10^{-3}	6.91×10^{-3}
LT10Sp	-1.133	0.477	6.83×10^{-3}	6.81×10^{-3}	6.86×10^{-3}
LT12Sp	-1.284	0.310	4.05×10^{-3}	3.91×10^{-3}	4.22×10^{-3}
HT4Sp	-2.961	0.512	4.87×10^{-3}	4.87×10^{-3}	4.87×10^{-3}
HT6Sp	-3.330	0.636	6.31×10^{-3}	6.31×10^{-3}	6.31×10^{-3}
HT8Sp	-3.602	0.673	6.52×10^{-3}	6.52×10^{-3}	6.52×10^{-3}
HT10Sp	-3.573	0.651	6.58×10^{-3}	6.56×10^{-3}	6.60×10^{-3}
HT12Sp	-3.523	0.665	6.38×10^{-3}	6.36×10^{-3}	6.40×10^{-3}

Additionally, it was noted that the temperature gradient within the solid regions of both Fused Silica (as indicated in Table 5.19) and LTCC micro thrusters was more pronounced compared to that of HTCC. This difference can be attributed to the lower thermal diffusivity and conductivity of these materials (notice the distinctions between temperatures at the solid-fluid interface, denoted as T_{int} and the solid wall in contact with the outside, denoted as T_{wall}). In the solid domain of materials with low thermal diffusivity, the temperature variation ranged from approximately 10 to 20 K, whereas in the case of HTCC, which boasts considerably higher thermal diffusivity, temperature variations were within the range of 1 to 3 K. The temperature gradient exhibited an inverse relationship with thermal conductivity, resulting in micro thrusters constructed from high thermal conductivity materials having inherently smaller temperature gradients.

5.6 Dynamics of steels materials

We will now start exploring the dynamics observed in the simulations using steels, more specifically stainless steels. These steels are a type of alloy composed mainly of iron and chromium, designed to resist rusting and corrosion and contain a minimum of 11% chromium and may include other elements like Nickel, Molybdenum and Titanium to attain specific properties such as improved corrosion resistance, higher tensile strength, and enhanced characteristics like malleability, toughness, ductility, and shear strength [203].

These stainless steels can be classified into five main groups [204]: austenitic, ferritic, martensitic, duplex, and precipitation-hardening. In our research, we have chosen to focus on two high-temperature austenitic⁽²⁷⁾ stainless steels, namely AISI 310 and 430, that can withstand high working temperatures, up to 1150 [°C] and are commonly used in the aerospace sector [205]. To distinguish between the two, despite both falling under the category of low carbon steels⁽²⁸⁾, we will refer to AISI 310 as **High Carbon Stainless Steel** (designated for simulations as CS4Sp to CS12Sp) and AISI 430 as **Low Carbon Stainless Steel** (designated for simulations as SS4Sp to SS12Sp).

Table 5.28: Chemical composition of two stainless steels: AISI 310 [196] and AISI 430 [197]

Stainless Steel	Iron (Fe)	Carbon (C)	Chromium (Cr)	Nickel (Ni)	Manganese (Mn)	Silicon (Si)	Sulfur (S)	Phosphorus (P)
AISI 310 (CS)	Balance	< 0.25%	24.0 ~ 26.0%	19.0 ~ 22.0%	< 2.00%	< 1.50%	< 0.045%	< 0.030%
AISI 430 (SS)	Balance	< 0.12%	16.0 ~ 18.0%	< 0.50%	< 1.00%	< 1.00%	< 0.040%	< 0.030%

The thermal properties of the materials are comparable to HTCC with three distinct differences. In comparison, these steels have a much higher density ($\rho \approx 7700$ [kg/m³]) and a much lower specific heat capacity ($C_p \approx 500$ [J/(kg · K)]). This translates to, respectively, the materials

⁽²⁷⁾Austenitic steels, which contain 16 to 26 percent chromium and up to 35 percent nickel (austenite-stabilizing elements), and are called “austenitic” because of their crystalline structure, of mostly iron and carbon, which is face-centered cubic (FCC) [203].

⁽²⁸⁾Steels with carbon content typically up to 0.25%, typically exhibit good ductility.

having a higher thermal mass, which allows them to store more heat energy for a given temperature change, and an inclination to heat up or cool down more rapidly in response to thermal input [37]. In practical terms, it means that the stainless steels will have more rapid temperature fluctuations in comparison to HTCC. Lastly, the final noteworthy difference is that they experience lower heat loss through radiation at the same surface temperature. This is because $\epsilon_{\text{rad@SS\&CS}} = 0.5$ is less than $\epsilon_{\text{rad@HTCC}} = 0.75$.

When comparing the two stainless steels, given that the ρ and C_p values of the materials are similar, the primary distinguishing factor lies in their thermal conductivity. Specifically, for AISI 310 (CS), the thermal conductivity is $\lambda_{s,\text{CS}} = 16.2 \text{ [W/(m} \cdot \text{K)]}$, whereas for AISI 430 (SS), it is $\lambda_s = 25 \text{ [W/(m} \cdot \text{K)]}$.

5.6.1 Stability map for steels materials

The stability map depicting various velocities and the two materials is provided in the subsequent Figure 5.58.

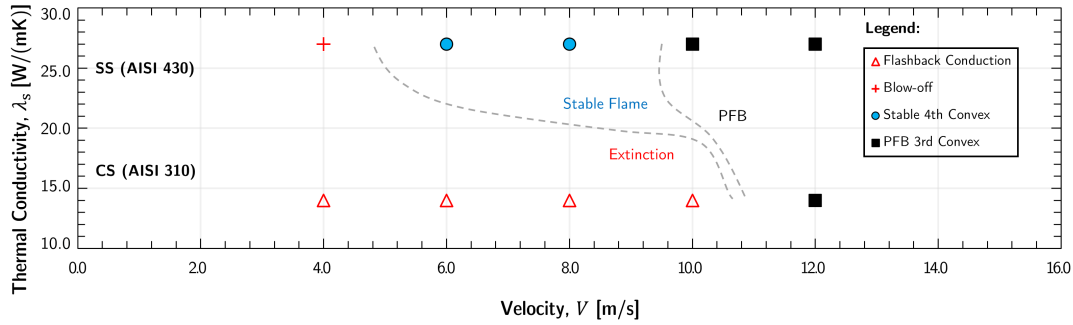


Figure 5.58: Stability map for the various simulations using a spark conducted for the stainless steels.

We observe that for SS, blow-off similar to what happen in LT4Sp happened in SS4Sp, due to not sufficient heat being produced in the initial stages of the spark, causing the walls to be too cold for the flame to anchor. As we increased inlet velocity, stable flames in the 4th were observed for both SS6Sp (Figure 5.59) and SS8Sp (Figure 5.60). Just like in HTCC, and previous observations, for the stable scenarios, higher velocities led to flames with larger flame lengths (ℓ_f).

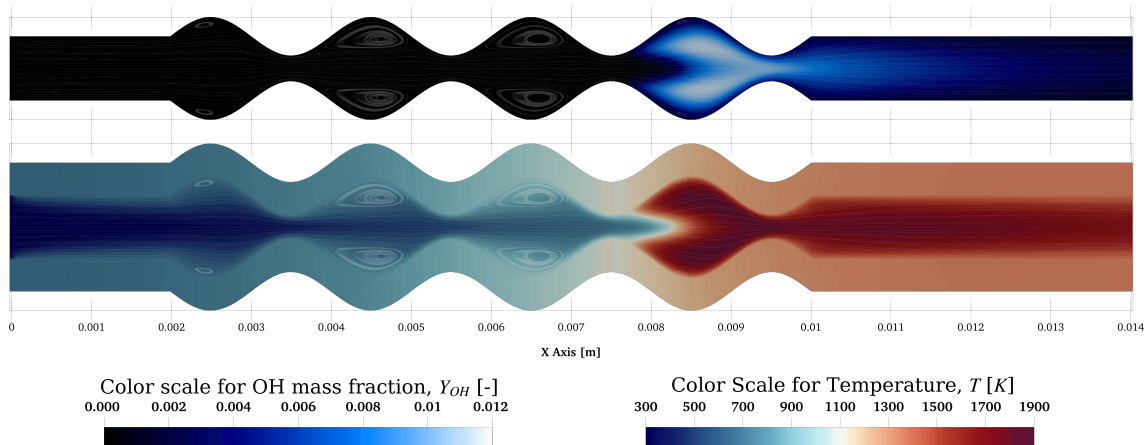


Figure 5.59: Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for SS6Sp (*FluidRegion* and *SolidRegion's*).

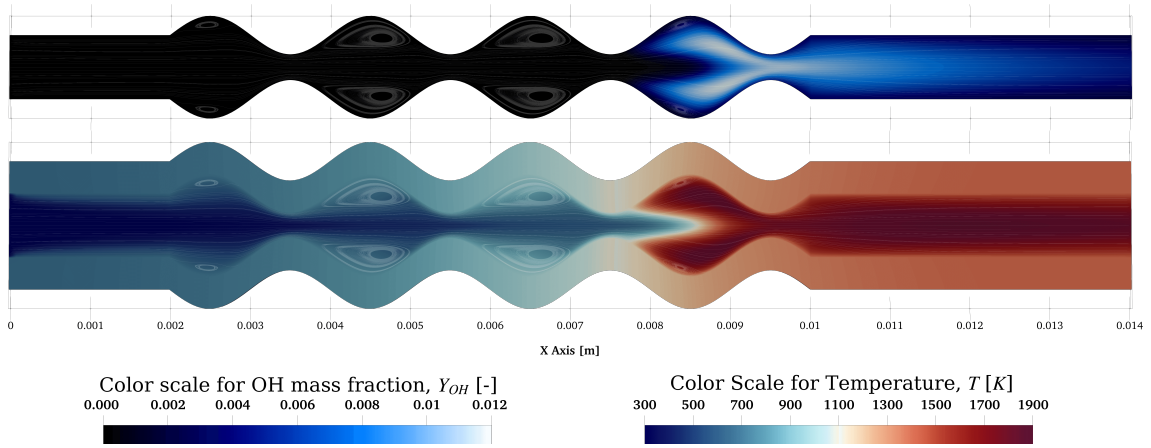


Figure 5.60: Streamlines of the flow field and distribution of the OH mass fraction (top) and temperature (bottom) for SS8Sp (*FluidRegion* and *SolidRegion*'s).

In the context of SS simulations conducted at elevated inlet velocities (specifically, SS10Sp and SS12Sp), and in the single CS simulation where flame extinction did not occur (CS12Sp), the interplay between fluid dynamics and combustion response became increasingly significant. This phenomenon was primarily attributed to the intensified vortices produced by the nonlinear burner geometry, leading to the Pulsatory Flame Burst dynamics. Across all scenarios, PFB manifested within the third convex zone, as illustrated in Figures 5.61 (depicting heat release rate) and 5.62 (H_2 mass fraction). It is evident that the dynamics exhibited striking similarities among these three cases. However, in instances where the inlet velocity (U_{in}) was set at 12, [m/s], akin to previous scenarios, the heat release rate displayed a recirculation pattern, resulting in an elevated H_2 concentration within the flame, as evidenced by the H_2 mass fraction. Furthermore, the flame front assumed a shape resembling that of a heart, in contrast to the more V-shaped configuration observed at lower U_{in} values.

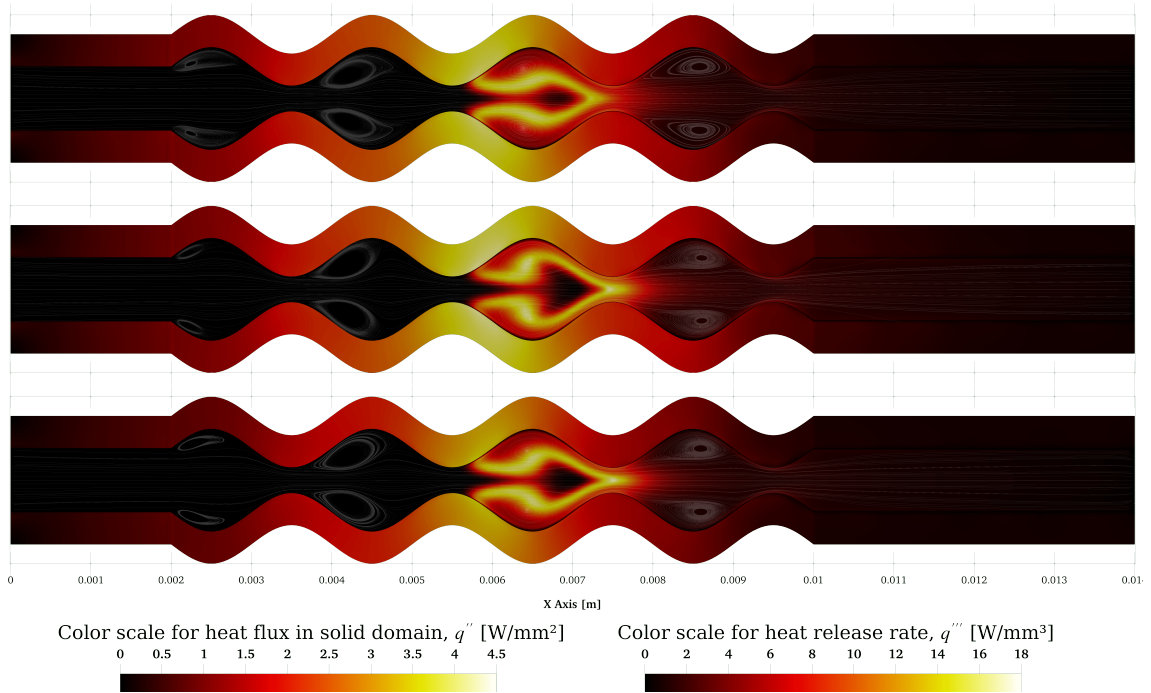


Figure 5.61: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for SS10Sp (top), SS12Sp (middle) and CS12Sp (bottom).

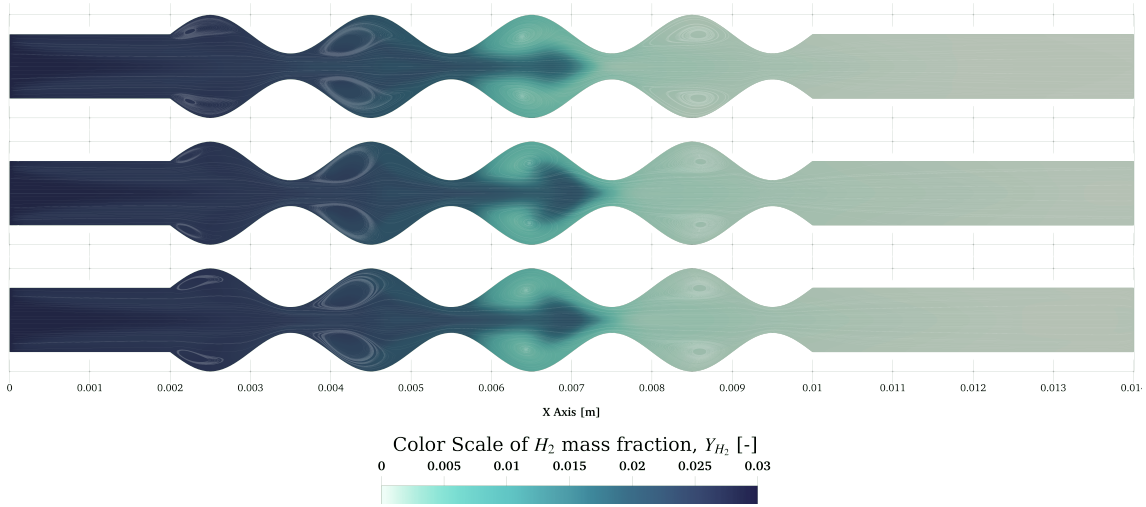


Figure 5.62: Streamlines of the flow field and distribution of the H_2 mass fraction for SS10Sp (top), SS12Sp (middle) and CS12Sp (bottom).

5.6.2 Backward Ignition Resurgence

A novel phenomenon was observed in simulations ranging from CS4Sp to CS10Sp. In all of these simulations, the flame undergoes a Pulsatory Flame Burst dynamic within the second convex zone. Throughout these scenarios, the flame gradually consolidates within this region, exhibiting a diminishing tPFB dynamic, with oscillations decreasing in magnitude over time. This suggests a trend toward achieving a stable flame state in all instances. Nevertheless, before the flame can complete its stabilization within the second convex zone, a new flame ignites within the preceding convex zone. This is attributed to an excessive retrograde flow of energy within the microchannel walls, driven by the backward heat conduction, which is substantial enough to initiate the ignition of the new flame. We have termed this phenomenon “Backward Ignition Resurgence” (BIR) because it entails the reignition of a new flame in the microchannel, that occurs behind the flame front, after a prolonged absence of combustion activity in the area.

In Figure 5.63 we show the evolution of q''_{avg} and T_{avg} over time for CS8Sp, to illustrate what happens during BIR to these average values of heat release rate and temperature during BIR.

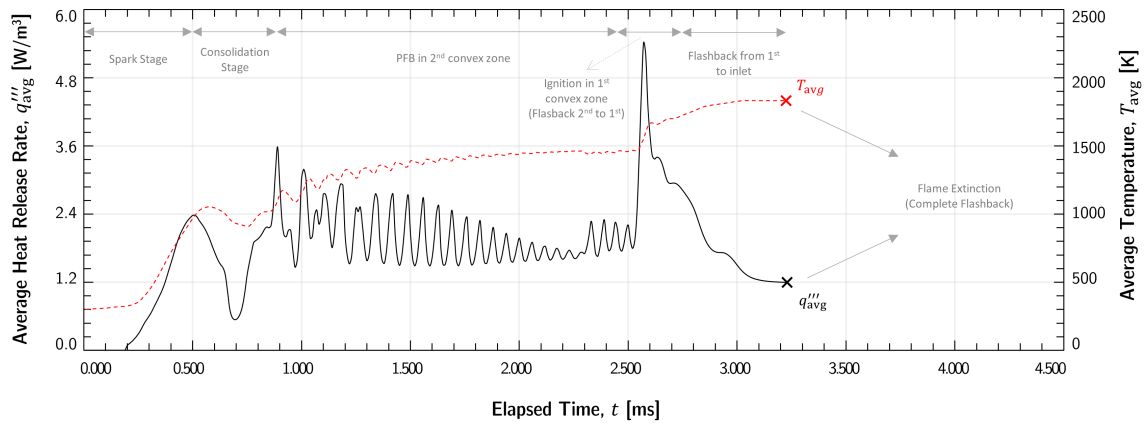


Figure 5.63: Temporal evolution of the average values of heat release rate and temperature for CS8Sp during $t = [0; 4.500]$ [s].

