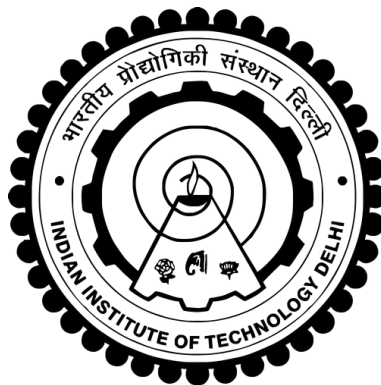


PRE-MIXED FLAME ACCELERATION AND INHIBITION IN PARTIALLY CONFINED GEOMETRIES

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by

Ayushi Mishra

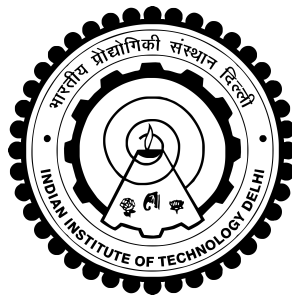
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CERTIFICATE

This is to certify that the thesis titled **Pre-mixed flame acceleration and inhibition in partially confined geometries**, submitted by **Mrs. Ayushi Mishra**, to the Indian Institute of Technology, Delhi, for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research work done by her under our supervision and guidance. The contents of this thesis, in full or in parts, have not been submitted to any other Institute or University for the award of any degree or diploma.

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ABSTRACT

Combustible gases such as ethylene, propane, methane, and hydrogen are widely used in petrochemical engineering, power generation, metallurgy, mining, transportation, and gas supply industries. However, during their manufacturing, transportation, storage, and use, these gases can pose significant hazards. When a premixed combustible gas and air mixture ignites, the flame can accelerate as it interacts with obstacles and confinement walls, potentially leading to highly dangerous explosions. The dynamics of flame propagation in such mixtures are strongly influenced by the geometrical characteristics of the confinement. This work explores the mechanisms of flame acceleration caused by both obstacles and walls, with an emphasis on reducing explosion overpressure to mitigate associated hazards.

In the obstacle study, most previous research has focused on linear plate-type blockages, which offer predominantly one-dimensional obstruction. In contrast, this work investigates the effects of obstacles with area (2D) and volume (3D) blockage, providing a more realistic representation of real-world geometries. The study involves numerical simulations using the XiFOAM solver in OpenFOAM. Four different Flame Surface Density (FSD) combustion models are evaluated, and the Weller model is selected along with a dynamic k -equation LES turbulence model. A correlation between the turbulent intensity of flame surface and the resulting overpressure is established, showing a strong linear relationship with an R^2 value of 0.85. The outcomes of this study offer valuable insights into the design of indoor spaces to minimize extreme overpressure caused by sudden ignition of premixed gases.

Another major cause of flame acceleration is wall confinement. In relatively narrow pipes, flame acceleration can be comparable to that produced by multiple obstacles with a blockage ratio of 50 %. The acceleration mechanism in plain pipes differs significantly from that in obstructed configurations; here, the flame undergoes repeated acceleration and deceleration phases, particularly in mixtures with low laminar burning velocities such as hydrocarbon fuels. During the first

deceleration phase, a tulip flame forms - a purely hydrodynamic phenomenon arising due to wall effects. Consequently, this work investigates the influence of wall boundary conditions on flame acceleration and tulip flame formation. The effects of constant wall temperature (T_{wall}) and wall roughness are examined, with roughness introduced numerically through modifications in the wall boundary condition of dynamic viscosity. Since tulip flame formation is flow-driven, additional studies are conducted by altering the flow field through natural and forced venting. The results show that natural vents located close to the ignition point are most effective in reducing flame acceleration and overpressure.

In addition, an experimental investigation is carried out to study flame inhibition through the introduction of solid aerosol additives. This part of the study examines both obstructed and unobstructed geometries. Two metal-salt aerosols are introduced into the premixed fuel-air mixture before ignition to assess their inhibitory effects. The synergistic influence of obstacle positioning and aerosol addition is also analyzed. The chosen geometry allows for studying aerosol inhibition in both laminar and turbulent flame regimes: the flame behavior before the tulip formation (first retardation point) is predominantly laminar, while after it, the flame becomes highly turbulent. For plain propane-air mixtures, a clear trend is observed where overpressure increases as the obstacle moves upstream; however, for aerosol-laden mixtures, a more complex relationship emerges, which is discussed in detail in the relevant chapter.

