

UNIVERSITÉ D'ORLÉANS
ÉCOLE DOCTORALE
Énergie, Matériaux, Sciences de la Terre et de l'Univers

LABORATOIRE PRISME

THÈSE présentée par :

Caio FILIPPO RAMALHO LEITE

soutenue le : **4 février 2025**

pour obtenir le grade de : **Docteur de l'Université d'Orléans**

Discipline/ Spécialité : **Énergétique**

**An Experimental Study on Aerodynamics, Combustion
and Cyclic Variability in Hydrogen-Fueled
Spark-Ignition Engines Under Ultra-Lean Conditions**

THÈSE DIRIGÉE PAR :

Fabrice FOUCHER
Jacques BORÉE

Professeur, Université d'Orléans
Professeur, ISAE-ENSMA

RAPPORTEURS :

Sebastian VERHELST
Brian PETERSON

Professeur, Ghent University
Professeur, University of Edinburgh

JURY :

Stefano FONTANESI
Fabrice FOUCHER
Jacques BORÉE
Sebastian VERHELST
Brian PETERSON
Andreas DREIZLER
Karine TRUFFIN
Pierre BREQUIGNY

Professeur, Univ. of Modena and Reggio Emilia, Président
Professeur, Université d'Orléans
Professeur, ISAE-ENSMA
Professeur, Ghent University
Professeur, University of Edinburgh
Professeur, TU Darmstadt
Ingénieure de Recherche, IFP Energies Nouvelles
Maître de Conférences, Université d'Orléans

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Étude expérimentale de l'aérodynamique, de la combustion et des variabilités cycliques dans les moteurs à allumage commandé alimentés en hydrogène dans des mélanges ultra-pauvres

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Pierre BREQUIGNY

Maître de Conférences, Université d'Orléans

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Résumé en français

Au cours des dernières années, l'urgence croissante de répondre à la dégradation environnementale et au changement climatique a été amplifiée par l'augmentation des concentrations de gaz à effet de serre, en particulier du dioxyde de carbone (CO_2). Cela a mis en évidence la nécessité impérieuse de développer des sources d'énergie alternatives durables. Parmi celles-ci, l'hydrogène décarboné s'impose comme un vecteur énergétique prometteur, en particulier pour réduire les émissions de CO_2 dans le secteur des transports grâce à son utilisation comme carburant dans les moteurs à combustion interne (MCI). Cependant, les propriétés intrinsèques de l'hydrogène diffèrent fondamentalement de celles des carburants conventionnels, nécessitant une compréhension approfondie de ses comportements dans les applications MCI. Les caractéristiques physiques et chimiques distinctives de l'hydrogène, telles que sa densité énergétique, ses propriétés de diffusion, son interaction avec la turbulence, sa dynamique de combustion et ses instabilités de flamme, influencent de manière significative les performances du moteur, comme présenté dans le **Chapitre 1**. En particulier, le comportement des flammes constitue un domaine de recherche prioritaire, mettant en avant l'urgence de développer des modèles de combustion spécifiques à l'hydrogène afin de soutenir le développement des moteurs à combustion interne fonctionnant à l'hydrogène (H_2MCI) et de contribuer à atteindre les objectifs européens de neutralité carbone à l'horizon 2050.

En plus de présenter des caractéristiques distinctes par rapport aux carburants conventionnels, les propriétés de l'hydrogène varient significativement en fonction de la richesse. La Table 1 récapitule les principales propriétés de l'hydrogène pour trois richesses (1,00, 0,50 et 0,25) et les compare à celles d'isooctane, propane et méthane à la stœchiométrie. On constate, d'abord, une différence significative dans l'occupation de l'espace dans la chambre de combustion selon les différents mélanges présentés. En raison du rapport air/carburant élevé requis pour atteindre la stœchiométrie, l'hydrogène occupe beaucoup plus de volume que les autres carburants. Par exemple, un mélange ultra-pauvre d'hydrogène ($\phi = 0,25$) est comparable en volume à un mélange stœchiométrique de méthane, le carburant standard le moins dense. Il est également important de rappeler que l'hydrogène a une densité énergétique volumique très faible, ce qui réduit la charge effective. Cependant, il possède une large plage de limites d'inflammabilité et une énergie minimale d'ignition extrêmement faible, lui permettant de s'enflammer dans une gamme étendue de richesse.

Une flamme hydrogène/air stœchiométrique dans des conditions ambiantes présente une vitesse de flamme de 230 cm/s, soit plus de cinq fois supérieure à celle d'autres carburants. À $\phi = 0,50$, la vitesse de flamme diminue d'un facteur quatre, se rapprochant de celle des flammes propane/air stœchiométriques. Dans la région ultra-pauvre ($\phi < 0,50$), la vitesse de flamme chute en dessous de 5 cm/s, ce qui peut devenir prohibitif pour les MCIs. Les flammes hydrogène/air stœchiométriques affichent une épaisseur environ trois fois inférieure à celles de l'isooctane et du méthane, mettant en évidence un développement rapide. À $\phi = 0,50$,

Table 1: Propriétés des mélanges hydrogène/air à 1 bar et 300 K*.