We note that at the instant of the new flame ignition, there is a distinct rise in q''' due to the temporary formation of two flame fronts. Subsequently, the flame front within the second convex zone merges with the newly ignited flame in the first convex zone. Afterwards, the flame continues its progression towards the inlet, ultimately leading to self-extinguishment due to flashback. This transition is visually depicted in Figure 5.64.

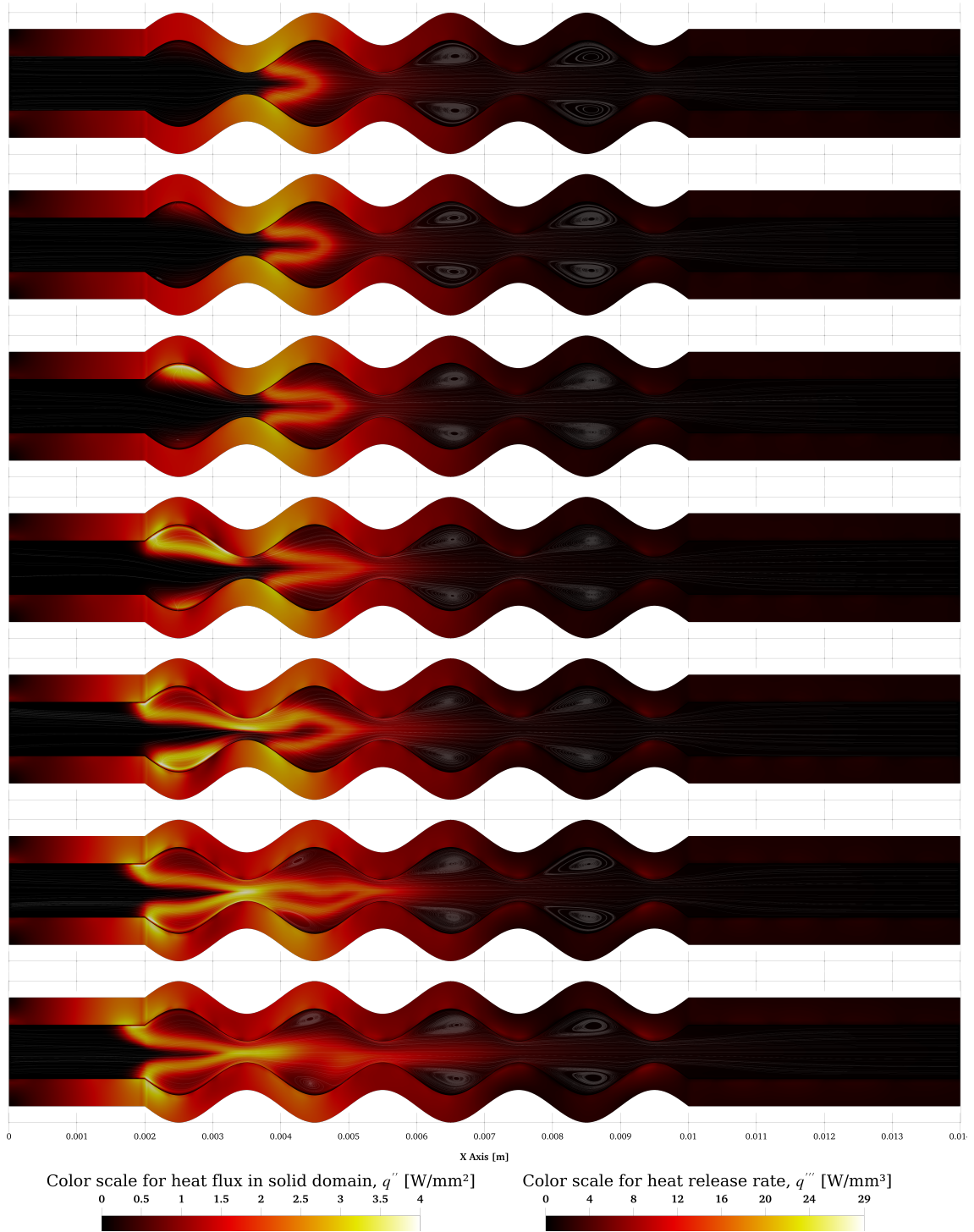


Figure 5.64: Streamlines of the flow field and distribution of heat release rate for fluidRegion and the heat flux due to conduction for solidRegion's for CS8Sp, during Backward Ignition Resurgence, in 10 [μ s] intervals.

It becomes increasingly apparent that, throughout the simulation, the convective heat flux from the microchannel walls into the first convex zone (filled with unburned mixture) continues to rise as the wall temperature escalates. With this intensifying heat transfer, the temperatures at the interface between the solid and fluid (notably, both maintained at the same temperature, represented as $T_{\text{int},s}$ and $T_{\text{int},f}$ respectively) eventually reach a critical threshold. At this point, these temperatures exceed the autoignition temperature of H_2 , prompting the mixture to initiate combustion in close proximity to the wall. Once ignited, this combustion rapidly propagates throughout the remaining convex region.

To better understand this evolution, we documented the conduction-induced heat flux and temperature data at the solid-fluid interface throughout the simulation. This data was collected from a specific point within the initial convex zone, situated approximately at $x \approx 3.0$, [mm].

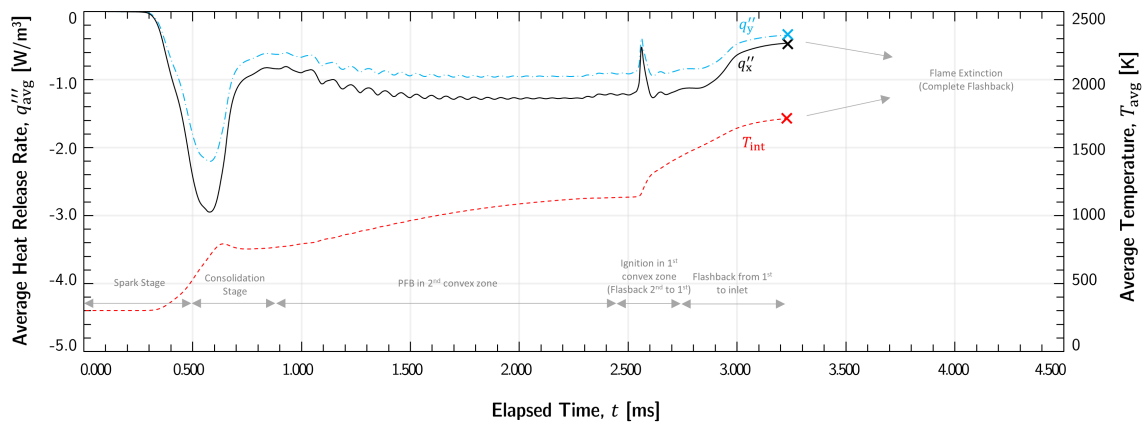


Figure 5.65: Temporal evolution of the average values of heat release rate and temperature for CS8Sp, in the solid-fluid interface on the first convex zone at $x \approx 3.0$ [mm], during $t = [0, 4.500]$ [s].

Until the occurrence of BIR, it is evident that there is a consistent and noticeable rise in the temperature at the solid-fluid interface, denoted as T_{int} , caused by the retrograde flow of energy through the walls, which is progressively heating the solid walls of the microchannel upstream from the flame front. The temperature eventually reaches approximately 1140 [K], considerably surpassing the Auto-Ignition Temperature (AIT) of both H_2 and air, as discussed in Section 2.1.5. At this point, the thermal energy in this region becomes sufficient to auto-ignite the mixture autonomously, without requiring a spark or involvement from the flame front. Consequently, a new flame initiates propagation within the first convex zone, resulting in a sudden elevation of T_{int} and a temporary reduction in $q''_{x,y}$. This reduction occurs because, as heat is generated within this zone due to combustion, there is a transient reversal of the heat flux.

A final question remains: WHY DOES THIS PHENOMENON OCCUR WITH CS, WHICH POSSESSES A THERMAL DIFFUSIVITY OF APPROXIMATELY $\alpha_T \approx 4.10$ [mm^2/s], BUT NOT WITH SS, WHICH HAS A HIGHER THERMAL DIFFUSIVITY OF $\alpha_T \approx 6.91$ [mm^2/s]? While it is true that the retrograde flow of energy through conduction is more pronounced in SS, which can be seen in the materials overview in Section 5.6.3, this increased thermal diffusivity also results in a more dispersed heat distribution within the solid walls and greater heat loss to the surroundings. Consequently, since the temperatures at the solid wall remain lower, they never reach a point where T_{int} significantly exceeds the AIT, preventing the occurrence of Backward Ignition Resurgence in SS.

5.6.3 Overview of steels materials

In the subsequent tables, in line with the methodology employed in this chapter, we offer a thorough overview of the simulations from SS6Sp to SS12Sp and SS12Sp. Much of the analysis conducted in Subsection 5.5.3 remains applicable in this context. We have observed that the trends previously seen remained constant, where in this case, the material SS is the one the highest thermal diffusivity, and CS, conversely, the lowest thermal diffusivity.

Within the CS scenario, both fluid and wall temperatures registered are notably higher. In contrast, akin to the comparison between HTCC and LTCC, the heightened thermal conductivity of SS facilitated a faster ignition of the flame. Consequently, each cycle involved the consumption of more H_2 , resulting in elevated heat release rates. Similar to the previous observations, materials characterized by higher thermal diffusivities and conductivities exhibited lower amplitude overall.

Table 5.29: Maximum and average temperature values for the fluid domain for the Stainless Steels simulations

Simulation	avg T_{avg} [K]	min T_{avg} [K]	max T_{avg} [K]	avg T_{max} [K]	min T_{max} [K]	max T_{max} [K]
SS6Sp	984.33	984.33	984.33	1882.89	1882.89	1882.89
SS8Sp	964.57	964.57	964.57	1878.45	1878.45	1878.45
SS10Sp	1200.10	1153.92	1224.04	1951.19	1913.96	1973.36
SS12Sp	1153.11	1090.68	1198.30	1950.26	1933.64	1965.15
CS12Sp	1165.02	1121.59	1193.32	1971.75	1955.52	1990.50

Table 5.30: Maximum and average heat release rate values for the fluid domain for the Stainless Steels simulations

Simulation	avg q_{tot} [W]	min q_{tot} [W]	max q_{tot} [W]	avg q'''_{avg} [W/mm ³]	max q'''_{avg} [W/mm ³]	avg q'''_{max} [W/mm ³]	max q'''_{max} [W/mm ³]
SS6Sp	0.518	0.518	0.518	1.094	1.094	18.380	18.380
SS8Sp	0.741	0.741	0.741	1.526	1.526	16.776	16.776
SS10Sp	0.995	0.823	1.269	2.222	3.055	16.788	17.970
SS12Sp	1.192	0.907	1.648	2.596	3.942	17.110	22.078
CS12Sp	1.028	0.810	1.326	2.281	3.146	16.633	17.584

Table 5.31: Maximum and average temperature values for the solid domain for the Stainless Steels simulations

Simulation	avg T_{int} [K]	avg T_{wall} [K]	avg T_s [K]	max T_s [K]	avg $T_{s,max}$ [K]	max $T_{s,max}$ [K]
SS6Sp	1005.23	1004.43	1004.82	1004.82	1359.87	1359.87
SS8Sp	1007.93	1007.12	1007.52	1007.52	1418.20	1418.20
SS10Sp	1225.24	1223.82	1224.53	1239.01	1525.47	1534.48
SS12Sp	1196.48	1195.15	1195.82	1211.96	1534.63	1544.70
CS12Sp	1202.34	1200.25	1201.32	1202.19	1565.03	1566.50

Table 5.32: Maximum and average values for heat flux within the solid domain and total heat dissipated to the surroundings for the Stainless Steels simulations

Simulation	avg $q''_{x,\max}$ [W/mm ²]	avg $q''_{y,\max}$ [W/mm ²]	avg q_{out} [W/mm ²]	min q_{out} [W]	max q_{out} [W]
SS6Sp	3.762	0.590	5.49×10^{-3}	5.49×10^{-3}	5.49×10^{-3}
SS8Sp	4.008	0.631	5.56×10^{-3}	5.56×10^{-3}	5.56×10^{-3}
SS10Sp	4.110	0.618	7.05×10^{-3}	6.90×10^{-3}	7.15×10^{-3}
SS12Sp	4.134	0.631	6.86×10^{-3}	6.70×10^{-3}	6.98×10^{-3}
CS12Sp	3.566	0.569	6.87×10^{-3}	6.81×10^{-3}	6.89×10^{-3}

Table 5.33: Signal spectral analysis results for amplitude values, A^{var} , for the Stainless Steels simulations that resulted in PFB

Simulation	f [Hz]	$A^{T_{\text{avg}}}$ [K]	$A^{T_{\text{max}}}$ [K]	$A^{q_{\text{tot}}}$ [W]	$A^{q''_{\text{avg}}}$ [W/mm ³]	$A^{q''_{\text{max}}}$ [W/mm ³]
SS10Sp	18750	47.71	53.11	0.41820	1.298	1.915
SS12Sp	17187	87.59	29.02	0.67600	2.014	5.383
CS12Sp	16406	67.53	33.91	0.5141	1.509	1.5962

Table 5.34: Signal spectral analysis results for scaled amplitude values, $A_{\sim}^{\text{var}}$, for the Stainless Steels simulations that resulted in PFB

Simulation	f [Hz]	$A_{\sim}^{T_{\text{avg}}}$ [—]	$A_{\sim}^{T_{\text{max}}}$ [—]	$A_{\sim}^{q_{\text{tot}}}$ [—]	$A_{\sim}^{q''_{\text{avg}}}$ [—]	$A_{\sim}^{q''_{\text{max}}}$ [—]
SS10Sp	18750	4.0%	2.7%	42.0%	58.4%	11.4%
SS12Sp	17187	7.60%	1.49%	56.7%	77.6%	31.5%
CS12Sp	16406	5.80%	1.72%	50.0%	66.1%	9.6%

5.7 Dynamics of conductor materials

We now arrive at the last group of materials, which are known for their excellent heat-conducting properties. Within this category, we will analyze three distinct materials commonly employed in aerospace applications:

- i) Pure Silicon (Si): Although silicon is generally not utilized in its purest form, we will, for the sake of simplicity, explore the properties of pure silicon. It boasts outstanding electrical conductivity, thermal stability, and dielectric characteristics. Additionally, it possesses a noteworthy thermal conductivity, with $\lambda_s = 130$ [W/(m · K)];
- ii) Generic Aluminium alloy (Al): renowned for their exceptional combination of lightweight properties and high strength, coupled with excellent heat conductivity, characterized by a thermal conductivity coefficient of $\lambda_s = 200$ [W/(m · K)]. However, a primary limitation often associated with these alloys is their relatively lower tolerance for extremely high temperatures, in comparison to other materials studied so far;

- iii) Copper-Tungsten Alloy (CT): these types of alloys find extensive application in aerospace, particularly in conjunction with tungsten and molybdenum alloys, where they play a crucial role in enhancing in-space propulsion performance. Although they are very dense, they exhibit exceptional heat resistance and outstanding thermal conductivity, with a thermal conductivity coefficient of $\lambda_s = 250 \text{ [W/(m} \cdot \text{K)]}$.

The materials remarkably high thermal conductivity gives rise to exceptionally high thermal diffusivity values. By way of comparison, among all the materials investigated so far, Stainless Steel (SS) stood out as having the highest thermal diffusivity, approximately $\alpha_{T,SS} \approx 6.91 \text{ [m}^2\text{/s]}$. However, the values seen in the excellent conductor materials values significantly surpass those found before, with Silicon exhibiting a thermal diffusivity of $\alpha_{T,Si} \approx 80.0 \text{ [m}^2\text{/s]}$, Aluminium at $\alpha_{T,Al} \approx 84.6 \text{ [m}^2\text{/s]}$, and Copper-Tungsten at $\alpha_{T,CT} \approx 106 \text{ [m}^2\text{/s]}$.

5.7.1 Stability map for thermal conductor materials

The stability map depicting various velocities and the three materials is provided in the subsequent Figure 5.66.

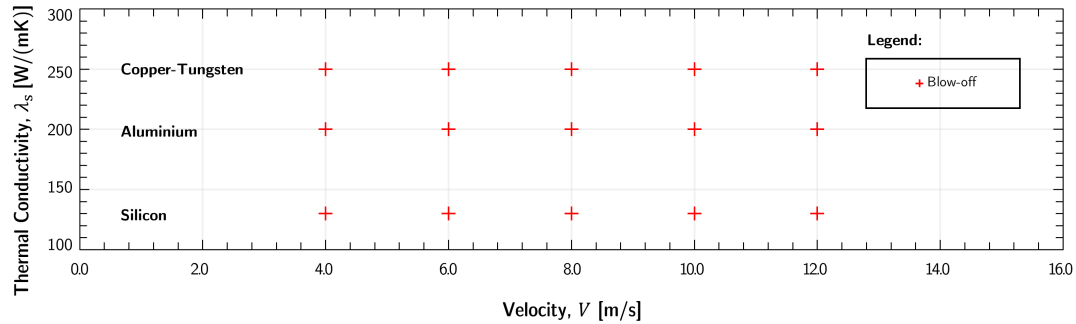


Figure 5.66: Stability map for the various simulations using a spark conducted with conductor materials.

We observe a consistent pattern in all simulations, regardless of the material or inlet velocity: there is excessive heat conduction, and the region near the flame lacks sufficient heat retention, ultimately leading to blow-off. This outcome aligns with theoretical expectations, primarily due to the rapid dissipation of heat on the walls. Consequently, the walls never reach the necessary temperature to support flame anchoring. This stands in contrast to the observations discussed in Section 5.5.2, but the end result remains the same: a lack of thermal energy within the microchannel to sustain the chemical reaction. Similar to the conditions observed in HTCC, the small temperature gradient (∇T_s) within the solid keeps the fluid temperature (T_f) at a level that can sustain the combustion reaction. But in contrast to HTCC, these materials excel in heat conduction, displaying significantly higher efficiency in distributing the heat thorough the microchannel. Consequently, the temperature at the wall near the flame never reaches a point where the flame can anchor itself. This ultimately leads to the complete extinguishment of the flame (full blow-off).

In summary, even under these simulations using high Fo values (pseudo-stationary approach assumes $\tau_s \approx \tau_c$), and with a spark duration of 0.5 milliseconds, these materials with very high thermal conductivity encounter challenges in preventing flame self-extinguishment within the context

of the complex wavy non-linear geometries. To ascertain whether stable flame or PFB dynamics can be achieved with sufficiently high wall temperatures, we conducted a new set of simulations, which will be discussed in the subsequent subsection.