The findings of this work contribute to a deeper understanding of flame acceleration mechanisms in confined geometries and the influence of obstacles, wall conditions, and venting on explosion behavior. The established correlation between flame turbulence and overpressure provides a useful predictive basis for safer structural design. Furthermore, the study on aerosol-based inhibition offers practical insights into flame suppression strategies, also providing a useful comparison between the two commonly used metal salts, KCl and KHCO_3 . Together, these results can guide future efforts toward developing more effective explosion mitigation and flame control techniques in industrial applications.

सारांश

एथिलीन, प्रोपेन, मीथेन और हाइड्रोजन जैसे दहनशील गैसों का व्यापक उपयोग पेट्रोकेमिकल इंजीनियरिंग, विद्युत उत्पादन, धातुकर्म, खनन, परिवहन तथा गैस आपूर्ति जैसी अनेक औद्योगिक और दैनिक जीवन की गतिविधियों में किया जाता है। तथापि, इन गैसों के निर्माण, परिवहन, भंडारण और उपयोग के दौरान गंभीर खतरे उत्पन्न हो सकते हैं। जब दहनशील गैस और वायु का मिश्रण प्रज्वलित होता है, तो लौ (फ्लेम) अपने मार्ग में उपस्थित अवरोधों तथा सीमित दीवारों के साथ पारस्परिक क्रिया के कारण तीव्र गति से फैल सकती है, जिससे अत्यंत खतरनाक विस्फोट हो सकते हैं। ऐसे मिश्रणों में लौ के प्रसार की गतिकी, परिबंध (confinement) की ज्यामितीय विशेषताओं पर अत्यधिक निर्भर होती है। यह शोध कार्य, अवरोधों तथा दीवारों द्वारा उत्पन्न लौ त्वरक (flame acceleration) तंत्र का अध्ययन करता है, जिसका उद्देश्य विस्फोट से उत्पन्न अधिकतम दाब (overpressure) को कम करके जोखिमों को नियंत्रित करना है।

अवरोधों से संबंधित अध्ययन में अब तक अधिकांश शोध रेखीय प्लेट-प्रकार की रुकावटों पर केंद्रित रहे हैं, जो मुख्यतः एक-आयामी (1D) अवरोध प्रदान करती हैं। इसके विपरीत, इस कार्य में क्षेत्रीय (2D) तथा आयतनात्मक (3D) अवरोधों के प्रभावों की जांच की गई है, जो वास्तविक जीवन की संरचनाओं का अधिक यथार्थवादी प्रतिरूप प्रस्तुत करते हैं। यह अध्ययन OpenFOAM सॉफ्टवेयर के XiFOAM सॉल्वर का उपयोग करते हुए संख्यात्मक रूप से किया गया है। चार विभिन्न फ्लेम सरफेस डेंसिटी (FSD) दहन मॉडलों का मूल्यांकन किया गया, जिनमें से Weller मॉडल को चुना गया और इसके साथ डायनेमिक k -इंक्लेशन LES टर्बुलेंस मॉडल का प्रयोग किया गया। लौ सतह की अशांतता तीव्रता (turbulent intensity) और उत्पन्न अतिदाब (overpressure) के बीच एक प्रत्यक्ष रैखिक संबंध स्थापित किया गया, जिसका $R^2 = 0.85$ प्राप्त हुआ। इस अध्ययन के निष्कर्ष इनडोर संरचनाओं के डिजाइन में सहायक हो सकते हैं ताकि मिश्रित गैसों की आकस्मिक प्रज्वलन से उत्पन्न अत्यधिक अतिदाब को कम किया जा सके।

लौ त्वरक का एक अन्य प्रमुख कारण दीवारों द्वारा उत्पन्न परिबंध है। अपेक्षाकृत संकीर्ण पाइपों में लौ की गति उतनी ही तीव्र हो सकती है जितनी कि 50% ब्लॉकज अनुपात वाले कई अवरोधों की उपस्थिति में होती है।