	C ₈ H ₁₈ /air ($\phi = 1.00$)	C ₃ H ₈ /air ($\phi = 1.00$)	CH ₄ /air ($\phi = 1.00$)		H ₂ /air ($\phi = 0.50$)	($\phi = 0.25$)
LFL $\rightarrow$ UFL (ϕ)	0.66 $\rightarrow$ 3.85	0.5 $\rightarrow$ 2.53	0.5 $\rightarrow$ 1.68		0.1 $\rightarrow$ 7.1	
LFL $\rightarrow$ UFL (% _v)	1.1 $\rightarrow$ 6	2.1 $\rightarrow$ 9.6	5 $\rightarrow$ 15		4 $\rightarrow$ 75	
x_F (% _v)	1.7	4.0	9.5	29.6	17.4	9.5
y_F (% _m)	6.2	6.0	5.5	2.9	1.4	0.7
$D_{F,Air}$ (cm ² ·s ⁻¹)	0.07	0.11	0.22	0.78	0.78	0.78
α_u (cm ² ·s ⁻¹)	0.20	0.20	0.22	0.44	0.34	0.28
ν_u (cm ² ·s ⁻¹)	0.14	0.15	0.16	0.22	0.19	0.17
s_L^0 (cm/s)	36	46	38	230	52	< 5
δ_L (mm)	0.06	0.04	0.06	0.02	0.07	> 10
T_b (K)	2,309	2,371	2,226	2,383	1,627	1,058
d_q (mm)	2.2	1.7	2.4	0.8	2.6	> 100
MIE (mJ)	0.23	0.25	0.28	0.02	0.05	0.20
$\sigma = \rho_u/\rho_b$ (-)	8.21	8.25	7.48	6.83	4.95	3.36
Le_D (-)	2.86	1.82	1.00	0.56	0.44	0.36

*Calculé avec Cantera software.

l'épaisseur devient comparable à celle des autres carburants, mais à $\phi = 0,25$, elle dépasse 10 cm, comme l'indiquent les simulations 0D/1D réalisées avec Cantera, ce qui soulève des questions sur leur pertinence. Enfin, la température de flamme adiabatique des mélanges hydrogène/air stœchiométriques, comprise entre 2 300 et 2 400 K, est similaire à celle des autres carburants. Cependant, elle diminue sensiblement pour atteindre environ 1 600 K à $\phi = 0,50$ et 1 000 K à $\phi = 0,25$. Cette combustion à basse température, bien qu'elle réduise l'efficacité indiquée maximale, pourrait offrir une efficacité absolue plus élevée grâce à une diminution des pertes thermiques et à des émissions de NOx considérablement réduites, les taux de formation chutant lorsque les températures de flamme descendent en dessous de 1 800 K.

En raison de la diffusivité massique de l'hydrogène, qui est supérieure à sa diffusivité thermique, des instabilités apparaissent dans les flammes d'hydrogène pauvres. Ces instabilités, gouvernées par le nombre de Lewis et appelées instabilités thermodiffusives, provoquent un plissement de la flamme et augmentent sa vitesse de propagation. Dans le tableau, on observe également la différence entre les nombres de Lewis des carburants conventionnels, qui sont soit égaux soit supérieurs à 1 (effet stabilisateur), et celui de l'hydrogène, inférieur à 1 (effet déstabilisateur). Ces phénomènes nécessitent encore des études approfondies pour être mieux compris et modélisés.

L'hydrogène, avec sa large plage de flammabilité et sa faible énergie d'ignition, présente des défis supplémentaires pour le fonctionnement des moteurs, notamment en raison des risques de pré-allumage, de cliquetis et de retours de flamme. Ces phénomènes peuvent survenir en présence de zones de mélange localement riches ou de points chauds dans la chambre de combustion. Pour atténuer ces problèmes, un contrôle précis des paramètres d'injection et une optimisation de l'aérodynamique interne sont essentiels pour garantir une combustion stable. Par ailleurs, les modèles actuels peinent encore à représenter pleinement les interactions complexes de combustion turbulente dans les conditions de moteur. Compte tenu des propriétés distinctes de l'hydrogène, un redimensionnement significatif des moteurs à combustion interne est également envisagé pour permettre leur application efficace.

Etant donné l'importance de caractériser les flammes hydrogène/air dans des conditions moteur et de la nécessité de données de haute fidélité, cette thèse se concentre sur l'étude des

flammes hydrogène/air ultra-pauvres en mélange homogène dans un moteur optique à allumage commandé. Les recherches visent principalement à comprendre le développement de la combustion, ainsi que l'influence des champs d'écoulement sur le comportement de la flamme turbulente. En éliminant la complexité liée à la préparation du mélange, cette étude garantit que toutes les analyses de variabilité et de sensibilité sont attribuées uniquement à l'interaction entre la dynamique des écoulements et celle des flammes.

Après avoir présenté les dispositifs expérimentaux et méthodologies, dans le **Chapitre 2**, et défini, à travers de multiples études, la géométrie des conduits d'admission et d'échappement, la position de l'injecteur d'hydrogène et le type de bougie d'allumage, le **Chapitre 3** réalise une première analyse de la combustion de l'hydrogène dans une configuration de moteur opaque. La méthodologie utilisée pour le post-traitement et l'analyse des pressions dans le cylindre ainsi que du dégagement de chaleur par cycle repose sur la méthode Three Pressure Analysis (TPA) intégrée au logiciel GT-Suite, avec un modèle de combustion à deux zones 0D/1D. L'hydrogène comme carburant en moteur à allumage commandé montre un fonctionnement stable jusqu'à des richesses aussi faible que 0.2 dans une plage de pression moyenne effective indiquée (PMI) de 1 à 4 bar.

La phase de combustion la plus affectée est celle de l'initiation de la flamme (de l'allumage jusqu'à 10% de la masse de carburant brûlée, MFB), étudiée en détail dans des conditions constantes de pression d'admission et de phasage de l'allumage, en comparant le développement de la combustion pour sept richesses ($0,25 \leq \phi \leq 0,55$) et trois vitesses de rotation moteur ($900 \leq N \leq 1500$ tr/min). Une analyse des échelles de temps caractéristiques révèle que la flamme dépend significativement de la turbulence et des instabilités de flamme, qui semblent interagir de manière synergique. Les conditions expérimentales sont positionnées sur le diagramme de Peters-Borghi, mettant en évidence que de faibles variations du mélange hydrogène/air influencent fortement le régime de combustion turbulente vu par la flamme prémélangée hydrogène/air (voir Figure 5 plus loin). Une analyse approfondie est proposée pour mieux comprendre les flammes turbulentes dans le moteur à travers des mesures des écoulements et du développement de la flamme.