5.7.2 Exploring the behavior of conductive materials with initial imposed temperature profiles

In this latest set of simulations, we incorporated an additional factor alongside the ignition spark. Specifically, we introduced a linear temperature profile ranging from 300 [K] at the entrance of the chamber to approximately 1300 [K], extending over a distance of approximately 5 [mm]. Furthermore, beyond the 5 [mm] mark and leading up to the outlet of the microchannel, the walls were maintained at a constant temperature of 1300 [K]. This temperature profile was derived from experimental observations of stable flames within microchannels, as detailed in the research conducted by Tsuboi et al. [110]. Also, this particular temperature profile has been widely accepted and employed in various research endeavors [88, 106, 110, 113, 206].

The temperature profile described was applied solely during the initial time-step, denoted as $t = 0$ [ms]. This operation was carried out through the utilization of an expression termed *Timposed*, found within the *funkySetField* Foam file (referenced in Listing 5.2), which modifies the T field. To execute this, 2 lines of code need to be included within the initialization bash shell script (as illustrated in Appendix D), with a snippet showcased in Listing 5.3.

```

1 FoamFile
2 {
3     version      2.0;
4     format       ascii;
5     class        dictionary;
6     object       funkySetFields;
7 }
8 // * * * * *
9
10 expressions
11 (
12     Timposed
13     {
14         field      T;
15         dimensions [0 0 0 1 0 0 0];
16         variables (
17     ↪ "xp=pos().x;minX=5.e-3;maxX=8.e-3;ttt=300+xp*(1600)/(maxX-0.);" );
18         expression "(xp > minX) ? 1300 : ttt";
19         keepPatches 1; //keep the boundary conditions that were set before
20     }
21 );

```

Code Listing 5.2: Snippet from the *funkySetFields* FoamFile for imposing wall temperatures in a microchannel during the first time-step using C++

```

1 funkySetFields -time 0 -region solidRegion1
2 funkySetFields -time 0 -region solidRegion2

```

Code Listing 5.3: Snippet of the Initialization .sh Bash shell script (Unix) used to change the temperature field of the walls during the first time-step.

Considering this, during the first time-step of the simulation, the temperature distribution of the microchannel is depicted in Figure 5.67.

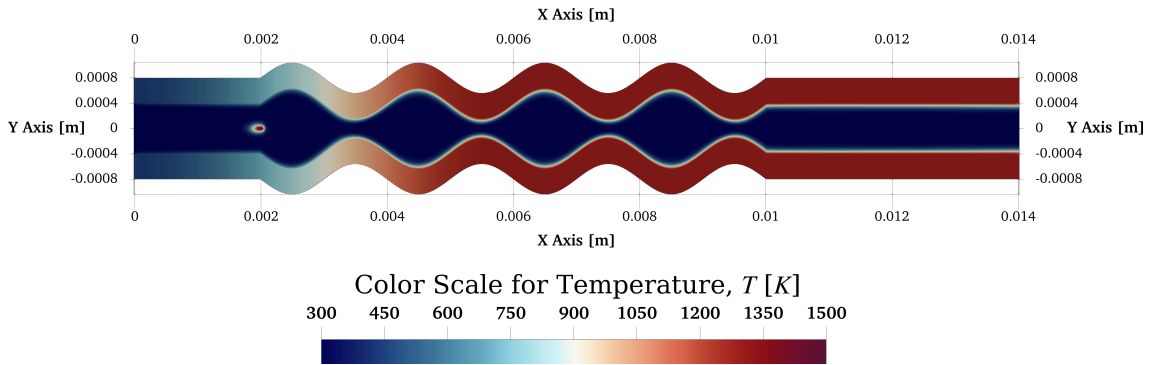


Figure 5.67: Visual representation of the initial temperature imposition on microchannel walls alongside the spark inside the microchannel.

A total of 15 additional simulations were conducted with inlet velocities ranging from $U_{in} = 4$ [m/s] to $U_{in} = 12$ [m/s] for the three different materials: Si4Im through Si12Im, Al4Im through Al12Im, and CT4Im through CT12Im. The stability map using initial imposed temperatures profiles and depicting the various velocities and the three materials is provided in the subsequent Figure 5.68.

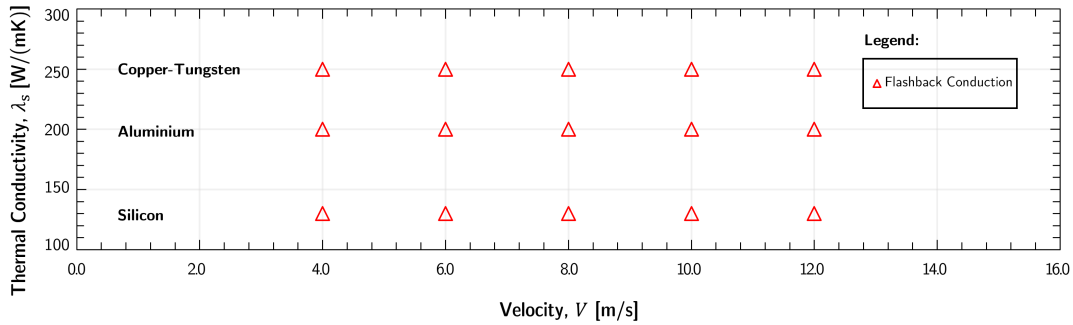


Figure 5.68: Stability map for the various simulations using a spark and imposed initial temperatures conducted with conductor materials.

Regardless of the selected material and velocity, it was consistently observed that in all simulations, there is a notable retrograde flow of energy within the microchannel walls, primarily driven by backward heat conduction. This phenomenon leads to the occurrence of Backward Ignition Resurgence (flashback) in all simulated scenarios. Consequently, it becomes evident that one of the primary challenges discussed in Subsection 2.3.2 related to micropropulsion becomes more prominent, especially in materials with extremely high thermal diffusivities. As the combustion chamber size decreases into the micro-scale range, the surface-to-volume ratio (S/V) experiences a rapid increase, significantly amplifying the heat loss ratio within the combustor. Therefore, we also establish that in the case of wavy microchannels, this challenge persists, making it challenging to anchor the flame, mainly due to the higher heat flux in the walls.

5.8 Materials overview

In order to conduct a comprehensive analysis of the obtained results, we present in Figures 5.69 and 5.70 the stability map for all performed simulations, as a function of the material's thermal conductivity, λ_s , and thermal diffusivity of the material, α_T , respectively.

As observed thus far, it becomes apparent that when considering most of the simulations with low λ_s resulting in flame extinction, the primary factor is the microchannel geometry. Considering this aspect, it suggests that lower thermal conductivity and diffusivity aid in preventing flame extinction. Conversely, when heat diffusivity/conductivity values are high, the issues of blow-off and flashback become more pronounced. Additionally, we noted that in the case of CS, despite its lower thermal diffusivity compared to HTCC and SS, the higher solid temperatures favor Backward Ignition Resurgence. This, as seen previously, causes a significant retrograde flow of energy to the convex zones ahead of the flame front, leading to reignition in that zone and causing the flame front to move in an upflow direction within the microchannel (flashback).

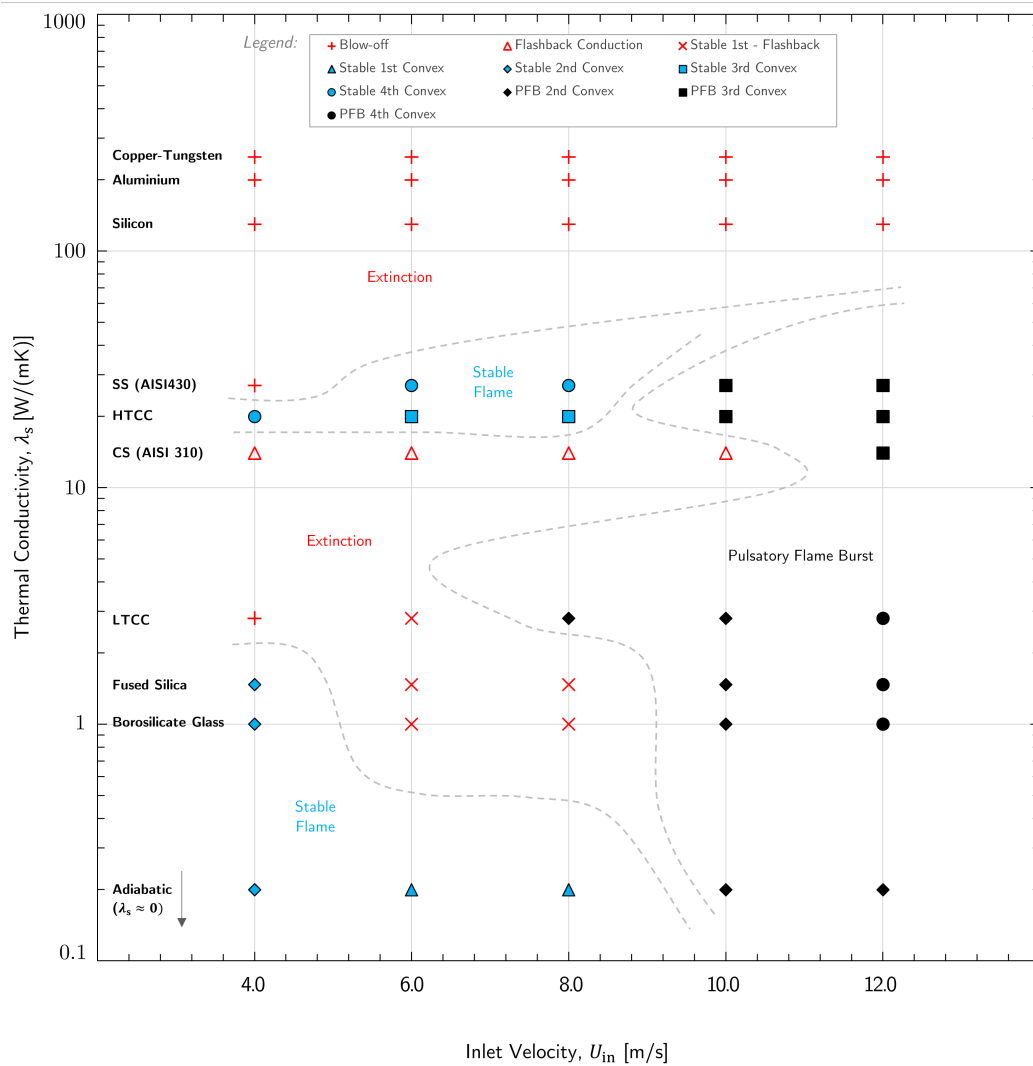


Figure 5.69: Stability map for the various simulations using a spark in function of the thermal conductivity of the materials.

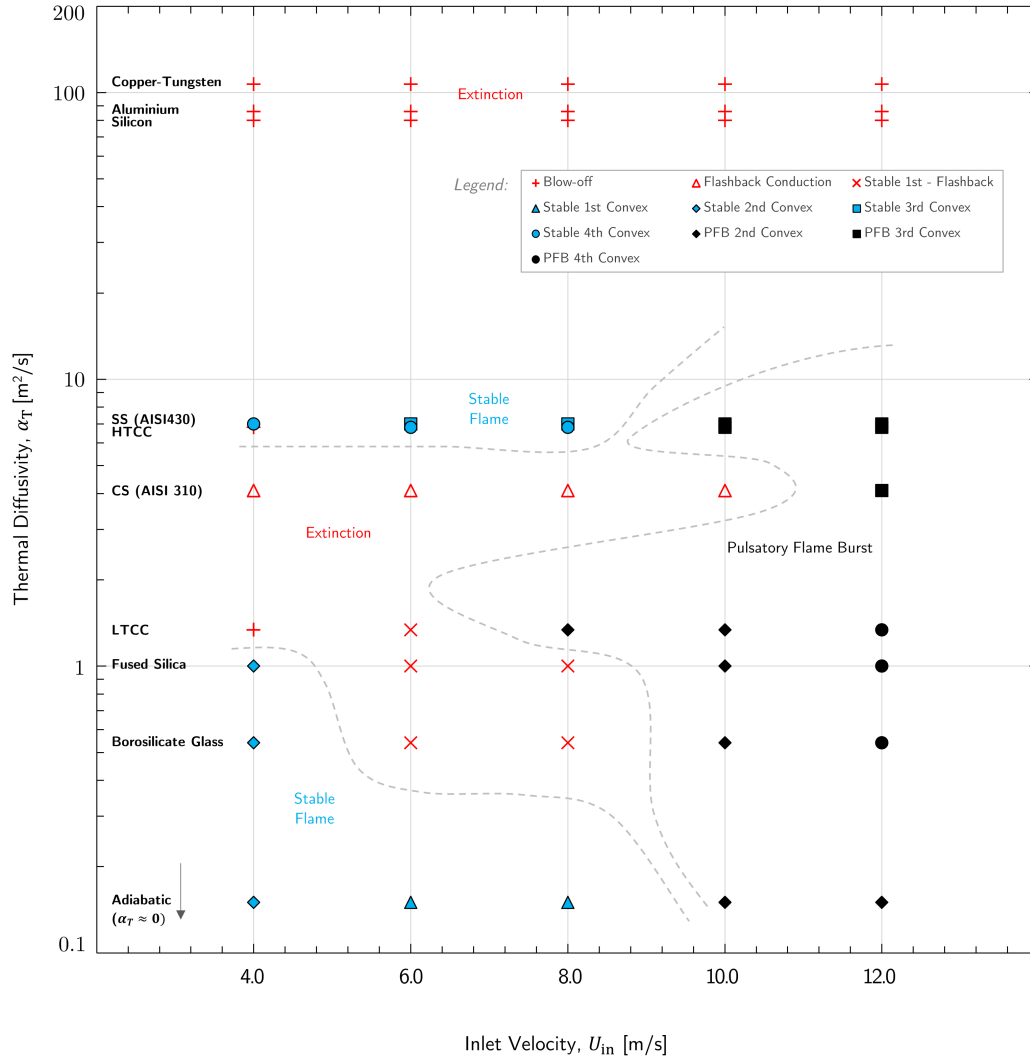


Figure 5.70: Stability map for the various simulations using a spark in function of the thermal diffusivity of the materials.

A thorough and comprehensive analysis has already been conducted throughout this chapter regarding the effect of heat loss and wall conduction on combustion dynamics and flow within the microchannel. Therefore, to prevent making this chapter overly cumbersome and repeating information, we will focus our overview analysis on three variables: the total heat release rate (average and maximum) within the microchannel, denoted as q_{tot} , the maximum temperature within the microchannel, denoted as T_{max} , and the maximum wall temperature, denoted as $T_{\text{s,max}}$.

Figure 5.71 illustrates the variations in maximum temperature within both the fluid (represented by the dotted lines and transparent colors) and solid phases (represented by solid lines and non-transparent colors) across different materials and velocities. It is essential to recognize the inherent complexity of the dynamics in this context, making it challenging to attribute changes solely to a single variable. As demonstrated earlier, the use of varying velocities and thermal diffusivities introduces a multitude of alterations, contributing to this complexity. Nonetheless, it is apparent that while temperatures generally exhibit a decrease as we introduce more heat loss into the system, the alterations in maximum values are not notably significant.

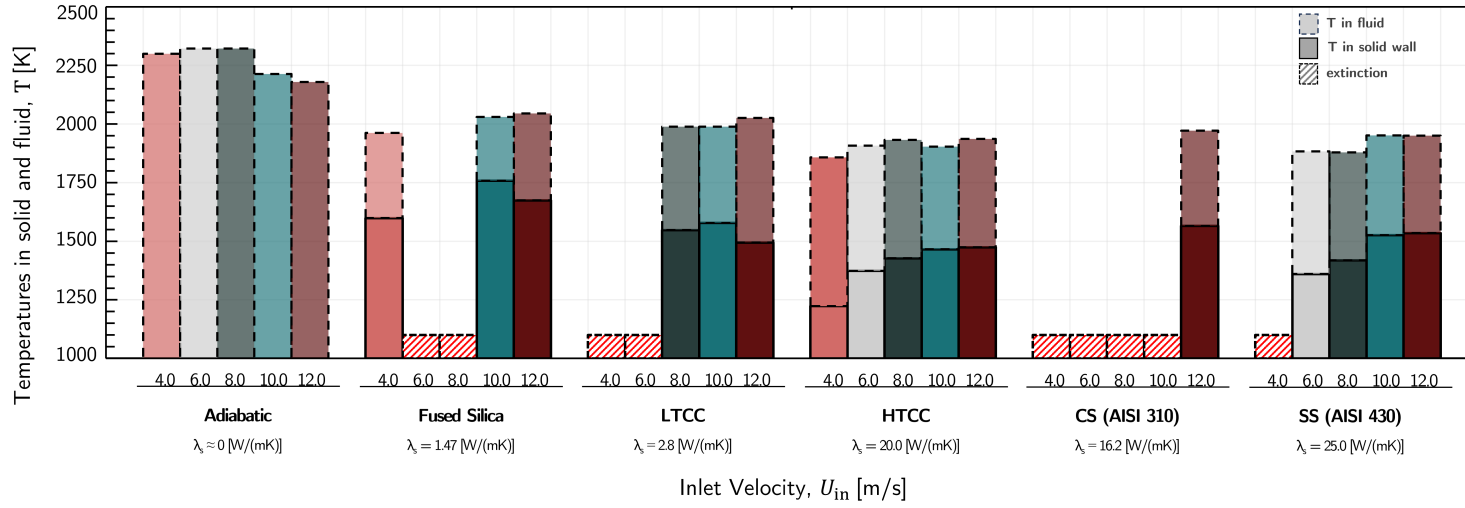


Figure 5.71: Temperatures in the solid and fluid domain for the different materials and simulations.

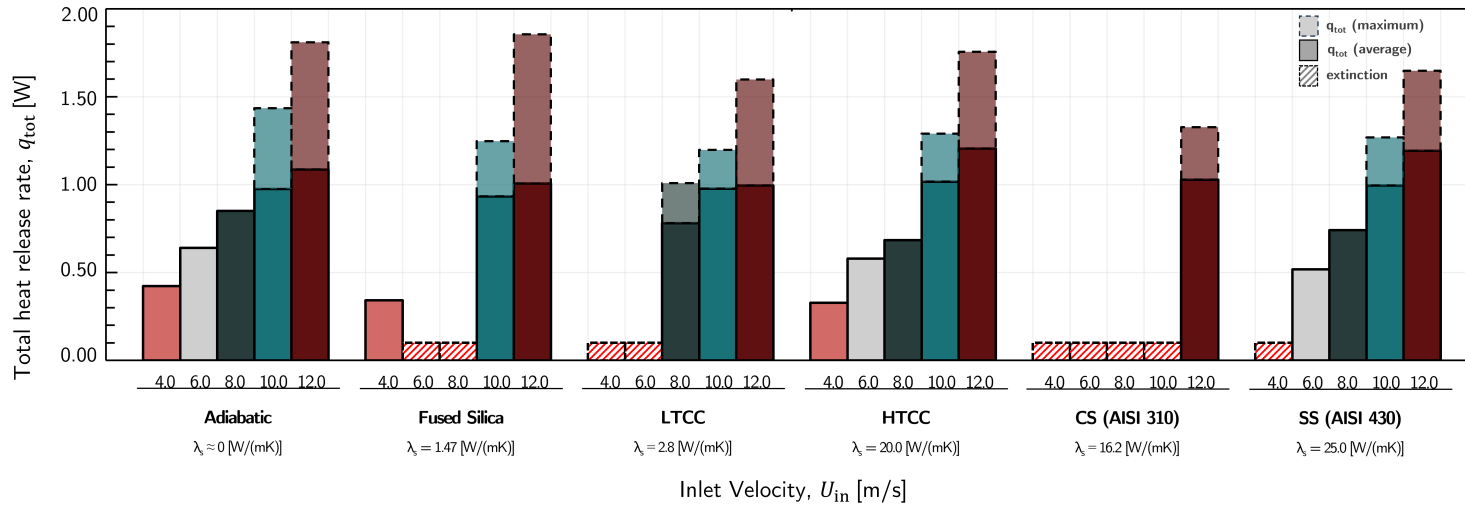


Figure 5.72: Maximum and average heat release rate for the different materials and simulations.