सादे पाइपों में लौ त्वरक का तंत्र अवरोधित ज्यामिति से काफी भिन्न होता है; यहाँ लौ, विशेष रूप से कम लैमिनर बर्निंग वेग वाले हाइड्रोकार्बन ईंधनों में, बार-बार त्वरित और मंदन (a चरणों से गुजरती है। पहले मंदन चरण के दौरान “ट्यूलिप फ्लेम” नामक संरचना बनती है, जो दीवारों की उपस्थिति से उत्पन्न एक शुद्ध हाइड्रोडायनामिक परिघटना है। इस कारण, इस शोध में दीवार सीमा परिस्थितियों (wall boundary conditions) का लौ त्वरक और ट्यूलिप लौ निर्माण पर प्रभाव का अध्ययन किया गया है। स्थिर दीवार तापमान (T_{wall}) और दीवार की खुरदरापन (roughness) के प्रभावों की जांच की गई है, जहाँ खुरदरापन को डायनेमिक विस्कॉसिटी की सीमा शर्तों में परिवर्तन कर के संख्यात्मक रूप से लागू किया गया। चूँकि ट्यूलिप लौ का निर्माण प्रवाह-चालित (flow-driven) प्रक्रिया है, इसलिए प्रवाह को बदलने के लिए प्राकृतिक तथा बाध्य (forced) वेंटिंग की स्थितियों का भी परीक्षण किया गया। परिणामों से पता चला कि प्रज्वलन बिंदु के निकट स्थित प्राकृतिक वेंट, लौ त्वरक और अतिदाब को न्यूनतम करने में सबसे अधिक प्रभावी हैं।

इसके अतिरिक्त, ठोस एरोसोल योजकों के माध्यम से लौ अवरोधन (flame inhibition) का अध्ययन करने के लिए एक प्रायोगिक जांच भी की गई। इस भाग में अवरोधित तथा अनवरोधित दोनों प्रकार की ज्यामितियों का परीक्षण किया गया। दो प्रकार के धातु-लवण एरोसोलों को प्रज्वलन से पूर्व ईंधन-वायु मिश्रण में सम्मिलित किया गया ताकि उनके दमनकारी प्रभावों का मूल्यांकन किया जा सके। अवरोध की स्थिति तथा एरोसोल की उपस्थिति के समन्वित प्रभाव (synergistic effects) का भी विश्लेषण किया गया। प्रयुक्त ज्यामिति ने लौ अवरोधन के अध्ययन को लैमिनर तथा टर्बुलेंट दोनों अवस्थाओं में संभव बनाया — जहाँ ट्यूलिप लौ के बनने से पूर्व का व्यवहार मुख्यतः लैमिनर होता है, जबकि उसके पश्चात लौ अत्यधिक अशांत हो जाती है। शुद्ध प्रोपेन-वायु मिश्रणों के लिए यह पाया गया कि जैसे-जैसे अवरोध प्रज्वलन बिंदु की ओर अग्रसर होता है, अतिदाब बढ़ता है; किंतु एरोसोल मिश्रणों के लिए यह संबंध अधिक जटिल पाया गया, जिसका विवरण संबंधित अध्याय में प्रस्तुत किया गया है।

इस कार्य के निष्कर्ष परिबंधित ज्यामितियों में लौ त्वरक तंत्र, अवरोधों, दीवार स्थितियों तथा वेंटिंग के प्रभावों की गहरी समझ प्रदान करते हैं। लौ की अशांतता और उत्पन्न अतिदाब के बीच स्थापित संबंध, सुरक्षित संरचनात्मक डिजाइन के लिए एक उपयोगी पूर्वानुमानात्मक आधार प्रस्तुत करता है। साथ ही, एरोसोल-आधारित लौ अवरोधन के अध्ययन से आकस्मिक गैस प्रज्वलन की स्थितियों में दमन रणनीतियाँ विकसित करने हेतु व्यावहारिक अंतर्दृष्टि प्राप्त होती है। समग्र रूप से, यह शोध औद्योगिक अनुप्रयोगों में विस्फोट नियंत्रण और लौ प्रबंधन की प्रभावी तकनीकों के विकास की दिशा में उपयोगी योगदान देता है।

Contents

CERTIFICATE	i
ACKNOWLEDGEMENTS	ii
ABSTRACT	iv
List of figures	xvi
List of tables	xvii
List of Abbreviations	xviii
1 Introduction	1
1.1 Flame acceleration	3
1.2 Flame inhibition	6
1.3 Objectives of the present study	9
1.4 Thesis organization	9
2 Literature review	11
2.1 Methodology	11
2.2 Experimental and numerical studies on flame acceleration	13
2.2.1 With obstacles	14
2.2.2 Plain pipes	16
2.3 Flame inhibition using aerosols	17
2.4 Literature gaps	19
3 Experimental methodology	21
3.1 Test chamber	21