Le **Chapitre 4** étudie le champ de vitesses dans le moteur optique à allumage commandé à l'aide de techniques de Vélocimétrie par Images de Particules (PIV) à haute vitesse et de Décomposition en Modes Empiriques (EMD), en se concentrant principalement sur l'analyse cyclique pendant les phases d'admission et de compression, ainsi que sur l'évaluation de l'énergie cinétique de la turbulence et des fluctuations de vitesses. La Figure 1 montre des exemples des champs de vitesses pour trois configurations PIVs (plans) non-simultanées à une pression d'admission de 0,7 bar et à 1200 tr/min pendant la phase de compression. Différentes méthodes de décomposition du champ d'écoulement sont également utilisées pour mieux comprendre ses structures variées. Les principales caractéristiques des phases d'admission et de compression, en termes d'écoulement moyen et de variabilité, sont analysées, révélant la génération et l'évolution du mouvement de rouleau, appelé "tumble", tout au long du cycle moteur jusqu'à sa phase de rupture, qui intensifie la turbulence et accélère la vitesse de flamme.

L'analyse de l'énergie cinétique à partir de multiples méthodes de décomposition est réalisée pour étudier l'évolution de chaque composante de vitesse et le comportement de son énergie cinétique dans la chambre de combustion. Les effets de la vitesse du moteur, de la pression d'admission et de la combustion sur le champ de vitesses sont également discutés et les résultats montrent l'effet linéaire de la vitesse de rotation sur l'écoulement et une insensibilité par rapport à la pression d'admission et la présence de la combustion. Les composantes de vitesse haute

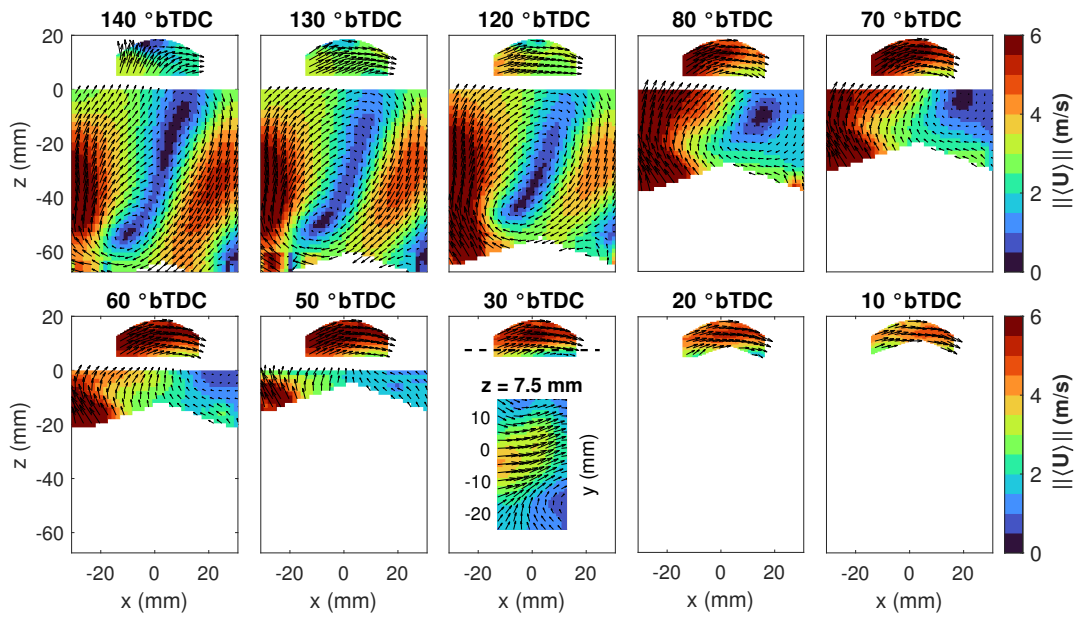


Figure 1: Magnitude de la vitesse moyenne d'ensemble pour les configurations VC, VCC et HCC à une pression d'admission de 0,7 bar et à 1200 tr/min à travers 10 angles vilebrequin différents.

fréquence, associées à la turbulence, influençant la propagation de la flamme, sont étudiées dans le cadre de l'analyse suivante. La vitesse des fluctuations turbulente de l'écoulement haute fréquence représente 22% de la vitesse moyenne du piston dans toutes les conditions de fonctionnement, et l'échelle spatiale caractéristique des composantes haute fréquence est déterminée à environ 1,5 mm, indépendamment des conditions opératoires.

Le **Chapitre 5** étudie l'évolution des flammes hydrogène/air ultra-pauvres dans le moteur, au cours de la phase initiale de la flamme à l'aide de la chimiluminescence (Figure 2), en évaluant leur impact sur les performances globales et en les comparant à un hydrocarbure conventionnel : le propane. L'étude débute par une analyse approfondie des facteurs clés influençant la combustion de l'hydrogène, notamment la richesse, la vitesse de rotation du moteur, la pression d'admission et l'énergie déposée (par la durée de charge de la bobine d'allumage). Les mélanges propane/air sont utilisés comme référence en raison de leurs caractéristiques de combustion bien établies, de leur état gazeux à pression et température normales, et de leur similarité en terme de dynamique de flamme avec les mélanges essence/air.