Figure 5.72 depicts the variations in the total heat release rate for the different simulations conducted. It is well understood that regions with vortices induced by velocity play a pivotal role in facilitating the retrograde flow of energy, where energy moves upstream, ultimately triggering the ignition of new flames, which is why the values increase with U_{in} . What becomes evident here is that, as we introduce heat conduction in the walls, we observe a corresponding increase in the heat flux due to conduction in the solid, especially in materials with higher thermal conductivity. Consequently, this amplifies the retrograde flow of energy, resulting in faster ignitions, greater consumption of H_2 , and consequently, higher heat release rates from combustion.

5.9 Micropropulsion performance analysis

As explained in Section 2.4.2, one of the most efficient ways to measure and analyze propulsion capability is by using the specific impulse indicator, I_{sp} . This indicator, as previously demonstrated in Equation (2.39), is calculated as the ratio of the total impulse (the integral of the momentum force, $\int F dt$) to the total mass of propellant consumed (the integral of mass flow rate, $\int \dot{m} dt$). By dividing these two quantities and multiplying by $1/g$, we are essentially comparing the momentum produced by the engine to the mass of propellant it uses while adjusting for Earth's gravity.

In simpler terms, we are assessing the efficiency of the micropropulsion system in converting its propellants into thrust. Consequently, higher values of I_{sp} indicate greater efficiency for the MPS. This means that it can generate more thrust using a given amount of propellant (or can sustain operation for a longer duration with the same quantity of propellant).

To obtain the values of I_{sp} for each simulation, we utilized the simplified equation show in Subsection 2.4.2.1 (Equation 2.40). Knowing that $\phi = 1.0$ for all simulations and that U_{in} is known, we only need to determine the average velocity (or mean velocity) at the system's outlet, denoted as U_{out} . Mathematically, this value is described by:

$$U_{out} = \frac{1}{A_{out}} \times \int ||\mathbf{v}_{out}|| dA_{out} \quad (5.3)$$

in other words, it's the integral of the magnitude of the velocity vector profile over the entire cross-sectional area (dA_{out}) at the outlet, divided by the cross-sectional outlet area.

This was accomplished using *ParaView*. Initially, we performed the integration of $||\mathbf{v}_{out}||$ across the cross-sectional outlet area using the *IntegrateVariables* filter. Subsequently, we divided this result by the microchannel outlet section's area, which, in this case, measures $4 \times 10^{-8} \text{ m}^2$. This yielded the mean velocity at the outlet, denoted as U_{out} . Finally, by employing Equation (2.40), we calculated the specific impulse.

In Figure 5.73 we show the outcomes obtained for all simulations conducted with various materials, and we include the results from Macedo [112] for adiabatic simulations using $\phi = 0.7$, $\phi = 1.1$ and $\phi = 1.3$.

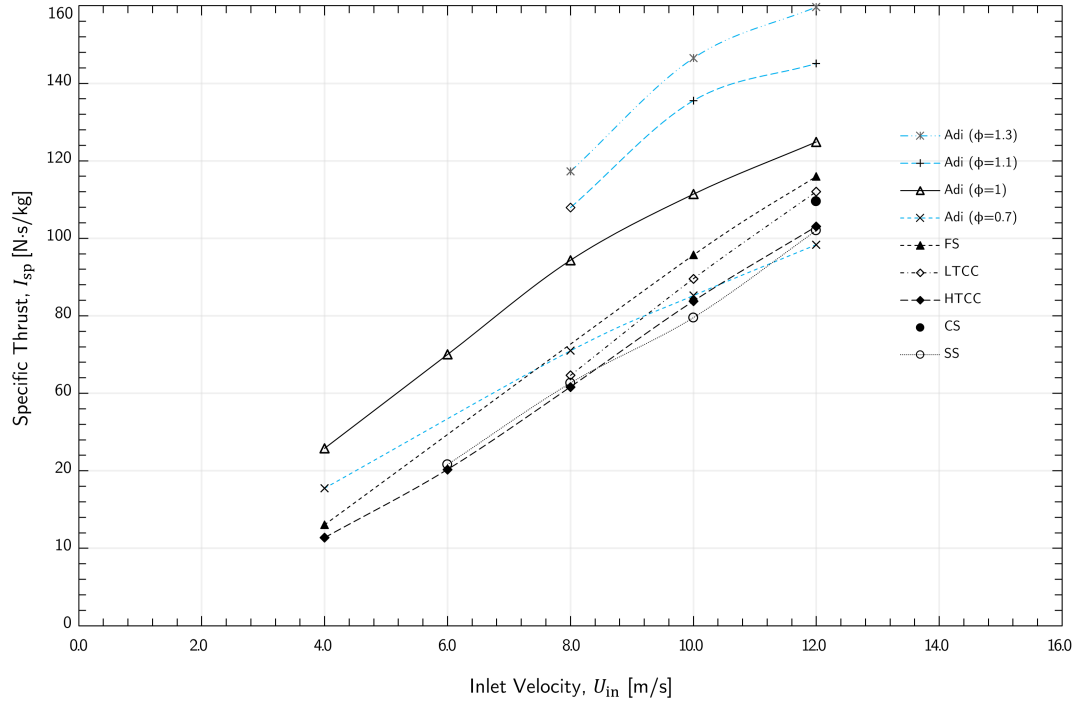


Figure 5.73: Specific thrust *versus* the inlet velocity for different materials.

In general, it is readily apparent that there is a clear influence of the inlet velocity on specific impulses. First, we observe that for the same material (blue lines), it is advantageous from a specific impulse standpoint to increase the equivalence ratio. This is because, if achievable, it results in significant enhancements of these values, as can be seen in the case of the adiabatic material, due to an increase in fuel flow rate. In the context of different materials, we observe a decreasing trend in the values as we increase the thermal diffusivity of the material. This illustrates that heat loss has a direct impact on the propulsion capabilities of the microchannel, with materials capable of retaining more thermal energy resulting in higher specific impulses. Nevertheless, it is important to note that velocity remains the variable with the most direct influence on the outcomes.

In Figure 5.74, we depict the outcomes obtained from simulations conducted with various materials using now a bar graph. Additionally, in Figure 5.75, we showcase the results for adiabatic regime but with different equivalence ratios. This extends the investigation initiated by Macedo [112], and includes results for $\phi = 1.0$. Since we also include the maximum values, we are able to see that PFB phenomenon leads to significantly higher specific impulse values, and as the inlet velocity increases, the gap between average and maximum values widens. This demonstrates that the oscillatory nature of the PFB is highly advantageous for its applicability in micro-propulsion systems. Another noteworthy observation is that for the majority of materials, there is a significant decrease in the maximum values of specific impulse as we increase the thermal conductivity/diffusivity, which can be undesirable in terms of efficiency and overall performance.

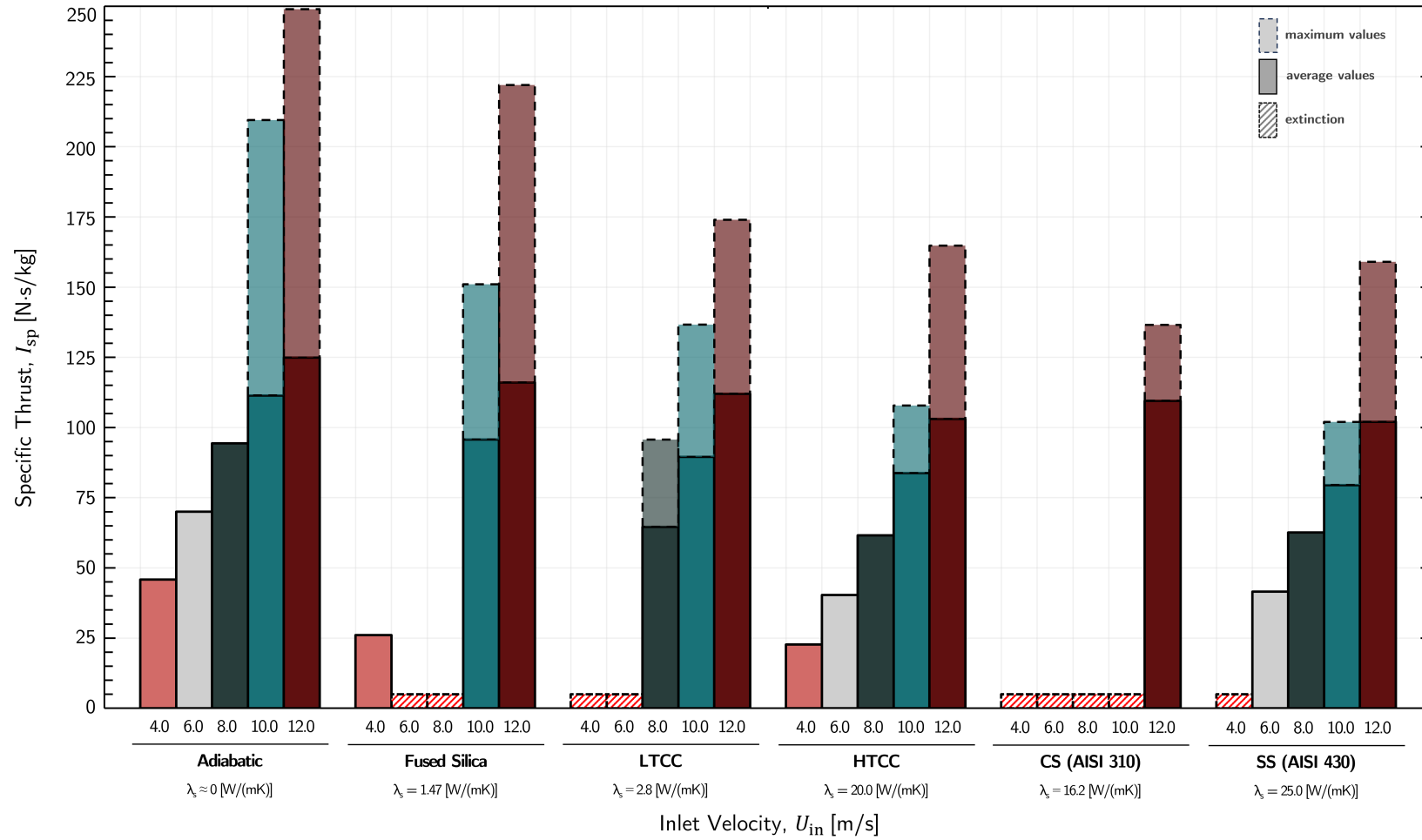


Figure 5.74: Average and maximum values of the specific thrust for different materials and simulations.

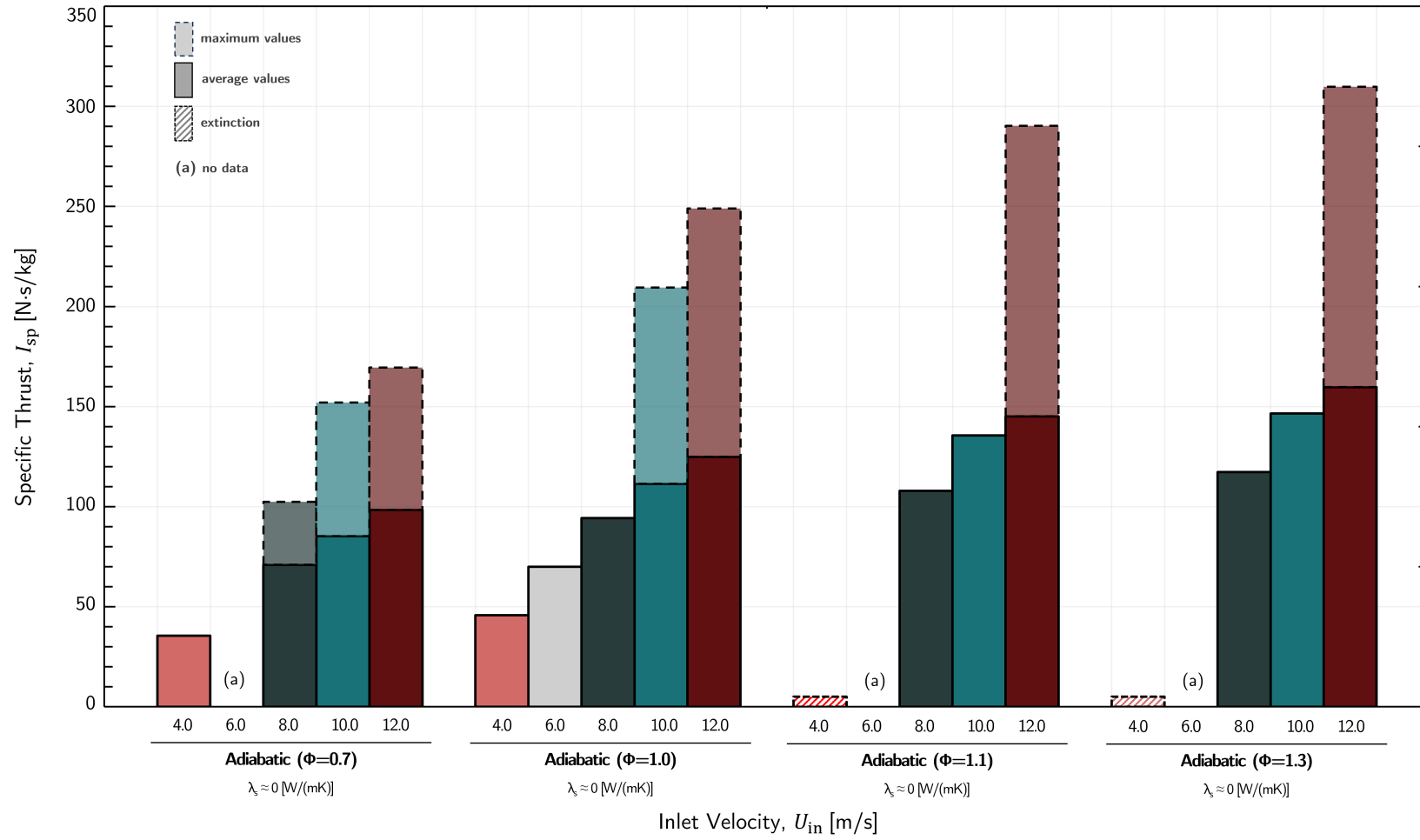


Figure 5.75: Average and maximum values of the specific thrust for adiabatic materials using different equivalency ratios.

Part IV

Conclusio Perpetua

CONCLUSIO:::(noun) *peroration,*
logical conclusion, deduction

PERPETUA:::(adj) *everlasting,*
lasting forever or for a long time

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Chapter 6

Summary and Outlook

*“To know that we know what we know, and to know
that we do not know what we do not know,
that is true knowledge.”*

Nicolaus Copernicus

6.1 Key findings

In this study, we conducted an comprehensive and meticulous study of microcombustion within wavy channel micropropulsion systems. The primary objective was to gain a deeper comprehension of the intricate dynamics within these complex non-linear geometries. Our investigation encompassed the analysis of various materials and their impact on various facets of combustion dynamics. This ranged from understanding heat transfer mechanisms within the combustor walls to examining the flow dynamics and kinetic reactions occurring within the microchannel.

6.1.1 Improvements on fundamental dynamics understanding

Our approach began with a comprehensive discretization of combustion phenomena in adiabatic materials, aiming to understand the conditions leading to a stable flame and the phenomenon of Pulsatory Flame Burst. Additionally, and more importantly, we have expanded upon the existing knowledge of PFB, refining the definition of its stages in a novel and highly detailed manner. In this enhanced PFB discretization, we have identified five distinct stages: propagation, ignition, burst, bifurcation, and extinction (or flow-assisted extinction). We provided explanations for how temperature, velocity, and heat release rate evolve during each of these five stages. Subsequently, we conducted an analysis of how these same parameters evolved throughout the entire simulation and subjected the data to Fast Fourier Transform analysis. This allowed us to examine the frequency and amplitude of the signals for temperature (T) and heat release rate (q''') in each simulation.

6.1.2 Understanding material impact on the microchannel dynamics

Consequently, we embarked on the exploration of simulations involving various selected material groups, which include adiabatic materials, ceramics (both LTCC and HTCC), metals (specifically

two types of stainless steel), amorphous materials (two variants of high-temperature glasses), and high thermal conductivity materials (such as silicon, aluminum, and copper-tungsten alloys).

We noticed that even with the introduction of finite walls, we still observed the same fundamental dynamics as seen in adiabatic scenarios. However, during this phase, we also observed novel and distinct dynamics that were solely induced by the wall conduction within the microchannel.

6.1.2.1 Novel dynamics discovered

One of these newly discovered dynamics is referred to as **Transitional Pulsatory Flame Burst**, abbreviated as **tPFB**. In this phenomenon, a flame located within a convex region initially displays dynamics resembling those of PFB. Nevertheless, as time progresses, the oscillations gradually diminish, leading the flame to transition into a stable dynamic state. The term "transition" signifies the shift from oscillatory behavior to a stable one, characterized by a progressively lower frequency in the signal after each oscillation.

The other newly discovered dynamic, termed **Stable to Flashback**, involves a scenario where the flame front started to anchor in the first convex zone, but *flashback* occurs and it gets pushed back to the inlet. This phenomenon also occurred in the adiabatic simulations, but in the former, due to heat loss, the flames are gradually pushed further inward as a result of horizontal (x-axis) wall conduction. Ultimately, this progression leads to flashback taking place at the inlet. Consequently, aroused an immediate need for a geometric adjustment.

As a response to this issue, a new design has been proposed for future research, since this occurred even for materials with low thermal conductivity (λ_s). This design aims to mitigate the problem since, otherwise, the effective length of the microchannel would be significantly reduced.