3.2	Aerosol generator	23
3.3	Measuring and recording	23
3.4	Flame image processing	24
3.5	Obstacle details and location	25
3.6	Ignition circuit	26
3.7	Test sequence	26
3.8	Repeatability and uncertainty	29
3.8.1	Pressure measurement	29
3.8.2	Flame tip speed	29
4	Numerical methodology	32
4.1	Numerical approach for obstacle cases	32
4.1.1	Geometry and mesh	32
4.1.2	Boundary and initial conditions	33
4.1.3	Numerical details	34
4.1.4	Effect of turbulence models	36
4.1.5	Effect of combustion models	38
4.1.6	Thermophysical and transport properties	41
4.2	Numerical approach for plain pipe cases	44
4.2.1	Geometry and mesh	44
4.2.2	Effect of turbulence model	44
4.2.3	Effect of combustion model	45
5	Effect of numerical schemes	47
5.1	Overpressure plots with old discretization schemes	48
5.2	Overpressure plots with new discretization schemes	51
5.3	Flame contours comparison	53
5.4	Effect of each discretization scheme	54
5.5	Summary	55
6	Effect of shape of obstacles and their configurations	58
6.1	Dependence on the shape of obstacles	59
6.2	Dependence on separation distance between the obstacles	60

6.3	Dependence on staggered vs in-line obstacles	64
6.4	Dependence on number of obstacles	68
6.5	Oscillatory pressure behavior	73
6.6	Maximum overpressure versus maximum flame surface area	77
6.7	Summary	80
7	Flame acceleration in plain pipes	82
7.1	Tulip flames	82
7.1.1	Stages of flame acceleration in plain pipes	83
7.1.2	Borghi diagram for flame acceleration in plain pipes	85
7.2	Effect of wall boundary conditions	88
7.2.1	Isothermal and adiabatic walls	88
7.2.2	Different wall temperatures	90
7.2.3	Varying wall roughness	95
7.3	Effect of vents	97
7.3.1	Natural vents	97
7.3.2	Forced vents	103
7.4	Summary	109
8	Experimental study on effects of obstacles and aerosols	113
8.1	Particle concentration and mass of aerosol for different molarities	113
8.2	Propane–air mixture with obstacles	115
8.2.1	No obstacle case	115
8.2.2	One obstacle at 79 cm	116
8.2.3	One obstacle at 69 cm	119
8.2.4	One obstacle at 59 cm	121
8.2.5	Comparison of all propane–air cases	122
8.3	Flame inhibition by potassium chloride	125
8.4	Flame inhibition by potassium bicarbonate	126
8.5	Flame inhibition by potassium chloride with obstacles	130
8.5.1	Obstacle at 79 cm	130
8.5.2	Obstacle at 69 cm	131

8.5.3	Obstacle at 59 cm	134
8.5.4	Comparison of all 3M KCl inhibition cases	136
8.6	Reasoning for complex behavior of aerosol flames	138
8.7	Summary	141
9	Conclusions and future work	143
	References	156
	Brief biodata and publications	157

List of Figures

1.1	Gas explosion at Kaohsiung, Taiwan [7]	2
1.2	Representation of turbulent flame [15]	3
1.3	Positive feedback mechanism [16]	4
1.4	Modified turbulent combustion diagram by Peters [17]	5
3.1	(a) Schematic of test channel, (b) real image of the test channel, and (c) various housing points in section A of the test channel	22
3.2	(a) Obstacle cutting by water jet machine, and (b) dimensions of obstacle with BR =30 %	25
3.3	Ignition circuit schematic	26
3.4	Experimental setup schematic	28
3.5	Mean pressure evolution with experimental uncertainty	29
3.6	Flame tip speed with experimental uncertainty	31
4.1	(a) Experimental setup schematic by Patel et al. [105], (b) computational domain with boundary conditions, and (c) hexahedral mesh details	33
4.2	Comparison of turbulence models	37
4.3	(a) Validation of overpressure for four combustion models, (b) validation of flame tip speed for Weller model with experimental results by Patel et al. [105], (c) flame morphology for experiments, and (d) flame morphology for simulations	42
4.4	Geometry and mesh details for plain pipe	45
4.5	Comparison of turbulence models for plain pipe	46
4.6	Comparison of combustion models for plain pipe	46
5.1	Overpressure variation plots with (a) k , (b) Δt , (c) Δx , and (d) $maxCo$ with old set of discretization schemes	50
5.2	Overpressure variation plots with (a) k , (b) Δt , (c) Δx , and (d) $maxCo$ with new set of discretization schemes	52