Comme discuté précédemment, les flammes hydrogène/air présentent un comportement significativement différent en fonction de la richesse, notamment dans des conditions ultra-pauvres, qui diffèrent fondamentalement des flammes d'hydrocarbures (Figure 3). La vitesse de flamme laminaire, dans des conditions similaires à celles d'un moteur, est sensiblement plus faible que celle des mélanges propane/air stœchiométriques, tandis que l'épaisseur de la flamme est plus importante, distinguant les différentes échelles de vitesse et d'épaisseur de flamme qui peuvent influencer le comportement global de la combustion. En outre, l'étude de mélanges propane/air sur une large gamme de richesse permet de mieux comprendre l'effet du nombre de Lewis sur le comportement de la combustion (passant de supérieur à 1 dans des conditions pauvres à inférieur à 1 dans des conditions riches) et l'impact potentiel des instabilités thermodiffusives. En analysant comment ces variables affectent la propagation de la flamme, cette étude vise à comprendre leur rôle dans la combustion et de la stabilité en conditions ultra-pauvres.

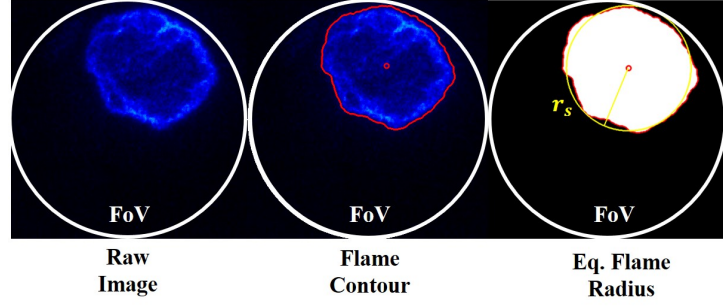


Figure 2: Traitement d'image par chimiluminescence pour une flamme hydrogène/air avec une richesse de 0.50. La figure montre le champ de vision (FoV) à travers le bol du piston en quartz, incluant le contour de la flamme et le rayon, r_s , calculé à partir de la surface projetée de la flamme.

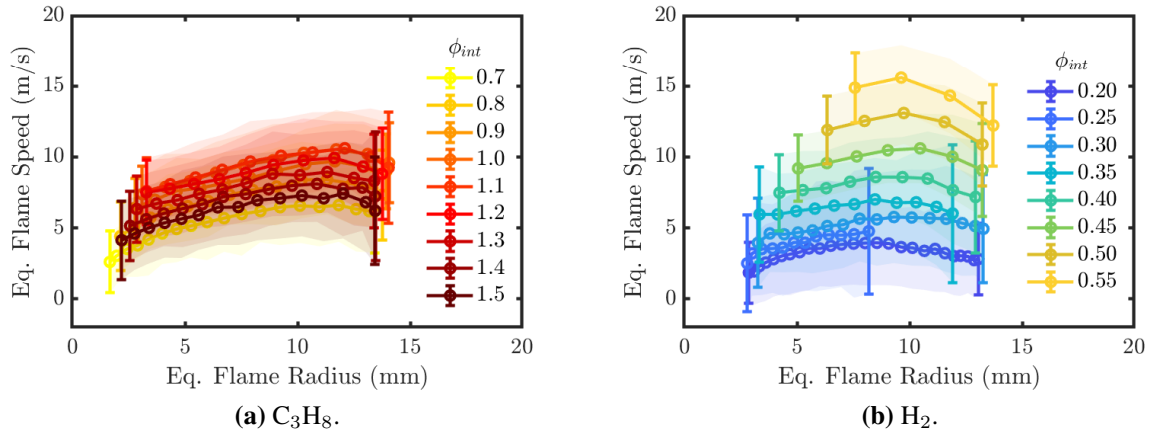


Figure 3: Effet de la richesse sur la vitesse de flamme en fonction du rayon. Les barres d'erreur indiquent $\pm$ deux écarts-types.

Un rapport est établie entre les images de flammes en cylindre et l'analyse du dégagement de chaleur afin d'évaluer si les caractéristiques observées lors de la phase initiale de la flamme peuvent prédire le taux de dégagement de chaleur de la combustion. Une corrélation entre les flammes turbulentes et les propriétés de flammes laminaires est développée sur pour toutes les conditions de fonctionnement testées. Cette corrélation est analysé avec le dégagement de chaleur et commenté à partir du diagramme de combustion pour fournir une perspective globale sur le potentiel de l'hydrogène comme carburant dans les moteurs à combustion interne. Des investigations expérimentales sont menées sur des flammes hydrogène/air très pauvres à ultra-pauvres ($0,20 \leq \phi \leq 0,55$) à différentes vitesses moteur ($900 \leq N \leq 1500$ tr/min), pressions d'admission ($0,6 \leq P_{int} \leq 0,9$ bar) et le temps de charge de la bobine d'allumage ($350 \leq \Delta t_D \leq 2000$ μ s) dans un moteur optique à allumage commandé. L'impact de chaque paramètre sur les flammes d'hydrogène est examiné, et des comparaisons avec les flammes de propane sont effectuées.

La phase de développement initial de la flamme est comparée à l'analyse du dégagement de chaleur basée sur la pression. Le temps nécessaire pour que la flamme atteigne un rayon spécifique est directement corrélé à la loi de fraction de masse brûlée: la vitesse moyenne de propagation équivalente de la flamme est directement corrélée à l'angle vilebrequin pour lequel 2% de carburant est brûlé, ce dernier étant lui même directement lié à l'ange vilebrequin pour

lequel 50% est brûlé. Cela démontre que la compréhension de la phase initiale de la flamme est essentielle pour prédire la durée totale de la combustion et l'évolution de la pression dans le cylindre.