We also discovered **Migrating Pulsatory Flame Burst** dynamic (**mPFB**), which essentially exhibits the same characteristics as those previously explored for PFB. However, here, the dynamics involve the flame's propagation from its initial position downstream of the microchannel. This migration predominantly takes place between convex zones, which typically act as the focal points for stabilizing the flame front.

Additionally, following each mPFB cycle, we observed an inverse tPFB phenomenon. In this case, the amplitude gradually increases over time until it stabilizes at a specific frequency and within a certain bandwidth.

Another phenomenon that has been previously studied and documented in microcombustion but was initially discovered in this research within wavy nonlinear geometries with finite walls is the occurrence of two types of **Blow-off**. Both of these occur during the initial stages of the simulation. The first type occurs when there is excessive localized heating of the microchannel wall, typically observed in materials with high thermal resistance. In this case, the temperature in the fluid drops as it heats the wall, leading to insufficient thermal energy to sustain combustion. The second type of blow-off happens with materials possessing very high thermal conductivity. Here, due to the rapid and widespread heat flux in the walls, the region of the wall adjacent to the

flame front remains excessively cold, causing the flame to be extinguished and blown towards the outlet.

The last dynamic uncovered in our research is known as **Backward Ignition Resurgence, (BIR)**. In this phenomenon, before a flame can fully stabilize within a convex zone, a new flame ignites within the preceding convex zone. This occurrence is attributed to an excessive retrograde flow of energy within the microchannel walls, driven by significant backward heat conduction, which has the capability to initiate the ignition of the new flame.

6.1.2.2 Comparison between materials

We successfully generated a comprehensive stability map applicable to nonlinear wavy microchannels. This map encompasses five inlet velocities and spans across ten materials, all characterized by significant variations in their thermal properties, including thermal conductivity, density, and specific heat.

In scenarios involving materials with exceptionally high thermal conductivities (λ_s), blowoff consistently occurred. Additionally, when we experimented with these specific materials and initiated a sufficiently hot temperature profile within the material walls, we weren't able to achieve flame stability, since the pronounced heat conduction in these materials led to flashback.

As for most materials, we saw that higher thermal diffusivities led to lower temperatures overall, both on the fluid and solid, due to more heat being lost. On the other hand, it's important to recognize the significance of regions with vortices induced by velocity, as they play a pivotal role in enabling the retrograde flow of energy, where energy moves upstream, subsequently initiating the ignition of new flames. When we introduce heat conduction into the walls, we observe that as the material's conductivity increases, the heat flux due to conduction in the solid becomes more pronounced. Consequently, this amplifies the already significant retrograde flow of energy, resulting in faster ignitions (which can be observed in the increase in the PFB frequencies). This is accompanied by an increase in heat release rates because more H_2 is able to be consumed.

Consequently, we observed a reduction in the amplitude of both temperature and heat release rate signals. This reduction is attributed to the faster unfolding of cycles, resulting in higher overall combustion intensity within the same time frame.

Finally, we conducted measurements and a thorough analysis of the propulsion performance of each microchannel constructed from various materials. To evaluate this performance, we employed the specific impulse metric, with higher values indicating more efficient propellant consumption. Our observations revealed that both velocity and the equivalence ratio play crucial roles in augmenting these specific impulse values. Additionally, materials with greater thermal dissipation exhibited a decrease in specific impulse values, particularly evident in the maximum values, which is detrimental in terms of overall efficiency and performance.

We also observed that achieving a stable flame or PFB is relatively easy for most velocities when working with materials possessing a low λ_s value. Therefore, these materials hold particular significance in experimental tests, as they exhibit the highest likelihood of sustaining a flame and

delivering superior propulsion performance. It's worth noting that most cases of extinction in these scenarios can be easily fixed with alterations in the channel geometry as mentioned earlier.

6.2 Limitations and weaknesses

The main limitation and challenge in this thesis result from the necessity of utilizing the pseudo-stationary approach for simulations. This research is significantly impacted by constraints related to computational resources and the substantial time required for simulations to reach steady-state conditions^(a). In many instances, if we did not simplified the simulation by equating the characteristic time of combustion, τ_c , and the characteristic time of diffusion in the solid, τ_s , it would substantially prolong the simulation duration. This is because it would involve heating the microchannel walls to a sufficiently high temperature to sustain the flame. Given the very small timescales required to accurately simulate the dynamics of the microchannel, this would result in exceptionally lengthy simulation times. Since there are ongoing issues with utilizing *CHT-laminarSMOKE* in parallel processing, there were limited alternatives available to achieve rapid temperature distributions. Therefore, the only viable option was to simplify the problem and adopt the pseudo-stationary approach in order to obtain the necessary results efficiently.

Another limitation of this study is that we did not account for the variation of thermal conductivity with time. In many real-world scenarios, especially in transient processes, the thermal conductivity of materials changes over time with temperature fluctuations, and although our results are valid for static λ_s , future studies could benefit from incorporating time and temperature-dependent λ_s .

Lastly, an essential area for improvement pertains to the calculation of specific impulse. In this dissertation, we employed a valid but simplified equation for this calculation. It is imperative to grasp the distinctions and benefits of utilizing a more accurate and precise equation, such as:

$$F = \int_{S_{\text{exit}}} \rho u_a (u \cdot n) dA + \int_{S_{\text{exit}}} (P_e - P_\infty) dA \quad (6.1)$$

where ρ is density, u_a is velocity component in an axial direction, u is a velocity vector, S_{exit} is the area of the fluid outlet, A is control surface, n is a unit vector normal to a plan A , P_e is the pressure at the fluid outlet, and P_∞ is the ambient pressure.

6.3 Future Research

In addition to the research presented in this dissertation, we are presently engaged in two distinct research endeavors. First, we are conducting a transient analysis of the Fourier number, establishing a relationship between τ_c and τ_s . This analysis seeks to offer a more profound insight into how varying Fourier numbers influence dynamics and impact the convergence of results.

^(a)The code is already capable of handling complete transient behavior; the decision was solely driven by computational limitations.

Furthermore, we are delving into the dynamics within anisotropic materials, where thermal conductivity properties vary according to direction. This research endeavor aims to enhance our understanding of how each direction influences the behavior of the flame. Other crucial research endeavors that have not yet commenced but should take precedence include:

1. The code for *CHTlaminarSMOKE* needs to be enhanced to support parallel processing for simulations. This enhancement would significantly accelerate result generation, regardless of grid refinement or the type of fuel under consideration. Otherwise, in some instances, obtaining results could potentially require years of simulation time;
2. Secondly, the absence of experimental data remains one of the primary challenges in micropropulsion research. The technological complexities associated with acquiring such data make the validation of simulations exceptionally difficult and will continue to be a significant drawback unless addressed differently. This is particularly true in the case of wavy channels, where experimental tests have not yet been conducted.

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In conclusion, given the current limitations in research on wavy channels, there is a substantial need for further exploration. This includes examining various parameters related to the sinusoidal nonlinear geometry, experimenting with different fuels, and exploring a range of equivalence ratios in simulations involving physical microchannel walls. There is still much to be uncovered and comprehended regarding the intricate and fascinating dynamics of microcombustion within wavy channels. The future holds great promise for the micropropulsion industry, but many more steps must be taken to unlock its full potential.

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Conference Talks

The majority of the work in this dissertation is currently either being prepared for submission or is in the planning stages. One upcoming contribution will be:

DIAS, D. M. ; RESENDE, P.R. AND AFONSO, A.M. (2023). NUMERICAL INVESTIGATION OF MICRO-COMBUSTION FOR THE DESIGN OF WAVY MICROPROPULSION SYSTEMS: MATERIALS AND PERFORMANCE ANALYSIS. 5TH RESEARCH CONGRESS FOAM@IBERIA MEETING (F@I23), GUIMARÃES, PORTUGAL, NOVEMBER, 2023.

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Part V

Appendices

APPENDICES:: (noun) *plural of appendix*

APPENDIX:: (noun) *an addition, continuation,
something attached*

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Appendix A

chtlaminarSMOKE solver files

A.1 chtlaminarSMOKE policy file

```
1 {
2     if(chtEquation == true)
3     {
4
5         /// SOLID 1 //////////////////////////////////////
6         // get the label for the interface boundary called solid_interface in solid region
7         label solidInterface = mesh2.boundaryMesh().findPatchID("solid_interface");
8         // get the label for the interface boundary called fluid_interface in fluid region
9         label fluidInterface = mesh.boundaryMesh().findPatchID("fluid_interface");
10
11         if (-1 == solidInterface || -1 == fluidInterface)
12         {
13             error err("no solid or fluid interface in solid 1");
14             err.exit();
15         }
16
17
18         // reads the scalar Temperature field at the first internal boundary
19         scalarField TsolidInterface = T2.boundaryField()[solidInterface];
20         // volScalarField& T1 = T;
21         scalarField TfluidInterface = T.boundaryField()[fluidInterface];
22
23         // calculates the gradient of Temperature in all the field
24         volVectorField gradT1cal = fvc::grad(T);
25         volVectorField gradT2cal = fvc::grad(T2);
26
27         // take the reference to the gradient value imposed to solid region
28         fixedGradientFvPatchScalarField& gradTsolidInterface =
↪ refCast<fixedGradientFvPatchScalarField>(T2.boundaryField()[solidInterface]);
29         scalarField& gradT2 = gradTsolidInterface.gradient();
30
31         //calculate the vector field of unit surface normals
32         surfaceVectorField unitNormals1 = mesh.Sf()/mesh.magSf();
33         surfaceVectorField unitNormals2 = mesh2.Sf()/mesh2.magSf();
34
35         //calculate the projection of the gradient onto the normal of the boundary
36         scalarField gradTlnorm = gradT1cal.boundaryField()[fluidInterface] &
↪ unitNormals1.boundaryField()[fluidInterface];
```

```

37     scalarField gradT2norm = gradT2cal.boundaryField()[solidInterface] &
    → unitNormals2.boundaryField()[solidInterface];
38
39     // set the gradient imposed to solid region equal to the gradient extracted
40     // from fluid region multiplied by the ratio of the conductivity of the
41     // two zones
42     //     scalarField coeff = thermo->alpha()*thermo->rho()*thermo->Cp()/K2;
43     //     scalarField coeff = lambda/ksolid;
44     dimensionedScalar ksolidxx = ksolid.component(tensor::XX);
45     dimensionedScalar ksolidyy = ksolid.component(tensor::YY);
46     dimensionedScalar ksolidzz = ksolid.component(tensor::ZZ);
47     dimensionedScalar ksolidMean = (ksolidxx + ksolidyy + ksolidzz) / 3.;
48
49     scalarField coeff = lambda/ksolidMean;
50
51     Info << "solid region 1:coeff " << max(coeff) <<"\n";
52     Info << "solid region 1:lambda " << max(lambda) <<"\n";
53     // original
54     // set the gradient on the solid equal to the gradient on fluid
55     gradT2 = -gradT1norm*coeff;
56
57     // print
58     //     deltagrad = max(gradT2norm)-max(-gradT1norm*coeff);
59     Info << "solid region 1:gradient at fluid side*coeff " << max(gradT2) <<"\n";
60     Info << "solid region 1:gradient at fluid side " << max(gradT1norm) <<"\n";
61     Info << "solid region 1:gradient at solid side " << max(gradT2norm) <<"\n";
62     Info << "solid region 1:delta grad " << max(gradT2norm)-max(-gradT1norm*coeff)
    → <<"\n";
63
64     // set the Temperature the boundary in solid region equal to Temperatur at the fluid
65     //     T2.boundaryField()[solidInterface] == T.boundaryField()[fluidInterface];
66     //     T2.correctBoundaryConditions();
67
68     fvScalarMatrix T2Eqn
69     (
70         dTdt0*fvm::ddt(rhosolid*cpsolid,T2) - fvm::laplacian(ksolid, T2)
71     //     dTdt0*fvm::ddt(rhosolid*cpsolid,T2) -
    → fvm::laplacian(ksolid.component(tensor::XX), T2)
72     //     dTdt0*fvm::ddt(T2) - fvm::laplacian(DiffT, T2)
73         );
74
75     T2Eqn.relax();
76     fvOptions.constrain(T2Eqn);
77     T2Eqn.solve(mesh2.solver("T"));
78     // solver("T") ou solver("T2")
79     T2.correctBoundaryConditions();
80     fvOptions.correct(T2);
81
82     // set the Temperature imposed to fluid region equal to temperature of
83     // the boundary in solid region
84
85     //     T.boundaryField()[fluidInterface] == TsolidInterface;
86     T.boundaryField()[fluidInterface] == T2.boundaryField()[solidInterface];
87     T.correctBoundaryConditions();
88     fvOptions.correct(T);
89

```

```

90     Info << "solid region 1: T fluid interface " << max(T.boundaryField()[fluidInterface])
↪ << "\n";
91     Info<< " * solid region 1:T min/max (solid transport) = " << min(T2).value() << ", "
↪ << max(T2).value() << endl;
92     runTime.write();
93
94     /// SOLID 1 //////////////////////////////////////
95
96     /// SOLID 2 //////////////////////////////////////
97     // get the label for the interface boundary called solid_interface in solid region
98     label solidInterface2 = mesh3.boundaryMesh().findPatchID("solid_interface2");
99     // get the label for the interface boundary called fluid_interface in fluid region
100    label fluidInterface2 = mesh.boundaryMesh().findPatchID("fluid_interface2");
101
102    if (-1 == solidInterface2 || -1 == fluidInterface2)
103    {
104        error err("no solid or fluid interface in solid 2");
105        err.exit();
106    }
107
108
109    // reads the scalar Temperature field at the first internal boundary
110    scalarField TsolidInterface2 = T3.boundaryField()[solidInterface2];
111    // volScalarField& T1 = T;
112    scalarField TfluidInterface2 = T.boundaryField()[fluidInterface2];
113
114    // calculates the gradient of Temperature in all the field
115    volVectorField gradT1cal2 = fvc::grad(T);
116    volVectorField gradT2cal2 = fvc::grad(T3);
117
118    // take the reference to the gradient value imposed to solid region
119    fixedGradientFvPatchScalarField& gradTsolidInterface2 =
↪ refCast<fixedGradientFvPatchScalarField>(T3.boundaryField()[solidInterface2]);
120    scalarField& gradT22 = gradTsolidInterface2.gradient();
121
122    //calculate the vector field of unit surface normals
123    surfaceVectorField unitNormals12 = mesh.Sf()/mesh.magSf();
124    surfaceVectorField unitNormals22 = mesh3.Sf()/mesh3.magSf();
125
126    //calculate the projection of the gradient onto the normal of the boundary
127    scalarField gradT1norm2 = gradT1cal2.boundaryField()[fluidInterface2] &
↪ unitNormals12.boundaryField()[fluidInterface2];
128    scalarField gradT2norm2 = gradT2cal2.boundaryField()[solidInterface2] &
↪ unitNormals22.boundaryField()[solidInterface2];
129
130    // set the gradient imposed to solid region equal to the gradient extracted
131    // from fluid region multiplied by the ratio of the conductivity of the
132    // two zones
133    // scalarField coeff = thermo->alpha()*thermo->rho()*thermo->Cp()/K2;
134    // scalarField coeff = lambda/ksolid;
135    dimensionedScalar ksolidxx2 = ksolid2.component(tensor::XX);
136    dimensionedScalar ksolidyy2 = ksolid2.component(tensor::YY);
137    dimensionedScalar ksolidzz2 = ksolid2.component(tensor::ZZ);
138    dimensionedScalar ksolidMean2 = (ksolidxx2 + ksolidyy2 + ksolidzz2) / 3.;
139
140    scalarField coeff2 = lambda/ksolidMean2;
141

```



```

142     Info << "solid region 2:coeff " << max(coeff2) << "\n";
143     Info << "solid region 2:lambda " << max(lambda) << "\n";
144 // original
145 // set the gradient on the solid equal to the gradient on fluid
146     gradT22 = -gradT1norm2*coeff2;
147
148 // print
149 //     deltagrad = max(gradT2norm)-max(-gradT1norm*coeff);
150     Info << "solid region 2:gradient at fluid side*coeff " << max(gradT22) << "\n";
151     Info << "solid region 2:gradient at fluid side " << max(gradT1norm2) << "\n";
152     Info << "solid region 2:gradient at solid side " << max(gradT2norm2) << "\n";
153     Info << "solid region 2:delta grad " << max(gradT2norm2)-max(-gradT1norm2*coeff2)
    => << "\n";
154
155 // set the Temperature the boundary in solid region equal to Temperatur at the fluid
156 //     T2.boundaryField()[solidInterface] == T.boundaryField()[fluidInterface];
157 //     T2.correctBoundaryConditions();
158
159     fvScalarMatrix T3Eqn
160     (
161         dTdt02*fvm::ddt(rhosolid2*cpsolid2,T3) - fvm::laplacian(ksolid2, T3)
162     );
163
164     T3Eqn.relax();
165     fvOptions.constrain(T3Eqn);
166     T3Eqn.solve(mesh3.solver("T"));
167 // solver("T") ou solver("T2")
168     T3.correctBoundaryConditions();
169     fvOptions.correct(T3);
170
171 // set the Temperature imposed to fluid region equal to temperature of
172 // the boundary in solid region
173
174 //     T.boundaryField()[fluidInterface] == TsolidInterface;
175     T.boundaryField()[fluidInterface2] == T3.boundaryField()[solidInterface2];
176     T.correctBoundaryConditions();
177     fvOptions.correct(T);
178
179     Info << "solid region 2: T fluid interface " << max(T.boundaryField()[fluidInterface2])
    => << "\n";
180     Info<< " * solid region 2:T min/max (solid transport) = " << min(T3).value() << ", "
    => << max(T3).value() << endl;
181     runTime.write();
182
183 }
184 }

```

Code Listing A.1: chtlaminarSMOKE policy file in C++.