5.3	(a) Flame contour and (b) overpressure with new discretization schemes, and (c) flame contour and (d) overpressure with old discretization schemes	54
5.4	Discretization scheme comparison (a) divergence terms, (b) temporal term, and (c) pressure-velocity coupling	56
6.1	(a) Four different shapes of obstacles with standard spacing, (b) squeezed-in and spaced-out configurations, (c) staggered configuration, and (d) squeezed-in configuration with five obstacles. The obstacle setups in (b), (c), and (d) are only shown for triangle, the study includes all the four shapes	60
6.2	Comparison of four different shape of obstacles (a) overpressure, (b) flame tip position, and (c) flame tip speed	61
6.3	Flame contours at specific locations for different shapes of obstacles (a) pre first obstacle, (b) post first obstacle, (c) post second obstacle, and (d) post third obstacle	62
6.4	Comparison of separation distance for triangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	64
6.5	Comparison of separation distance for rectangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	65
6.6	Comparison of separation distance for ellipse obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	66
6.7	Comparison of separation distance for circle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	67
6.8	Comparison of flame contours for separation distance (a) rectangle, (b) triangle, (c) ellipse, and (d) circle	68
6.9	Comparison of in-line and staggered setup for triangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	69
6.10	Comparison of in-line and staggered setup for rectangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	70
6.11	Comparison of in-line and staggered setup for ellipse obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	71
6.12	Comparison of in-line and staggered setup for circle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	72
6.13	Comparison of flame contours for in-line and staggered setup (a) rectangle, (b) triangle, (c) ellipse, and (d) circle	73
6.14	Comparison of number of obstacles for triangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	74
6.15	Comparison of number of obstacles for rectangle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	75
6.16	Comparison of number of obstacles for ellipse obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	76

6.17	Comparison of number of obstacles for circle obstacles (a) overpressure, (b) flame tip positions, and (c) flame tip speeds	77
6.18	Flame contours for squeezed-in setup with 5 obstacles (a) triangle, (b) rectangle, (c) ellipse, and (d) circle	78
6.19	(a) Oscillatory behavior with exponential curve fit and their difference for rectangle case, (b) for triangle case (c) FFT analysis for rectangle, and (d) triangle . . .	78
6.20	(a) Flame surface area, and (b) flame tip speed for triangle, rectangle and ellipse staggered cases	79
6.21	Comparison of maximum flame surface area and peak overpressure using scatter plot	79
7.1	Flame evolution in plain pipe (a) experimental results, and (b) simulation results	83
7.2	Flame propagation behavior in plain pipes (a) flame tip speed, and (b) overpressure	84
7.3	Stages of flame acceleration in plain pipes with experimental images by Ponizy et al. [68]	86
7.4	(a) Borghi diagram for flame acceleration in plain pipes, and (b) v'/S_l and flame tip speed with time	87
7.5	Structural evolution for flame acceleration in plain pipes, shaded with v'/S_l . .	88
7.6	Comparison of iso-thermal and adiabatic wall boundary conditions with experimental results (a) flame tip speed, and (b) overpressure	89
7.7	Flame morphology for iso-thermal and adiabatic wall boundary at different time instances	90
7.8	(a) Flame tip distance, and (b) flame tip speed for different wall temperatures .	92
7.9	Flame morphology for different wall temperatures	92
7.10	Temperature and velocity contours for $T_{wall} = 1500$ K at $t = 28, 40$ and 55 ms .	93
7.11	Pressure distribution inside the pipe for different wall temperatures	94
7.12	Pressure and velocity contours for first 5 ms for $T_{wall} = 1500$ K	95
7.13	Comparison of different wall roughness cases (a) flame tip speed, and (b) overpressure	96
7.14	Flame morphology for (a) 0.0005 m, and (b) 0.005 m wall roughness	97
7.15	Vent location for (a) middle vent, and (b) start vent	99
7.16	Effect of vent location (a) flame tip position, (b) flame tip speed, and (c) overpressure	100
7.17	Flame structural evolution and flow behavior for middle vent (left, (a), and (c)) and start vent (right, (b), and (d))	100