Un modèle pour les vitesses de flammes turbulentes prémélangées d'hydrogène, basé sur l'équation de Zimont (Figure 4), est proposé en utilisant les données expérimentales pour prédire le comportement de la combustion lors des phases initiales. Une équation pour la prédiction de la durée de combustion en 0D/1D jusqu'à 10% de la fraction massique brûlée (MFB) est également proposé. La corrélation est valable pour le régime des flammes plissées jusqu'au régime des flammes épaissies ($Ka < 100$ et $\phi \geq 0,25$) du diagramme de Peters-Borghi dans les conditions expérimentales étudiées ici. Cependant, pour des richesses plus faibles, où les propriétés de flamme laminaire n'ont pas été validées, les résultats suggèrent des quantités non physiques, comme une épaisseur de flamme laminaire théorique équivalente à la moitié du rayon mesuré de la flamme. Cela indique que des données spécifiques et des mécanismes cinétiques affinés sont nécessaires pour ces conditions. Il serait également pertinent de positionner les flammes hydrogène/air ultra-pauvres sur le diagramme de combustion turbulente (Figure 5) tout en tenant compte des instabilités de flamme qui se manifestent dans ces conditions, notamment à des pressions élevées. Cela pourrait être réalisé en utilisant, par exemple, le modèle ω_2 , qui caractérise l'augmentation de la vitesse de flamme laminaire avec les effets thermodiffusifs.

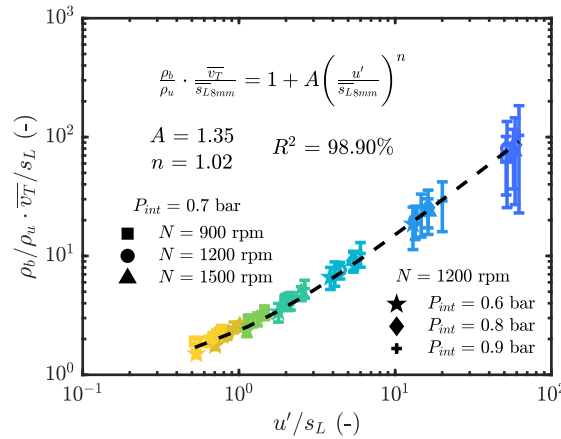


Figure 4: Augmentation de la vitesse de flamme en fonction de u'/s_L pour toutes les conditions expérimentales. La corrélation de la vitesse de flamme turbulente de Zimont, ajustée aux mesures de cette étude, montre une bonne concordance globale ($R^2 = 98.90\%$).

Le **Chapitre 6** caractérise la variabilité de la combustion hydrogène/air dans les moteurs à combustion interne à allumage commandé par trois principales analyses. Premièrement, une analyse globale utilise à la fois la méthode d'analyse du dégagement de chaleur et l'imagerie de chimiluminescence pour identifier les principales différences dans la pression cylindre (Figure 6), les images de flamme et les paramètres dérivés de ces mesures pour les flammes de propane et d'hydrogène. Deuxièmement, les effets de la richesse, de la vitesse du moteur, de la pression d'admission et du temps de charge de la bobine sur la variabilité de la flamme sont explorés. Enfin, les conditions extrêmes identifiées lors de l'analyse globale sont examinées sur une base cycle par cycle, en triant les cycles mesurés en catégories rapides et lents. Les modèles aérodynamiques et la propagation de la flamme des cycles rapides et lents sont comparés afin de

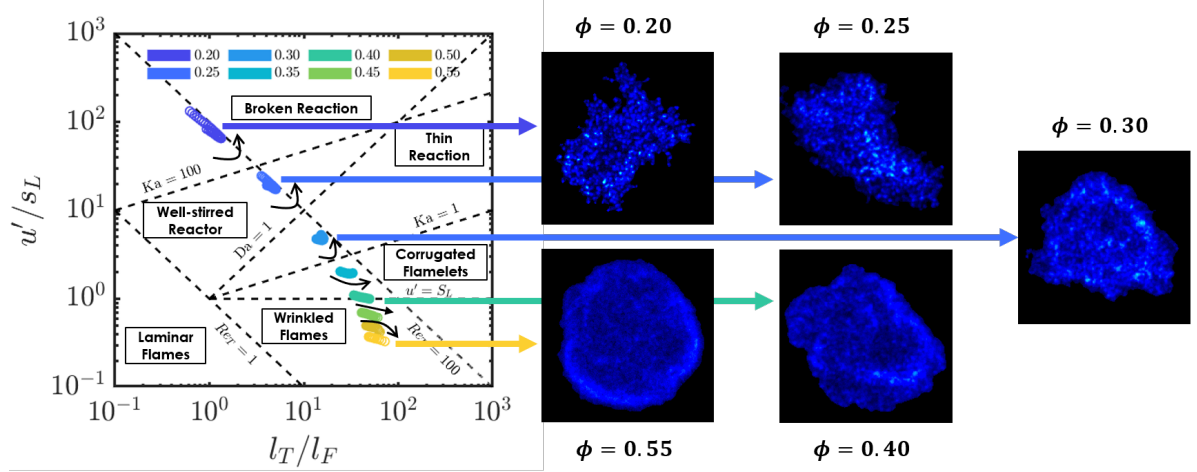


Figure 5: Diagramme de Peters-Borghi pour toutes les richesses à 1200 tr/min. Chaque mélange est représenté par une couleur différente. Le parcours de développement de la combustion est affiché pour chaque angle de vilebrequin, depuis le moment de l'allumage jusqu'à 10% de masse brûlée, avec la direction indiquée par des flèches. Des images chimiluminescentes illustrent les caractéristiques de la flamme dans différentes zones de combustion turbulente, toutes capturées à un rayon de flamme équivalent proche de 8 mm.

comprendre l'impact du champ d'écoulement sur la variabilité de la flamme. La performance moteur et la variabilité de la flamme d'hydrogène sont comparées à celles du propane pour mieux comprendre les facteurs clés influençant chaque type de flamme. Tant la pression cylindre que les paramètres de la flamme sont analysés en tant que métriques globales et sur une base cycle par cycle afin de saisir les différences fondamentales entre les cycles rapides et lents. De plus, l'impact de plusieurs paramètres sur la variabilité est étudié.