A.2 system Files

```

1  /*-----*\
2  | ===== |
3  |  \ \      /  F i e l d      | OpenFOAM: The Open Source CFD Toolbox |
4  |  \ \      /  O peration     | Version: 1.0 |
5  |   \ \      /  A nd          | Web:      http://www.openfoam.org |
6  |    \ \ /    M anipulation   | |
7  \*-----*/
8  FoamFile
9  {
10     version      2.0;
11     format        ascii;
12     root          "";
13     case          "";
14     instance      "";
15     local         "";
16     class         dictionary;
17     object        fvSchemes;
18  }
19  // ***** //
20  ddtSchemes
21  {
22     default       Euler;
23  }
24  gradSchemes
25  {
26     default       Gauss linear;
27     grad(T)       fourth;
28  }
29  divSchemes
30  {
31     default       Gauss linear;
32  }
33  laplacianSchemes
34  {
35     default       none;
36     laplacian(ksolid,T) Gauss linear uncorrected;
37  }
38  interpolationSchemes
39  {
40     default       linear;
41  }
42  snGradSchemes
43  {
44     default       corrected;
45  }
46  fluxRequired
47  {
48     default       no;
49     T;
50  }
51  // ***** //

```

Code Listing A.2: *fvSchemes* file in C++.

```

1  /*-----*\
2  | ===== |
3  |  \ \      /  F ield      | OpenFOAM: The Open Source CFD Toolbox |
4  |  \ \      /  O peration  | Version: 1.0 |
5  |   \ \      /   A nd      | Web:      http://www.openfoam.org |
6  |    \ \ /      M anipulation | |
7  \*-----*/
8  FoamFile
9  {
10     version      2.0;
11     format        ascii;
12     root          "";
13     case          "";
14     instance      "";
15     local         "";
16     class         dictionary;
17     object        fvSolution;
18 }
19 // ***** //
20 solvers
21 {
22     T
23     {
24         solver      PCG;
25         preconditioner DIC;
26         tolerance   1e-06;
27         relTol      0.0;
28     }
29 }
30 SIMPLE
31 {
32     nNonOrthogonalCorrectors 0;
33     residualControl
34     {
35         default      1e-7;
36         T            1e-7;
37     }
38 }
39 relaxationFactors
40 {
41     equations
42     {
43         T            0.5;
44     }
45 }
46 PIMPLE
47 {
48     momentumPredictor no;
49     nOuterCorrectors 1;
50     nCorrectors      2;
51     nNonOrthogonalCorrectors 0;
52 }
53 // ***** //

```

Code Listing A.3: fvSolution file in C++.

```

1  /*-----* C++ -*-----*\
2  | ===== |
3  | \ \      / F i e l d      | OpenFOAM: The Open Source CFD Toolbox |
4  | \ \      / O p e r a t i o n      | Version: 2.3.0 |
5  | \ \      / A n d      | Web: www.OpenFOAM.com |
6  | \ \ /      M a n i p u l a t i o n      | |
7  \*-----*\
8  FoamFile
9  {
10     version      2.0;
11     format        binary;
12     class          dictionary;
13     location       "system";
14     object         controlDict;
15 }
16 // *****
17 application      reactingFoam;
18
19 startFrom         latestTime;
20
21 stopAt            endTime;
22
23 endTime           4.5e-3;
24
25 deltaT            1e-8;
26
27 writeControl      adjustableRunTime;
28
29 writeInterval     1e-5;
30
31 purgeWrite        0;
32
33 writeFormat        ascii;
34
35 writePrecision    11;
36
37 writeCompression  uncompressed;
38
39 timeFormat         general;
40
41 timePrecision      11;
42
43 runTimeModifiable yes;
44
45 adjustTimeStep    no;
46
47 maxCo             0.1;
48 // *****
49 libs (
50     "libOpenFOAM.so"
51     "libsimpleSwakFunctionObjects.so"
52     "libswakFunctionObjects.so"
53     "libgroovyBC.so"
54 );

```

Code Listing A.4: controlDict file in C++.

A.3 constant Files

```

1  /*-----*\
2  | ===== |
3  |  \ \      /  F i e l d      | OpenFOAM: The Open Source CFD Toolbox |
4  |  \ \      /  O p e r a t i o n | Version: 1.0 |
5  |  \ \      /  A n d      | Web: http://www.openfoam.org |
6  |  \ \ /      M a n i p u l a t i o n | |
7  \*-----*/
8
9  FoamFile
10 {
11     version      2.0;
12     format       ascii;
13
14     root         "";
15     case         "";
16     instance     "";
17     local        "";
18
19     class        dictionary;
20     object       transportProperties;
21 }
22
23 // * * * * *
24
25
26 ksolid          ksolid [1 1 -3 -1 0 0 0] (200 0. 0. 0. 200 0. 0. 0. 200);
27
28 rhesolid        rhesolid [1 -3 0 0 0 0 0] 2750.;
29
30 cpsolid         cpsolid [0 2 -2 -1 0 0 0] 860.;
31
32 DiffT           DiffT [0 2 -1 0 0 0 0] (8.55e-05 0. 0. 0. 8.55e-05 0. 0. 0.
33   → 8.55e-05);
34
35 dTdt0           dTdt0 [0 0 0 0 0 0 0] 0.000;
36
37 // * * * * *

```

Code Listing A.5: *transportProperties* file for *solidRegion1* in C++.

```

1  /*-----*\ C++ -*\
2  | ===== |
3  |  \ \      /  F i e l d      | OpenFOAM: The Open Source CFD Toolbox |
4  |  \ \      /  O p e r a t i o n | Version: 2.2.0 |
5  |  \ \      /  A n d      | Web: www.OpenFOAM.org |
6  |  \ \ /      M a n i p u l a t i o n | |
7  \*-----*/
8
9  FoamFile
10 {
11     version      2.3;
12     format       ascii;
13     class        dictionary;
14     location     "constant";
15     object       solverOptions;
16 }

```

```

16 // * * * * *
17
18 Kinetics
19 {
20     folder
21     ↪      ".../laminarSMOKE-0.3.0/cases/Toro-Flames/kinetics/kinetics-POLIMI/";
22     inertSpecies      N2;
23 }
24 PhysicalModel
25 {
26     strangAlgorithm      "MomentumTransportReaction";
27     homogeneousReactions      on;
28     momentumEquations      on;
29     speciesEquations      on;
30     energyEquation      on;
31     constPressureBatchReactor      true;
32     sparseJacobian      false;
33     massDiffusionInEnergyEquation      true;
34     diffusivityModel      "multi-component";
35     thermophoreticEffect      true;
36     soRETEffect      true;
37     includeDpDt      off;
38     thermodynamicPressure      101325.;
39     tauEquation      off;
40     zMixEquation      off;
41     zMixDmixSpecies      N2;
42 }
43 ChtOptions
44 {
45     chtEquation      on;
46     usedTdt      off;
47     userhocp      off;
48 }
49 Radiation
50 {
51     radiationModel      "none";
52     environmentTemperature      300.;
53 }
54 Output
55 {
56     formationRates      off;
57     diffusivities      off;
58 }
59 PolimiSoot
60 {
61     thermophoreticEffectTag      "BIN";
62     physicalSootDiffusivity      off;
63 }
64 OdeHomogeneous
65 {
66     odeSolver      "OpenSMOKE";
67     relTolerance      1e-7;
68     absTolerance      1e-12;
69     maximumOrder      5;
70     fullPivoting      false;
71 }
72 Spark

```

```

72  {
73      spark                on;
74      //spark              off; //for the simulations without spark
75      position              (0.002  0.0 5e-5);
76      time                  0.;
77      temperature           1500;
78      duration              0.0005;
79      diameter              0.1e-3;
80  }
81  PostProcessing
82  {
83      moleFractions         off;
84      concentrations        off;
85      mixtureFraction       off;
86      soot                  off;
87      PolimiSoot
88      {
89          onTheFlyFill      on;
90          integralUpdate    10;
91          planckCoefficient  "none";
92          boundaries        ();
93          sootPrecursors    (C10H8);
94          binMinimum        "BIN5";
95          binIndexZero      10;
96          binIndexFinal     20;
97          binDensityZero    1500.;
98          binDensityFinal   1500.;
99          fractalDiameter   3;
100     }
101 }
102 DRG
103 {
104     drg                off;
105 }
106 #include "isatOptions"
107 LewisNumbers
108 {
109     N2 0.987;O2 1.045;H2 0.290;H2O 0.777;H2O2 1.058;CO 1.058;CO2 1.347;CH2O 1.209;CH4
    ↪ 0.955;CH3OH 1.237;C2H2 1.246;CH2CO 1.430;C2H4 1.258;CH3CHO 1.443;C2H6 1.383;C3H6 1.453;O
    ↪ 0.679;H 0.174;OH 0.692;HO2 1.051;CH 0.634;HCO 1.199;CH2S 0.928;CH3 0.950; CH2OH
    ↪ 1.237;CH3O 1.237;HCCO 0.843;C2H3 1.259;CH3CO 1.437;CH2CHO 1.437;C2H5 1.371;CH2CHCH2
    ↪ 1.479;NC3H7 1.724;C2H 1.233;C4H3 1.969;CYC5H5 2.082;C6H5 2.175;C6H5O 2.358;C6H4C2H
    ↪ 2.535;C10H7 2.903;C3H2 1.364;AC3H4 1.653;PC3H4 1.653;C2H3CHO 1.572;C4H2 1.961;C4H4
    ↪ 1.975;CYC5H6 2.087;C6H6 2.179;C6H5OH 2.361;MCPTD 2.145;C6H5C2H 2.533;C10H8 2.906;CH2
    ↪ 0.928;C3H3 1.644;
110 }
111 // *****

```

Code Listing A.6: solverOptions file for fluidRegion in C++.

Appendix B

Kinetic Mechanism of the Combustion Reaction

This appendix introduces the kinetic mechanism named POLIMI-H₂CO-NO_x-1412 .

CHEMICAL REACTIONS			
Units:			
[kmol], [m ³], [s], [—] and [cal/mol]			
Coefficients of the Arrhenius Equation (<i>k</i> _Δ):			
Pre-exponential factor, <i>A</i>			
Temperature exponent, (<i>γ</i>) ^{<i>T</i>}			
Activation energy, <i>E</i> _{ati}			
1. O ₂ + H → O + OH	<i>k</i> _Δ : 9.600000 × 10 ¹¹	−0.20	16625.00
2. H ₂ + O → H + OH	<i>k</i> _Δ : 4.330000 × 10 ¹⁰	0.00	10000.00
3. O ₂ + H(+ M) → HO ₂ (+ M)	Fall-off (Troe)		
	<i>k</i> ₀ : 8.400000 × 10 ¹¹	−0.80	0.00
	<i>k</i> _∞ : 5.580000 × 10 ⁹	0.40	0.00
	Troe Parameters		
	<i>a</i> : 5.00 × 10 ^{−1}		
	<i>T</i> ^{***} : 1.00 × 10 ^{−30}		
	<i>T</i> [*] : 1.00 × 10 ³⁰		
	<i>T</i> ^{**} : 0.00 × 10 ⁰		
	H ₂ O enhanced by 18.000		
	H ₂ enhanced by 2.500		
	N ₂ enhanced by 1.260		
	Ar enhanced by 0.800		
	He enhanced by 0.800		
	CO enhanced by 1.200		
	CO ₂ enhanced by 2.400		
4. OH + HO ₂ → O ₂ + H ₂ O	<i>k</i> _Δ : 5.000000 × 10 ¹⁰	0.00	1000.00
5. H + HO ₂ → 2 OH	<i>k</i> _Δ : 2.500000 × 10 ¹¹	0.00	1900.00
6. O + HO ₂ → O ₂ + OH	<i>k</i> _Δ : 3.250000 × 10 ¹⁰	0.00	0.00
7. 2 OH → H ₂ O + O	<i>k</i> _Δ : 3.570000 × 10 ¹	2.40	−2110.00
8. H ₂ + M → 2 H + M	<i>k</i> _Δ : 1.115000 × 10 ¹¹	0.00	96081.00
	H ₂ enhanced by 2.500		
	H ₂ O enhanced by 12.000		
	Ar enhanced by 0.500		
	CO enhanced by 1.900		
	CO ₂ enhanced by 3.800		
9. O ₂ + M → 2 O + M	<i>k</i> _Δ : 1.550000 × 10 ¹¹	0.00	115120.00
	H ₂ enhanced by 2.500		
	H ₂ O enhanced by 12.000		
	Ar enhanced by 0.200		
	He enhanced by 0.200		
	CO enhanced by 1.900		

CO₂ enhanced by 3.800

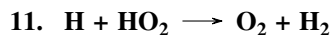


$$k_{\Delta} : 4.500000 \times 10^{16} \quad -2.00 \quad 0.00$$

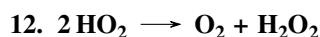
H₂O enhanced by 16.000

H₂ enhanced by 2.000

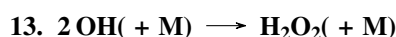
CO₂ enhanced by 1.900



$$k_{\Delta} : 2.500000 \times 10^{10} \quad 0.00 \quad 700.00$$



$$k_{\Delta} : 2.110000 \times 10^9 \quad 0.00 \quad 0.00$$



Fall-off (Troe)

$$k_0 : 1.300000 \times 10^{12} \quad -0.90 \quad -1700.00$$

$$k_{\infty} : 7.400000 \times 10^{10} \quad -0.37 \quad 0.00$$

Troe Parameters

$$a : 7.35 \times 10^{-1}$$

$$T^{***} : 9.40 \times 10^1$$

$$T^* : 1.76 \times 10^3$$

$$T^{**} : 5.18 \times 10^3$$

H₂ enhanced by 2.000

H₂O enhanced by 6.000

CO enhanced by 1.500

CO₂ enhanced by 2.000

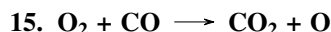
Ar enhanced by 0.700

He enhanced by 0.700

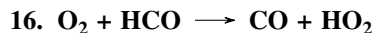
N₂ enhanced by 0.900



$$k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$$



$$k_{\Delta} : 2.530000 \times 10^9 \quad 0.00 \quad 47700.00$$



$$k_{\Delta} : 3.000000 \times 10^9 \quad 0.00 \quad 0.00$$



Fall-off (Lindemann)

$$k_0 : 2.070000 \times 10^{20} \quad -3.34 \quad 7610.00$$

$$k_{\infty} : 9.640000 \times 10^7 \quad 0.00 \quad 3800.00$$

H₂O enhanced by 12.000

H₂ enhanced by 2.000

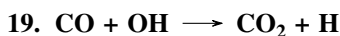
CO enhanced by 1.500

CO₂ enhanced by 2.000

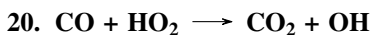
Ar enhanced by 0.500



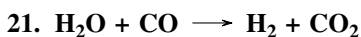
$$k_{\Delta} : 9.600000 \times 10^8 \quad 0.14 \quad 7352.00$$



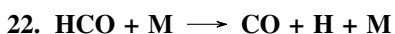
$$k_{\Delta} : 7.320000 \times 10^7 \quad 0.03 \quad -16.00$$



$$k_{\Delta} : 3.000000 \times 10^{10} \quad 0.00 \quad 23000.00$$



$$k_{\Delta} : 2.000000 \times 10^8 \quad 0.00 \quad 38000.00$$



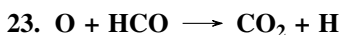
$$k_{\Delta} : 1.200000 \times 10^{14} \quad -1.00 \quad 17000.00$$

H₂O enhanced by 5.000

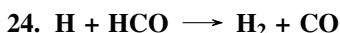
CO₂ enhanced by 3.000

H₂ enhanced by 1.900

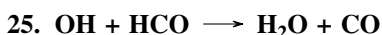
CO enhanced by 1.900



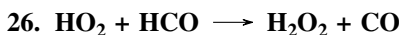
$$k_{\Delta} : 3.000000 \times 10^{10} \quad 0.00 \quad 0.00$$



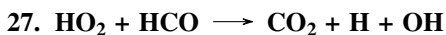
$$k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$$



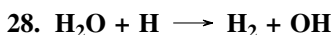
$$k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$$



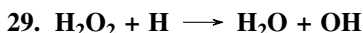
$$k_{\Delta} : 4.000000 \times 10^8 \quad 0.00 \quad 0.00$$



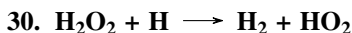
$$k_{\Delta} : 3.000000 \times 10^{10} \quad 0.00 \quad 0.00$$



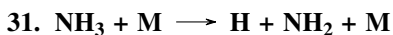
$$k_{\Delta} : 4.800000 \times 10^7 \quad 1.00 \quad 19000.00$$



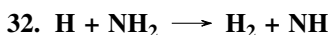
$$k_{\Delta} : 2.410000 \times 10^{10} \quad 0.00 \quad 3970.00$$



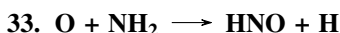
$$k_{\Delta} : 6.025000 \times 10^{10} \quad 0.00 \quad 7950.00$$