7.18	Effect of vent area and number for centrally located vents (a) flame tip position, (b) flame tip speed, and (c) overpressure	102
7.19	Effect of vent area and number for vents located near ignition (a) flame tip position, (b) flame tip speed, and (c) overpressure	104
7.20	Flame structural evolution for (a) single vent with size $9mm^2$, and (b) double vents with size $2 \times 4mm^2$	104
7.21	Forced vent condition for (a) middle vent, and (b) start vent	105
7.22	Effect of forced vent condition for centrally located vent (a) flame tip position, (b) flame tip speed, (c) overpressure, and (d) flame surface area	107
7.23	Flame structural evolution and flow behavior for (a) inlet-vent, and (b) outlet-vent located centrally	107
7.24	Effect of forced vent condition for vent located close to ignition (a) flame tip position, (b) flame tip speed, (c) overpressure, and (d) flame surface area	110
7.25	Flame structural evolution and flow behavior for (a) inlet-vent, and (b) outlet-vent located close to ignition	110
8.1	Number concentration with particle size for different molarities of aqueous solutions	115
8.2	Overpressure and flame tip speed plot for without obstacle case	117
8.3	Flame morphology for without obstacle case	117
8.4	Overpressure and flame tip speed plot for obstacle at 79 cm	119
8.5	Flame morphology for obstacle at 79 cm	119
8.6	Overpressure and flame tip speed plot for obstacle at 69 cm	120
8.7	Flame morphology for obstacle at 69 cm	121
8.8	Overpressure and flame tip speed plot for obstacle at 59 cm	122
8.9	Flame morphology for obstacle at 59 cm	122
8.10	Comparison of all propane–air cases (a) flame tip position, (b) flame tip speed, and (c) overpressure	124
8.11	Comparison of KCl inhibition cases (a) flame tip position, (b) flame tip speed, and (c) overpressure	127
8.12	Flame morphology for (a) 1M KCl aerosol, and (b) 3M KCl aerosol	127
8.13	Comparison of $KHCO_3$ inhibition cases (a) flame tip position, (b) flame tip speed, and (c) overpressure	129
8.14	Flame morphology for (a) 1M $KHCO_3$ aerosol, and (b) 3M $KHCO_3$ aerosol	129
8.15	KCl inhibition with obstacle at 79 cm (a) flame tip position, (b) flame tip speed, and (c) overpressure	132

8.16	Flame morphology for KCl with obstacle at 79 cm	133
8.17	KCl inhibition with obstacle at 69 cm (a) flame tip position, (b) flame tip speed, and (c) overpressure	133
8.18	Flame morphology for KCl with obstacle at 69 cm	134
8.19	KCl inhibition with obstacle at 59 cm (a) flame tip position, (b) flame tip speed, and (c) overpressure	135
8.20	Flame morphology for KCl with obstacle at 59 cm	135
8.21	Comparison of KCl inhibition cases with varying obstacle locations (a) flame tip position, (b) flame tip speed, and (c) overpressure	139
8.22	Flame morphology for different obstacle locations for KCl inhibition (left), and plain propane–air mixture (right)	141
8.23	Peak pressure for 3M KCl cases for (a) KCl inhibition, and (b) plain propane–air mixture	141

List of Tables

4.1	Initial and boundary conditions for different variables used in the simulation . .	34
5.1	Updated discretization schemes	50
5.2	Comparison of three discretization schemes separately	55
6.1	Summary of different configuration comparison	72
8.1	Comparison of propane–air cases with different obstacle locations	124
8.2	Effect of KCl addition on pressure and flame tip speed for cases with obstacle .	138

List of Abbreviations

CFD	Computational Fluid Dynamics
FSD	Flame Surface Density
AFSW	Algebraic Flame Surface Wrinkling
TFC	Turbulent Flame Closure
LES	Large Eddy Simulation
RANS	Reynolds-Averaged Navier-Stokes
DDT	Deflagration to Detonation Transitions
CPV	Combustion Progress Variable
FFT	Fast Fourier Transform
LBV	Laminar Burning Velocity
BR	Blockage Ratio
LPM	Liters Per Minute
MFC	Mass Flow Controller
RTV	Room Temperature Vulcanizing
TKE	Turbulent Kinetic Energy
SGS	Sub-grid Scale
EDM	Eddy Dissipation Model
URF	Under Relaxation Factor
SMPS	Scanning Mobility Particle Sizer