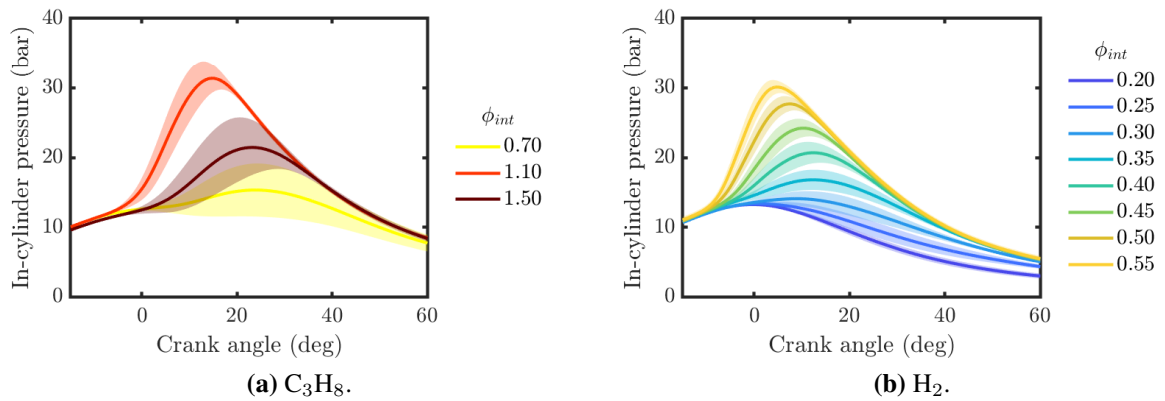


Figure 6: Pression cylindre en fonction de l'angle de vilebrequin pour des mélanges propane/air à trois richesses (0,70, 1,00 et 1,50) et des mélanges hydrogène/air à huit richesses (0,20 - 0,55).

La combustion de l'hydrogène dans un MCI présente un comportement globalement stable en termes de pression cylindre, notamment en ce qui concerne la variabilité de la pression maximale (Figure 7), qui diffère significativement de celle du propane. La variabilité de la PMI pour les deux carburants montre des valeurs similaires, bien que la PMI moyenne pour l'hydrogène soit plus faible en raison de sa densité énergétique réduite. Cependant, l'hydrogène

présente une variabilité minimale, même pour des richesses ultra-pauvres (aussi faible que $\phi_{cyl} = 0,17$), sans compromettre la stabilité de fonctionnement du moteur. Cela est probablement dû à la faible énergie d'allumage minimale de l'hydrogène, à sa large plage de flammabilité et à sa faible densité énergétique (sur une base volumétrique). En outre, l'écart type des durées de combustion pour l'hydrogène et le propane dépend largement de la vitesse de flamme laminaire, avec une relation inverse observée.

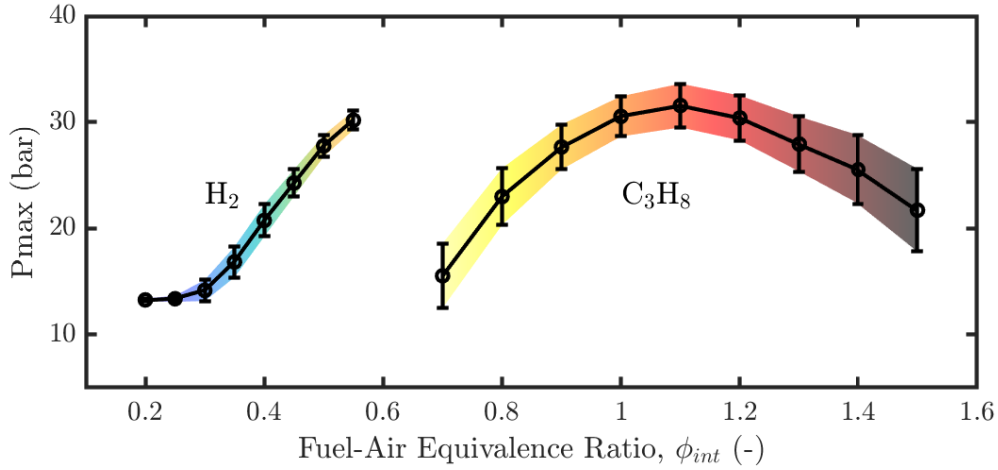


Figure 7: Pression cylindre maximale en fonction de la richesse pour les mélanges hydrogène/air et propane/air. Les barres d'erreur représentent deux fois l'écart-type.

Lors de la comparaison du comportement des flammes à un angle de vilebrequin donné, aucun impact significatif de la richesse sur la variabilité de la flamme n'est observé, tant pour l'hydrogène que pour le propane. Cependant, pour un rayon de flamme donné, des vitesses de flamme plus élevées entraînent une variabilité de flamme plus faible, ce qui est cohérent avec l'analyse de la durée de combustion. La vitesse du moteur influence principalement la variabilité de la vitesse de flamme pour les flammes d'hydrogène à faibles richesses. Inversement, la variation de la pression d'admission affecte principalement les mélanges à des richesses plus élevées, et aucune conclusion définitive ne peut être tirée concernant l'effet de la variation du temps de charge de la bobine.

Les cycles rapides et lents sont analysés en utilisant à la fois la pression en cylindre et le rayon équivalent de la flamme. Un développement plus rapide de la flamme correspond à des cycles de pression cylindre plus élevés, une tendance observée pour les deux carburants. Pour l'hydrogène, les cycles rapides sont associés à un champ d'écoulement plus intense près de la bougie d'allumage au moment de l'allumage (Figure 8). Les cycles de flamme d'hydrogène présentent moins de variation entre les extrêmes par rapport aux cycles de flamme de propane. Globalement, une corrélation modérée entre le champ d'écoulement et le développement de la flamme est observée. Une pression d'admission plus élevée réduit la corrélation entre les composantes de vitesse à faible et haute fréquence et le développement de la combustion, probablement en raison de la vitesse de flamme laminaire. Des vitesses de moteur plus élevées entraînent des corrélations plus fortes entre les composantes de vitesse à haute fréquence et le développement de la flamme. Enfin, les flammes avec des richesses plus élevées sont moins influencées par le champ d'écoulement à basse fréquence et plus affectées par les composantes de vitesse à haute fréquence (turbulentes).