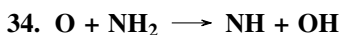
$$k_{\Delta} : 2.200000 \times 10^{13} \quad 0.00 \quad 93470.00$$



$$k_{\Delta} : 4.000000 \times 10^{10} \quad 0.00 \quad 3650.00$$



$$k_{\Delta} : 6.600000 \times 10^{11} \quad -0.50 \quad 0.00$$



$$k_{\Delta} : 6.800000 \times 10^9 \quad 0.00 \quad 0.00$$

35. $\text{O} + \text{NH}_2 \longrightarrow \text{NO} + \text{H}_2$
 $k_A : 1.300000 \times 10^5 \quad 1.02 \quad -627.00$
36. $\text{O}_2 + \text{NH}_2 \longrightarrow \text{HNO} + \text{OH}$
 $k_A : 4.500000 \times 10^9 \quad 0.00 \quad 25000.00$
37. $\text{OH} + \text{NH}_2 \longrightarrow \text{H}_2\text{O} + \text{NH}$
 $k_A : 4.000000 \times 10^3 \quad 2.00 \quad 1000.00$
38. $\text{HO}_2 + \text{NH}_2 \longrightarrow \text{OH} + \text{H}_2\text{NO}$
 $k_A : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
39. $\text{O} + \text{H}_2\text{NO} \longrightarrow \text{O}_2 + \text{NH}_2$
 $k_A : 2.000000 \times 10^{11} \quad 0.00 \quad 0.00$
40. $\text{N} + \text{NH}_2 \longrightarrow \text{N}_2 + {}_2\text{H}$
 $k_A : 7.000000 \times 10^{10} \quad 0.00 \quad 0.00$
41. $\text{NH} + \text{NH}_2 \longrightarrow \text{N}_2\text{H}_2 + \text{H}$
 $k_A : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
42. $2\text{NH}_2 \longrightarrow \text{H}_2 + \text{N}_2\text{H}_2$
 $k_A : 8.500000 \times 10^8 \quad 0.00 \quad 0.00$
43. $2\text{NH}_2 \longrightarrow \text{NH}_3 + \text{NH}$
 $k_A : 5.000000 \times 10^{10} \quad 0.00 \quad 10000.00$
44. $2\text{NH}_2 (+\text{M}) \longrightarrow \text{N}_2\text{H}_4 (+\text{M})$
Fall-off (Lindemann)
 $k_0 : 1.000000 \times 10^{12} \quad 0.00 \quad 0.00$
 $k_\infty : 1.500000 \times 10^{10} \quad 0.00 \quad 0.00$
 N_2 enhanced by 2.500
 H_2O enhanced by 5.000
 NH_3 enhanced by 10.000
45. $\text{NO} + \text{NH}_2 \longrightarrow \text{NNH} + \text{OH}$
 $k_A : 8.900000 \times 10^9 \quad -0.35 \quad 0.00$
46. $\text{NO} + \text{NH}_2 \longrightarrow \text{N}_2 + \text{H}_2\text{O}$
 $k_A : 1.720000 \times 10^{16} \quad -2.29 \quad 1058.00$
47. $\text{NO}_2 + \text{NH}_2 \longrightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$
 $k_A : 3.200000 \times 10^{15} \quad -2.20 \quad 0.00$
48. $\text{NO}_2 + \text{NH}_2 \longrightarrow \text{NO} + \text{H}_2\text{NO}$
 $k_A : 3.500000 \times 10^9 \quad 0.00 \quad 0.00$
49. $\text{H} + \text{NH} \longrightarrow \text{H}_2 + \text{N}$
 $k_A : 3.000000 \times 10^{10} \quad 0.00 \quad 0.00$
50. $\text{O} + \text{NH} \longrightarrow \text{NO} + \text{H}$
 $k_A : 9.200000 \times 10^{10} \quad 0.00 \quad 0.00$
51. $\text{NH} + \text{OH} \longrightarrow \text{HNO} + \text{H}$
 $k_A : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
52. $\text{NH} + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{N}$
 $k_A : 5.000000 \times 10^8 \quad 0.50 \quad 2000.00$
53. $\text{NH} + \text{OH} \longrightarrow \text{NO} + \text{H}_2$
 $k_A : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
54. $\text{O}_2 + \text{NH} \longrightarrow \text{HNO} + \text{O}$
 $k_A : 4.600000 \times 10^2 \quad 2.00 \quad 6500.00$
55. $\text{O}_2 + \text{NH} \longrightarrow \text{NO} + \text{OH}$
 $k_A : 1.300000 \times 10^3 \quad 1.50 \quad 100.00$
56. $2\text{NH} \longrightarrow \text{N}_2 + {}_2\text{H}$
 $k_A : 2.500000 \times 10^{10} \quad 0.00 \quad 0.00$
57. $\text{N} + \text{NH} \longrightarrow \text{N}_2 + \text{H}$
 $k_A : 3.000000 \times 10^{10} \quad 0.00 \quad 0.00$
58. $\text{NO} + \text{NH} \longrightarrow \text{N}_2 + \text{OH}$
 $k_A : 2.200000 \times 10^{10} \quad -0.23 \quad 0.00$
59. $\text{NO}_2 + \text{NH} \longrightarrow \text{N}_2\text{O} + \text{OH}$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
60. $\text{N} + \text{OH} \longrightarrow \text{NO} + \text{H}$
 $k_A : 3.800000 \times 10^{10} \quad 0.00 \quad 0.00$
61. $\text{O}_2 + \text{N} \longrightarrow \text{NO} + \text{O}$
 $k_A : 6.400000 \times 10^6 \quad 1.00 \quad 6280.00$
62. $\text{NO} + \text{N} \longrightarrow \text{N}_2 + \text{O}$
 $k_A : 3.300000 \times 10^9 \quad 0.30 \quad 0.00$
63. $\text{N}_2\text{H}_4 + \text{H} \longrightarrow \text{H}_2 + \text{N}_2\text{H}_3$
 $k_A : 1.300000 \times 10^{10} \quad 0.00 \quad 2500.00$
64. $\text{N}_2\text{H}_4 + \text{O} \longrightarrow \text{N}_2\text{H}_2 + \text{H}_2\text{O}$
 $k_A : 8.500000 \times 10^{10} \quad 0.00 \quad 1200.00$
65. $\text{N}_2\text{H}_4 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{N}_2\text{H}_3$
 $k_A : 4.000000 \times 10^{10} \quad 0.00 \quad 0.00$
66. $\text{N}_2\text{H}_4 + \text{NH}_2 \longrightarrow \text{NH}_3 + \text{N}_2\text{H}_3$
 $k_A : 3.900000 \times 10^9 \quad 0.00 \quad 1500.00$
67. $\text{N}_2\text{H}_3 + \text{M} \longrightarrow \text{N}_2\text{H}_2 + \text{H} + \text{M}$
 $k_A : 3.500000 \times 10^{13} \quad 0.00 \quad 46000.00$
68. $\text{H} + \text{N}_2\text{H}_3 \longrightarrow 2\text{NH}_2$
 $k_A : 1.600000 \times 10^9 \quad 0.00 \quad 0.00$
69. $\text{O} + \text{N}_2\text{H}_3 \longrightarrow \text{N}_2\text{H}_2 + \text{OH}$
 $k_A : 5.000000 \times 10^9 \quad 0.00 \quad 5000.00$
70. $\text{O} + \text{N}_2\text{H}_3 \longrightarrow \text{HNO} + \text{NH}_2$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$

71. $\text{OH} + \text{N}_2\text{H}_3 \longrightarrow \text{N}_2\text{H}_2 + \text{H}_2\text{O}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
72. $\text{OH} + \text{N}_2\text{H}_3 \longrightarrow \text{HNO} + \text{NH}_3$
 $k_{\Delta} : 1.000000 \times 10^9 \quad 0.00 \quad 15000.00$
73. $\text{NH} + \text{N}_2\text{H}_3 \longrightarrow \text{N}_2\text{H}_2 + \text{NH}_2$
 $k_{\Delta} : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
74. $\text{N}_2\text{H}_2 + \text{M} \longrightarrow \text{H} + \text{NNH} + \text{M}$
 $k_{\Delta} : 5.000000 \times 10^{13} \quad 0.00 \quad 50000.00$
 N_2 enhanced by 2.000
 H_2 enhanced by 2.000
 O_2 enhanced by 2.000
 H_2O enhanced by 15.000
75. $\text{N}_2\text{H}_2 + \text{H} \longrightarrow \text{H}_2 + \text{NNH}$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
76. $\text{N}_2\text{H}_2 + \text{O} \longrightarrow \text{NO} + \text{NH}_2$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
77. $\text{N}_2\text{H}_2 + \text{O} \longrightarrow \text{NNH} + \text{OH}$
 $k_{\Delta} : 2.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
78. $\text{N}_2\text{H}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{NNH}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
79. $\text{NO} + \text{N}_2\text{H}_2 \longrightarrow \text{N}_2\text{O} + \text{NH}_2$
 $k_{\Delta} : 4.000000 \times 10^9 \quad 0.00 \quad 11922.00$
80. $\text{N}_2\text{H}_2 + \text{NH} \longrightarrow \text{NNH} + \text{NH}_2$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
81. $\text{N}_2\text{H}_2 + \text{NH}_2 \longrightarrow \text{NH}_3 + \text{NNH}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
82. $\text{NNH} \longrightarrow \text{N}_2 + \text{H}$
 $k_{\Delta} : 1.000000 \times 10^7 \quad 0.00 \quad 0.00$
83. $\text{H} + \text{NNH} \longrightarrow \text{N}_2 + \text{H}_2$
 $k_{\Delta} : 1.000000 \times 10^{11} \quad 0.00 \quad 0.00$
84. $\text{O} + \text{NNH} \longrightarrow \text{N}_2\text{O} + \text{H}$
 $k_{\Delta} : 1.000000 \times 10^{11} \quad 0.00 \quad 0.00$
85. $\text{O} + \text{NNH} \longrightarrow \text{NO} + \text{NH}$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
86. $\text{NNH} + \text{OH} \longrightarrow \text{N}_2 + \text{H}_2\text{O}$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
87. $\text{O}_2 + \text{NNH} \longrightarrow \text{N}_2 + \text{HO}_2$
 $k_{\Delta} : 6.670000 \times 10^{10} \quad 0.00 \quad 0.00$
88. $\text{O}_2 + \text{NNH} \longrightarrow \text{N}_2 + \text{O}_2 + \text{H}$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
89. $\text{NH} + \text{NNH} \longrightarrow \text{N}_2 + \text{NH}_2$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
90. $\text{NNH} + \text{NH}_2 \longrightarrow \text{N}_2 + \text{NH}_3$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
91. $\text{NO} + \text{NNH} \longrightarrow \text{N}_2 + \text{HNO}$
 $k_{\Delta} : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
92. $\text{HNNO} + \text{M} \longrightarrow \text{N}_2\text{O} + \text{H} + \text{M}$
 $k_{\Delta} : 2.200000 \times 10^{12} \quad 0.00 \quad 21600.00$
93. $\text{HNNO} + \text{M} \longrightarrow \text{N}_2 + \text{OH} + \text{M}$
 $k_{\Delta} : 1.000000 \times 10^{12} \quad 0.00 \quad 25600.00$
94. $\text{HNNO} + \text{H} \longrightarrow \text{N}_2\text{O} + \text{H}_2$
 $k_{\Delta} : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
95. $\text{HNNO} + \text{H} \longrightarrow \text{NNH} + \text{OH}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
96. $\text{HNNO} + \text{O} \longrightarrow \text{N}_2\text{O} + \text{OH}$
 $k_{\Delta} : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
97. $\text{HNNO} + \text{O} \longrightarrow \text{O}_2 + \text{NNH}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
98. $\text{HNNO} + \text{OH} \longrightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$
 $k_{\Delta} : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
99. $\text{HNNO} + \text{OH} \longrightarrow \text{NNH} + \text{HO}_2$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
100. $\text{NO} + \text{HNNO} \longrightarrow \text{N}_2\text{O} + \text{HNO}$
 $k_{\Delta} : 1.000000 \times 10^9 \quad 0.00 \quad 0.00$
101. $\text{NO} + \text{HNNO} \longrightarrow \text{NO}_2 + \text{NNH}$
 $k_{\Delta} : 3.200000 \times 10^9 \quad 0.00 \quad 270.00$
102. $\text{NO}_2 + \text{HNNO} \longrightarrow \text{NO}_3 + \text{NNH}$
 $k_{\Delta} : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
103. $\text{NO}_2 + \text{HNNO} \longrightarrow \text{N}_2\text{O} + \text{HONO}$
 $k_{\Delta} : 1.000000 \times 10^9 \quad 0.00 \quad 0.00$
104. $\text{NO} + \text{HO}_2 \longrightarrow \text{NO}_2 + \text{OH}$
 $k_{\Delta} : 2.100000 \times 10^9 \quad 0.00 \quad -480.00$
105. $\text{NO} + \text{O} + \text{M} \longrightarrow \text{NO}_2 + \text{M}$
 $k_{\Delta} : 7.500000 \times 10^{13} \quad -1.41 \quad 0.00$
 N_2 enhanced by 1.700
 O_2 enhanced by 1.500

- H₂O enhanced by 10.000
106. $\text{NO} + \text{OH} (+ \text{M}) \longrightarrow \text{HONO} (+ \text{M})$
 Fall-off (Lindemann)
 $k_0 : 2.330000 \times 10^{17} \quad -2.40 \quad 0.00$
 $k_\infty : 2.000000 \times 10^{10} \quad 0.00 \quad 0.00$
107. $\text{NO} + \text{HCO} \longrightarrow \text{HNO} + \text{CO}$
 $k_A : 7.200000 \times 10^9 \quad 0.00 \quad 0.00$
108. $\text{NO} + \text{H} + \text{M} \longrightarrow \text{HNO} + \text{M}$
 $k_A : 4.000000 \times 10^{14} \quad -1.75 \quad 0.00$
 N₂ enhanced by 1.000
 H₂O enhanced by 4.100
 H₂ enhanced by 1.250
109. $\text{HNO} + \text{H} \longrightarrow \text{NO} + \text{H}_2$
 $k_A : 4.400000 \times 10^8 \quad 0.72 \quad 650.00$
110. $\text{HNO} + \text{O} \longrightarrow \text{NO} + \text{OH}$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
111. $\text{HNO} + \text{OH} \longrightarrow \text{NO} + \text{H}_2\text{O}$
 $k_A : 3.600000 \times 10^{10} \quad 0.00 \quad 0.00$
112. $\text{O}_2 + \text{HNO} \longrightarrow \text{NO} + \text{HO}_2$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 25000.00$
113. $\text{HNO} + \text{NH}_2 \longrightarrow \text{NO} + \text{NH}_3$
 $k_A : 2.000000 \times 10^{10} \quad 0.00 \quad 1000.00$
114. $\text{NO} + \text{HNO} \longrightarrow \text{N}_2\text{O} + \text{OH}$
 $k_A : 2.000000 \times 10^9 \quad 0.00 \quad 26000.00$
115. $\text{NO}_2 + \text{HNO} \longrightarrow \text{NO} + \text{HONO}$
 $k_A : 6.000000 \times 10^8 \quad 0.00 \quad 2000.00$
116. $2 \text{HNO} \longrightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$
 $k_A : 9.000000 \times 10^5 \quad 0.00 \quad 3100.00$
117. $\text{NO}_2 + \text{H}_2 \longrightarrow \text{HONO} + \text{H}$
 $k_A : 3.000000 \times 10^{10} \quad 0.00 \quad 29000.00$
118. $\text{HONO} + \text{O} \longrightarrow \text{NO}_2 + \text{OH}$
 $k_A : 1.200000 \times 10^{10} \quad 0.00 \quad 6000.00$
119. $\text{HONO} + \text{OH} \longrightarrow \text{NO}_2 + \text{H}_2\text{O}$
 $k_A : 4.000000 \times 10^9 \quad 0.00 \quad 0.00$
120. $\text{HONO} + \text{NH} \longrightarrow \text{NO}_2 + \text{NH}_2$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
121. $\text{HONO} + \text{NH}_2 \longrightarrow \text{NO}_2 + \text{NH}_3$
 $k_A : 5.000000 \times 10^9 \quad 0.00 \quad 0.00$
122. $2 \text{HONO} \longrightarrow \text{NO} + \text{NO}_2 + \text{H}_2\text{O}$
 $k_A : 1.020000 \times 10^{10} \quad 0.00 \quad 8540.00$
123. $\text{H}_2\text{NO} + \text{M} \longrightarrow \text{HNO} + \text{H} + \text{M}$
 $k_A : 1.000000 \times 10^{13} \quad 0.00 \quad 50000.00$
124. $\text{H} + \text{H}_2\text{NO} \longrightarrow \text{HNO} + \text{H}_2$
 $k_A : 3.000000 \times 10^4 \quad 2.00 \quad 2000.00$
125. $\text{H} + \text{H}_2\text{NO} \longrightarrow \text{OH} + \text{NH}_2$
 $k_A : 5.000000 \times 10^{10} \quad 0.00 \quad 0.00$
126. $\text{O} + \text{H}_2\text{NO} \longrightarrow \text{HNO} + \text{OH}$
 $k_A : 3.000000 \times 10^4 \quad 2.00 \quad 2000.00$
127. $\text{OH} + \text{H}_2\text{NO} \longrightarrow \text{HNO} + \text{H}_2\text{O}$
 $k_A : 2.000000 \times 10^4 \quad 2.00 \quad 1000.00$
128. $\text{NO} + \text{H}_2\text{NO} \longrightarrow {}_2\text{HNO}$
 $k_A : 2.000000 \times 10^1 \quad 2.00 \quad 13000.00$
129. $\text{NH}_2 + \text{H}_2\text{NO} \longrightarrow \text{HNO} + \text{NH}_3$
 $k_A : 3.000000 \times 10^9 \quad 0.00 \quad 1000.00$
130. $\text{NO}_2 + \text{H}_2\text{NO} \longrightarrow \text{HNO} + \text{HONO}$
 $k_A : 6.000000 \times 10^8 \quad 0.00 \quad 2000.00$
131. $\text{NO}_3 + \text{H} \longrightarrow \text{NO}_2 + \text{OH}$
 $k_A : 6.000000 \times 10^{10} \quad 0.00 \quad 0.00$
132. $\text{O} + \text{NO}_3 \longrightarrow \text{O}_2 + \text{NO}_2$
 $k_A : 1.000000 \times 10^{10} \quad 0.00 \quad 0.00$
133. $\text{NO}_3 + \text{OH} \longrightarrow \text{NO}_2 + \text{HO}_2$
 $k_A : 1.400000 \times 10^{10} \quad 0.00 \quad 0.00$
134. $\text{NO}_3 + \text{HO}_2 \longrightarrow \text{O}_2 + \text{NO}_2 + \text{OH}$
 $k_A : 1.500000 \times 10^9 \quad 0.00 \quad 0.00$
135. $\text{NO}_2 + \text{NO}_3 \longrightarrow \text{NO} + \text{O}_2 + \text{NO}_2$
 $k_A : 5.000000 \times 10^7 \quad 0.00 \quad 2940.00$
136. $\text{NO}_3 \longrightarrow \text{NO} + \text{O}_2$
 $k_A : 2.500000 \times 10^6 \quad 0.00 \quad 12000.00$
137. $2 \text{NO}_3 \longrightarrow \text{O}_2 + {}_2\text{NO}_2$
 $k_A : 5.100000 \times 10^8 \quad 0.00 \quad 6750.00$
138. $\text{NO}_2 + \text{HCO} \longrightarrow \text{NO} + \text{CO}_2 + \text{H}$
 $k_A : 8.400000 \times 10^{12} \quad -0.75 \quad 1930.00$
139. $\text{NO}_2 + \text{H} \longrightarrow \text{NO} + \text{OH}$
 $k_A : 1.320000 \times 10^{11} \quad 0.00 \quad 360.00$
140. $\text{NO}_2 + \text{O} \longrightarrow \text{NO} + \text{O}_2$
 $k_A : 3.900000 \times 10^9 \quad 0.00 \quad -238.00$