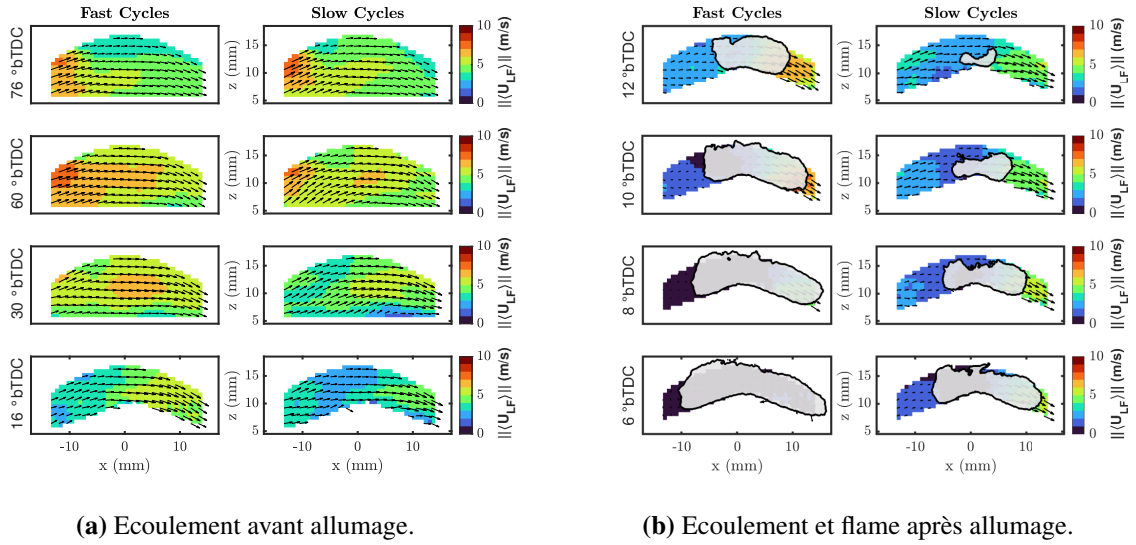


Figure 8: Mesures simultanées de PIV et de chimiluminescence pour un mélange hydrogène/air avec une richesse de 0,40.

Le **Chapitre 7** discute les résultats, en ouvrant un large éventail de perspectives académiques et industrielles sur les aspects fondamentaux des flammes hydrogène/air ultra-pauvres dans le cylindre et leur comportement dans des environnements turbulents, ainsi que leur modélisation et utilisation pour des concepts de conception industrielle innovants. À partir de cette base, plusieurs lignes directrices sont proposées pour aborder les problématiques de recherche complexes à l’avenir.

L’étude du développement de la combustion de l’hydrogène à travers différentes richesses démontre qu’une seule corrélation de la vitesse de flamme turbulente peut représenter une large gamme des régimes de combustion turbulents sur le diagramme de Peters-Borghi. Cette découverte suggère que les régimes de combustion rencontrés par ces flammes ne sont pas intrinsèquement différents, car le même modèle et ses hypothèses peuvent expliquer leur comportement. Ces résultats mettent en évidence des pistes intéressantes pour une exploration plus poussée des flammes hydrogène/air, tant dans des environnements laminaire que turbulent.

Il est à noter que les vitesses de flamme laminaire non étirées – couramment utilisées pour modéliser les premières étapes de la combustion – ne sont pas très bien déterminées pour les flammes d’hydrogène ultra-pauvres, notamment en conditions de pression et température représentative d’un moteur. Les instabilités intrinsèques, telles que les instabilités hydrodynamiques, thermodiffusives et gravitationnelles, influencent rapidement la flamme après l’allumage en conditions laminaires, rendant difficile la mesure précise des vitesses de flamme laminaire. Cela est particulièrement critique pour la modélisation de flammes turbulentes, qui reposent sur des propriétés de flamme laminaire. De plus, des investigations détaillées sur les instabilités de la flamme, en particulier les effets thermodiffusifs, dans des conditions accessibles tant dans des chambres de combustion canoniques que dans des moteurs, sont cruciales pour faire progresser les connaissances sur la combustion des mélanges en contenant d’hydrogène.

La modélisation des flammes représente un autre domaine de recherche crucial, englobant tout, des modèles cinétiques pour les simulations de combustion 0D/1D – souvent non validés dans des conditions proches de celles des moteurs, mais toujours largement utilisés dans la

modélisation des moteurs à combustion interne et pour la prédiction des paramètres fondamentaux comme vitesse et épaisseur de flamme laminaire – aux phénomènes physiques tels que l’allumage, la combustion turbulente, le transfert de chaleur aux parois et les effets de quenching. Les données expérimentales fournies dans cette thèse pourraient grandement contribuer à ces efforts. Par exemple, elles pourraient permettre de prédire le rayon de flamme à des angles de vilebrequin spécifiques et sa variabilité selon différentes conditions de fonctionnement (par exemple, la richesse, la vitesse du moteur, la pression d’admission) pour affiner les modèles d’allumage. La corrélation de combustion turbulente développée pourrait être étendue à d’autres configurations, en incorporant les instabilités thermodiffusives pour améliorer la modélisation des flammes turbulentes en cylindre. De plus, les données de pression cylindre pourraient être utilisées pour améliorer les modèles d’échanges thermiques aux parois et de quenching, notamment après le CA50, en liant potentiellement ces effets aux richesses. Des techniques avancées, telles que la diffusion de Mie pour les mesures de morphologie de flammes bidimensionnelles, pourraient améliorer la modélisation des facteurs de plissement turbulent et d’étirement dans les simulations Reynolds Averaged Navier-Stokes (RANS) et simulations aux grandes échelles (LES) des H_2 MCI. Ces simulations permettent de modéliser les interactions complexes au sein de la chambre de combustion, un élément clé pour prédire le comportement de la combustion et optimiser les performances du moteur. Ces données 2D fourniraient, alors, une base plus solide que la simple utilisation de projections basées sur la chimiluminescence.