141. $\text{NO}_2 + \text{O} + \text{M} \longrightarrow \text{NO}_3 + \text{M}$
 $k_A : 2.940000 \times 10^{15} \quad -2.00 \quad 0.00$
142. $\text{NO}_2 + \text{HO}_2 \longrightarrow \text{O}_2 + \text{HONO}$
 $k_A : 6.310000 \times 10^5 \quad 1.25 \quad 5000.00$
143. $2\text{NO}_2 \longrightarrow 2\text{NO} + \text{O}_2$
 $k_A : 1.600000 \times 10^9 \quad 0.00 \quad 26123.00$
144. $2\text{NO}_2 \longrightarrow \text{NO} + \text{NO}_3$
 $k_A : 9.600000 \times 10^6 \quad 0.73 \quad 20923.00$
145. $2\text{NO}_2 \longrightarrow \text{NO} + \text{NO}_3$
 $k_A : 1.600000 \times 10^9 \quad 0.00 \quad 26123.00$
146. $\text{NO}_2 + \text{CO} \longrightarrow \text{NO} + \text{CO}_2$
 $k_A : 9.040000 \times 10^{10} \quad 0.00 \quad 33800.00$
147. $\text{NO}_2 + \text{HCO} \longrightarrow \text{HONO} + \text{CO}$
 $k_A : 1.200000 \times 10^{20} \quad -3.29 \quad 2355.00$
148. $\text{CO}_2 + \text{N} \longrightarrow \text{NO} + \text{CO}$
 $k_A : 1.900000 \times 10^8 \quad 0.00 \quad 3400.00$
149. $\text{N}_2\text{O} + \text{M} \longrightarrow \text{N}_2 + \text{O} + \text{M}$
 $k_A : 4.000000 \times 10^{11} \quad 0.00 \quad 56100.00$
 N_2 enhanced by 1.700
 O_2 enhanced by 1.400
 H_2O enhanced by 12.000
 CO enhanced by 1.500
 CO_2 enhanced by 3.000
150. $\text{N}_2\text{O} + \text{H} \longrightarrow \text{N}_2 + \text{OH}$
 $k_A : 3.300000 \times 10^7 \quad 0.00 \quad 4729.00$
151. $\text{N}_2\text{O} + \text{H} \longrightarrow \text{N}_2 + \text{OH}$
 $k_A : 4.400000 \times 10^{11} \quad 0.00 \quad 19254.00$
152. $\text{NO} + \text{NH} \longrightarrow \text{N}_2\text{O} + \text{H}$
 $k_A : 3.190000 \times 10^{11} \quad -0.46 \quad 0.00$
153. $\text{N}_2\text{O} + \text{O} \longrightarrow 2\text{NO}$
 $k_A : 2.900000 \times 10^{10} \quad 0.00 \quad 23150.00$
154. $\text{N}_2\text{O} + \text{O} \longrightarrow \text{N}_2 + \text{O}_2$
 $k_A : 1.400000 \times 10^9 \quad 0.00 \quad 10800.00$
155. $\text{N}_2\text{O} + \text{OH} \longrightarrow \text{N}_2 + \text{HO}_2$
 $k_A : 2.000000 \times 10^9 \quad 0.00 \quad 40000.00$
156. $\text{HNO}_2 + \text{H} \longrightarrow \text{NO}_2 + \text{H}_2$
 $k_A : 2.400000 \times 10^5 \quad 1.50 \quad 5087.00$
157. $\text{HNO}_2 + \text{O} \longrightarrow \text{NO}_2 + \text{OH}$
 $k_A : 1.700000 \times 10^5 \quad 1.50 \quad 3020.00$
158. $\text{HNO}_2 + \text{OH} \longrightarrow \text{NO}_2 + \text{H}_2\text{O}$
 $k_A : 1.200000 \times 10^3 \quad 2.00 \quad -596.00$
159. $\text{HNO}_2 \longrightarrow \text{HONO}$
 $k_A : 1.300000 \times 10^{29} \quad -5.47 \quad 52814.00$
160. $\text{NO}_2 + \text{OH}(=\text{M}) \longrightarrow \text{HONO}_2(=\text{M})$
Fall-off (Troe)
 $k_0 : 6.420000 \times 10^{26} \quad -5.49 \quad 2351.00$
 $k_\infty : 2.400000 \times 10^{10} \quad 0.00 \quad 0.00$
Troe Parameters:
 $a : 5.25 \times 10^{-1}$
 $T^* = T^{**} : 1.00 \times 10^{-15}$
 $T^{***} : 1.00 \times 10^{15}$
 H_2O enhanced by 5.000
161. $\text{HONO}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{NO}_3$
 $k_A : 1.030000 \times 10^7 \quad 0.00 \quad -1240.00$
162. $\text{H}_2 + \text{NH}_2 \longrightarrow \text{NH}_3 + \text{H}$
 $k_A : 1.576000 \times 10^2 \quad 2.00 \quad 3954.86$
163. $\text{H}_2\text{O} + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{OH}$
 $k_A : 5.388000 \times 10^2 \quad 2.00 \quad 28780.05$
164. $\text{H}_2\text{O} + \text{NH}_2 \longrightarrow \text{NH}_3 + \text{OH}$
 $k_A : 1.126000 \times 10^2 \quad 2.00 \quad 8169.13$
165. $\text{NO}_2 + \text{H}_2\text{O}_2 \longrightarrow \text{HONO} + \text{HO}_2$
 $k_A : 6.831000 \times 10^2 \quad 2.00 \quad 14711.89$
166. $\text{H}_2\text{O}_2 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{HO}_2$
 $k_A : 3.195000 \times 10^2 \quad 2.00 \quad -4169.95$
167. $\text{H}_2\text{O}_2 + \text{O} \longrightarrow \text{OH} + \text{HO}_2$
 $k_A : 1.083000 \times 10^3 \quad 2.00 \quad -1657.32$
168. $\text{H}_2\text{O}_2 + \text{NH}_2 \longrightarrow \text{NH}_3 + \text{HO}_2$
 $k_A : 9.005000 \times 10^0 \quad 2.00 \quad -1507.20$
169. $\text{O}_2 + \text{NH}_3 \longrightarrow \text{HO}_2 + \text{NH}_2$
 $k_A : 5.111000 \times 10^4 \quad 2.00 \quad 60086.33$
170. $\text{NH}_3 + \text{H} \longrightarrow \text{H}_2 + \text{NH}_2$
 $k_A : 7.220000 \times 10^4 \quad 2.00 \quad 15302.86$
171. $\text{NH}_3 + \text{OH} \longrightarrow \text{H}_2\text{O} + \text{NH}_2$
 $k_A : 1.198000 \times 10^4 \quad 2.00 \quad 4067.13$
172. $\text{NH}_3 + \text{O} \longrightarrow \text{OH} + \text{NH}_2$
 $k_A : 4.060000 \times 10^4 \quad 2.00 \quad 13586.66$
173. $\text{NH}_3 + \text{HO}_2 \longrightarrow \text{H}_2\text{O}_2 + \text{NH}_2$
 $k_A : 1.616000 \times 10^3 \quad 2.00 \quad 27340.80$

Appendix C

OpenFOAM Standard Boundary Conditions

In this appendix, we provide an overview of the standard boundary conditions available in OpenFOAM that can be utilized by users.

Table C.1 presents the basic boundary conditions, while Table C.2 demonstrates the constraint-based boundary conditions. Generic boundary conditions are detailed in Table C.3 and wall boundary conditions in Table C.4. For inlet, outlet and coupled boundary conditions relevant information, one can access [183], where a comprehensive guide can be found. These tables serve as valuable references for users seeking to apply appropriate boundary conditions in their OpenFOAM simulations.

Table C.1: Basic boundary conditions [183]

<i>calculated</i>	This boundary condition is not designed to be evaluated; it is assumed that the value is assigned via field assignment, and not via a call to e.g. <code>updateCoeffs</code> or <code>evaluate</code>
<i>fixedValue</i>	This boundary condition supplies a fixed value constraint, and is the base class for a number of other boundary conditions
<i>fixedGradient</i>	This boundary condition supplies a fixed gradient condition, such that the patch values are calculated using:
<i>zeroGradient</i>	This boundary condition applies a zero-gradient condition from the patch internal field onto the patch faces
<i>mixed</i>	This boundary condition provides a base class for 'mixed' type boundary conditions, i.e. conditions that mix fixed value and patch-normal gradient conditions
<i>directionMixed</i>	Base class for direction-mixed boundary conditions
<i>extrapolatedCalculated</i>	This boundary condition applies a zero-gradient condition from the patch internal field onto the patch faces when evaluated but may also be assigned. <code>snGrad</code> returns the patch gradient evaluated from the current internal and patch field values rather than returning zero

Table C.2: Constraint boundary conditions [183]

<i>cyclic</i>	This boundary condition enforces a cyclic condition between a pair of boundaries
<i>cyclicACMI</i>	This boundary condition enforces a cyclic condition between a pair of boundaries, whereby communication between the patches is performed using an arbitrarily coupled mesh interface (ACMI) interpolation
<i>cyclicAMI</i>	This boundary condition enforces a cyclic condition between a pair of boundaries, whereby communication between the patches is performed using an arbitrary mesh interface (AMI) interpolation
<i>cyclicSlip</i>	This boundary condition is a light wrapper around the cyclicFvPatchField condition, providing no new functionality
<i>empty</i>	This boundary condition provides an 'empty' condition for reduced dimensions cases, i.e. 1- and 2-D geometries. Apply this condition to patches whose normal is aligned to geometric directions that do not constitute solution directions
<i>jumpCyclic</i>	This boundary condition provides a base class for coupled-cyclic conditions with a specified 'jump' (or offset) between the values
<i>jumpCyclicAMI</i>	This boundary condition provides a base class that enforces a cyclic condition with a specified 'jump' (or offset) between a pair of boundaries, whereby communication between the patches is performed using an arbitrary mesh interface (AMI) interpolation
<i>nonuniformTransformCyclic</i>	This boundary condition enforces a cyclic condition between a pair of boundaries, incorporating a non-uniform transformation
<i>processor</i>	This boundary condition enables processor communication across patches
<i>processorCyclic</i>	This boundary condition enables processor communication across cyclic patches
<i>symmetry</i>	This boundary condition enforces a symmetry constraint
<i>symmetryPlane</i>	This boundary condition enforces a symmetryPlane constraint
<i>wedge</i>	This boundary condition is similar to the cyclic condition, except that it is applied to 2-D geometries

Table C.3: Generic boundary conditions [183]

<i>codedFixedValue</i>	Constructs on-the-fly a new boundary condition (derived from fixedValueFvPatchField) which is then used to evaluate
<i>codedMixed</i>	Constructs on-the-fly a new boundary condition (derived from mixedFvPatchField) which is then used to evaluate
<i>fixedInternalValue-FvPatchField</i>	This boundary condition provides a mechanism to set boundary (cell) values directly into a matrix, i.e. to set a constraint condition. Default behaviour is to act as a zero gradient condition

(table continues on next page)

Table C.3: Continuation of previous Table [183]

<i>fixedNormalSlip</i>	This boundary condition sets the patch-normal component to a fixed value
<i>fixedProfile</i>	This boundary condition provides a fixed value profile condition
<i>interfaceCompression</i>	Applies interface-compression to the phase-fraction distribution at the patch by setting the phase-fraction to 0 if it is below 0.5, otherwise to 1
<i>mappedField</i>	This boundary condition provides a self-contained version of the mapped condition. It does not use information on the patch; instead it holds the data locally
<i>mappedFixedInternalValue</i>	This boundary condition maps the boundary and internal values of a neighbour patch field to the boundary and internal values of *this
<i>mappedFixedPushed-InternalValue</i>	This boundary condition maps the boundary values of a neighbour patch field to the boundary and internal cell values of *this
<i>mappedFixedValue</i>	This boundary condition maps the value at a set of cells or patch faces back to *this
<i>partialSlip</i>	This boundary condition provides a partial slip condition. The amount of slip is controlled by a user-supplied field
<i>phaseHydrostaticPressure</i>	This boundary condition provides a phase-based hydrostatic pressure condition, calculated as:
<i>prghPressure</i>	This boundary condition provides static pressure condition for p_rgh, calculated as:
<i>prghTotalHydrostaticPressure</i>	This boundary condition provides static pressure condition for p_rgh, calculated as:
<i>prghTotalPressure</i>	This boundary condition provides static pressure condition for p_rgh, calculated as:
<i>rotatingWallVelocity</i>	This boundary condition provides a rotational velocity condition
<i>scaledFixedValue</i>	This condition applies a scalar multiplier to the value of another boundary condition
<i>slip</i>	This boundary condition provides a slip constraint
<i>surfaceNormalFixedValue</i>	This boundary condition provides a surface-normal vector boundary condition by its magnitude
<i>translatingWallVelocity</i>	This boundary condition provides a velocity condition for translational motion on walls
<i>uniformDensityHydrostaticPressure</i>	This boundary condition provides a hydrostatic pressure condition, calculated as:
<i>uniformFixedGradient</i>	This boundary condition provides a uniform fixed gradient condition
<i>uniformFixedValue</i>	This boundary condition provides a uniform fixed value condition
<i>uniformNormalFixedValue</i>	This boundary condition provides a uniform surface-normal vector boundary condition by its magnitude

Table C.4: Wall boundary conditions [183]

<i>fixedFluxExtrapolated-Pressure</i>	This boundary condition sets the pressure gradient to the provided value such that the flux on the boundary is that specified by the velocity boundary condition
<i>fixedFluxPressure</i>	This boundary condition sets the pressure gradient to the provided value such that the flux on the boundary is that specified by the velocity boundary condition
<i>fixedNormalSlip</i>	This boundary condition sets the patch-normal component to a fixed value
<i>movingWallVelocity</i>	This boundary condition provides a velocity condition for cases with moving walls
<i>noSlip</i>	This boundary condition fixes the velocity to zero at walls
<i>partialSlip</i>	This boundary condition provides a partial slip condition. The amount of slip is controlled by a user-supplied field
<i>rotatingWallVelocity</i>	This boundary condition provides a rotational velocity condition
<i>slip</i>	This boundary condition provides a slip constraint
<i>translatingWallVelocity</i>	This boundary condition provides a velocity condition for translational motion on walls

Appendix D

Setting up a simulation

Ensure that your file organization aligns with the guidelines presented in Chapter 4, specifically detailed in Section 4.2. In this process, it's essential to establish a proper file structure. Additionally, you'll need to generate two supplementary files. The first is a **.sh** script, shown in Listing D.1, which serves to initiate the simulation on the cluster. This script coordinates the simulation.

```
1  #!/bin/bash
2  #SBATCH --time=720:00:00           # maximum simulation time
3  #SBATCH --ntasks=1                # number of processor cores (i.e. tasks)
4  #SBATCH --nodes=1                 # number of nodes
5  #SBATCH -J "SimName"              # job name (maximum of 8 digits)
6  #SBATCH --mail-user=local@domain  # email address
7  #SBATCH --mail-type=BEGIN
8  #SBATCH --mail-type=END
9
10 # Setting up the environment (loads paths and configurations) for OpenFOAM version 2.3.0
11 module load openfoam/2.3.0
12 source $FOAM
13
14 # Setting up Boost libraries for programs to access.
15 export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:$HOME/NumericalLibraries/Boost/boost_1_58_0/lib
16
17 # Tells the shell to change the current directory to a directory located at the specified
18 ↪ absolute path.
19 cd /homes/UserDirectory/runs/GeneralSimFolder/SpecificSimFolder
20
21 # Used to apply custom initial (t=0) temperature profiles to different regions in your
22 ↪ simulation geometry (for non-cold wall start, with imposed temperature)
23 funkySetFields -time 0 -region solidRegion1
24 funkySetFields -time 0 -region solidRegion2
25
26 # Lines of code for orchestrating a parallel simulation in OpenFOAM
27 #decomposePar
28 #decomposePar -allRegions -constant
29 #mpirun -np 4 chtDoublelaminarPimpleSMOKE > log_U10_H2_CHT_Imposed_LTCC_HQm -parallel
30
31 # Lines of code for orchestrating a singular core simulation in OpenFOAM
32 chtDoublelaminarPimpleSMOKE > log_U10_H2_CHT_Imposed_LTCC_HQm
```

Code Listing D.1: Initialization **.sh** Bash shell script (Unix), to start a job in HPC.

The next file, a **.foam** file, essentially functions as a placeholder, serving as a beacon for ParaView to access the simulation's data output, enabling data visualization during later OpenFOAM simulation stages. Although this file doesn't hold any actual data, it operates as a linkage or signpost directing ParaView to the simulation results. This streamlines data loading and structured visualization.

As seen in Section 4.6, we used the HPC Cluster from FEUP, using a Secure Shell (SSH) connection. To initially start a simulation, you first need to ascertain the current availability of computational resources, specifically the unused CPUs in the cluster, and for that, users can employ the command:

```
1 $ qtop
```

which will basically give the user an interactive overview of the ongoing activities and resource utilization within the HPC cluster's job scheduling system. After confirming the availability of computational resources, initiating the simulation involves a two-step process. Initially, you must ensure the executability of the designated .sh script (makes the **SimName.sh** script executable, allowing it to be run like a program.), and after, submit a batch job^(a) to the cluster's job scheduler. This is achieved by writing the following line in the shell:

```
1 $ chmod a+x SimName.sh
2 $ sbatch SimName.sh
```

As a final remark, if one wants to generate the mesh and refine it, you can add the following lines to the initialization script shown in Listing D.1 (this does not need to be done if in the files it's already present *PolyMesh* files).

```
1 # Generates and manipulates meshes, which includes mirroring through mirrorMesh, and scaling
   ↳ down mesh points using transformPoints.
2 blockMesh
3 gmshToFoam Channel_undulate_PR_M8_1.msh
4 mirrorMesh
5 transformPoints -scale '(0.00001 0.00001 0.00001)'
6
7 # Defines topological set and then applies mesh refinement based on the provided
   ↳ dictionaries.
8 topoSet -dict system/myTopoSet.topoSet
9 refineMesh -overwrite -dict system/refineMeshDictf
```

Code Listing D.2: Snippet of the Mesh generation and refinement Bash shell script (Unix).

^(a)A batch job is a task or a series of tasks that can be run independently. When you use sbatch, you're essentially telling the cluster to queue up and execute a specified job script.

Appendix E

Data analysis programs

E.1 Fast Fourier Transform

```
1  % read in file with textscan (must be power 2^n)
2  a = load('U10_QnT.dat');
3  % time
4  t=a(:,1);
5  % sinal
6  s=a(:,2);
7  %delta time
8  dt=t(2)-t(1)
9  m=length(s)
10 y=fft(s);
11 power=y.*conj(y)/m;
12 power(1)=0.;
13 f=(0:m-1)*(1/dt)/m;
14
15 %plot(f,power);
16 if mod(m,2)==0
17     m = m;
18 else
19     m = m - 1;
20 end
21
22 ppp = zeros(m/2+1, 2);
23
24 % save half file
25 for n = 1:m/2+1
26     ppp(n,1)=f(n);
27     ppp(n,2)=power(n);
28 end
29
30 dlmwrite('fft_sinal.dat',ppp,'precision',8,'delimiter',' ');
31 [num idx] = max(ppp(:,2));
32 freqpeak=ppp(idx,1)
33
34 plot(t,s)
```

Code Listing E.1: Fast Fourier Transform script file in MATLAB.

E.2 Cumulative integral

```
1  % Load data from the .dat file
2  data = load('dataint.dat');
3  time = data(:, 1);
4  var = data(:, 2);
5
6  % Calculate cumulative variable using cumtrapz
7  cintvar = cumtrapz(time, var);
8
9  % Create a table to display time and cumulative integrated variable
10 T = table(time, cintvar, 'VariableNames', {'Time', 'CumulativeIntVar'});
11
12 % Display the table
13 disp(T);
14
15 % Plot the cumulative integrated variable
16 plot(time, cintvar);
17 title('Cumulative variable per unit time');
18 xlabel('Time');
19 ylabel('Integrated Variable');
20
21 % Save the table to a new data file
22 writetable(T, 'cumint.dat', 'Delimiter', '\t');
23 disp('Data saved to output_data.dat');
```

Code Listing E.2: Cumulative integral script file in MATLAB.