Une fois ces phénomènes bien compris, il devient essentiel d’élargir le champ d’étude pour inclure des configurations impliquant des effets de mélange. Par exemple, explorer différentes stratégies de mélange, telles que l’injection indirecte/directe et les variations de pression d’injection, peut aider à analyser l’impact de la stratification du mélange au moment de l’allumage. Les recherches indiquent que les applications industrielles se concentrent de plus en plus sur des mélanges non homogènes pour atténuer les risques de sécurité. Des techniques optiques avancées devraient être utilisées pour valider les phénomènes de mélange, établissant un lien crucial entre les effets des mélanges inhomogènes et les modèles de flammes turbulentes homogènes validés.

La dissociation des contributions de la turbulence et des instabilités à l’accélération des flammes hydrogène/air en cylindre représente une voie passionnante pour faire progresser la science de la combustion et les technologies de propulsion durable. Les données expérimentales de haute fidélité issues de cette étude pourraient compléter les simulations DNS existantes dans des conditions proches de celles des moteurs, permettant d’obtenir des aperçus plus profonds du comportement des flammes. Obtenir un accord entre les calculs DNS et les résultats expérimentaux permettrait d’accéder à une vaste quantité de données non mesurées, améliorant ainsi les prévisions et la compréhension des propriétés des flammes. L’adaptation des géométries des collecteurs ou des pistons pour modifier les structures turbulentes au moment de l’allumage, telles que la force du tumble ou du swirl, pourrait fournir des informations précieuses sur les effets de la turbulence sur la dynamique des flammes. De plus, en complément du projet ANR Alekcia, les techniques d’assimilation de données pourraient améliorer les simulations numériques de haute fidélité, notamment pour les simulations LES, permettant des investigations détaillées du développement des flammes d’hydrogène lors de cycles extrêmes mesurés spécifiques, tels que des événements de combustion anormale, dans des conditions de fonctionnement bien connues.

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Chapter 1

Introduction

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1.1 Environmental challenges

1.1.1 Context

In recent years, concerns over environmental degradation and climate change have intensified, largely due to increasing concentrations of greenhouse gases, particularly carbon dioxide (CO₂). The rise in CO₂ levels in the atmosphere is primarily attributed to human activities related to energy consumption, including the burning of fossil fuels, deforestation, and industrial

processes. Since the Industrial Revolution, with a big increase in energy demand and consumption, as illustrated in Figure 1.1, atmospheric CO₂ levels have increased from about 280 parts per million (ppm) to over 420 ppm, a record high that has not been seen in recent times. This rise in greenhouse gases has a significant impact on the Earth's climate, contributing to global temperature variation, ocean acidification, and other environmental challenges that pose risks to ecosystems, biodiversity, and human societies [1, 2].

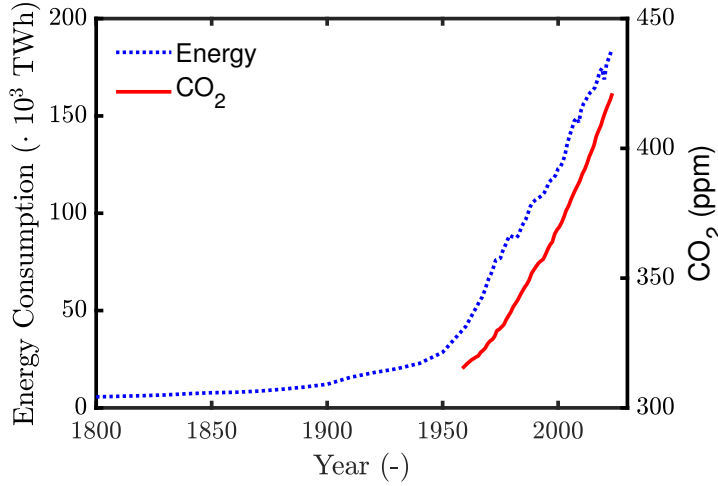


Figure 1.1: Energy consumption and atmospheric CO₂ levels over the years. Original data from [1, 2].

One of the primary concerns with elevated CO₂ levels is the greenhouse effect. CO₂ and other greenhouse gases trap heat in the Earth's atmosphere, creating a warming effect. While necessary for sustaining life on Earth, it has been greatly amplified, leading to an increase in global temperatures. This phenomenon, together with other natural influences in smaller scales, has led to a series of cascading effects, such as melting polar ice, rising sea levels, and increased frequency of extreme weather events like hurricanes, wildfires, and droughts [3]. These climate-related impacts threaten not only natural ecosystems but also human infrastructure, agriculture, and water resources, creating a pressing need for effective strategies to mitigate CO₂ emissions [4].

According to the International Energy Agency (IEA) reports [5, 6], transport is responsible for approximately one-fifth of global carbon dioxide emissions, rising to 24% considering energy-related alone. Within this sector, road travel is the largest contributor, accounting for almost three-quarters of transport emissions. Passenger vehicles, including cars and buses, contribute to 45.1%, while trucks carrying freight make up the remaining 29.4%. Since the transport sector accounts for 21% of total emissions and road transport represents three-quarters of that, road transport alone contributes to approximately 15% of global CO₂ emissions. Moreover, transport demand is projected to rise globally in the coming decades due to population growth, increasing incomes, and more widespread access to cars, trains, and air travel. The *Energy Technology Perspectives* report anticipates that global transport, measured in passenger kilometers, will double by 2070, with car ownership increasing by 60% and demand for passenger and freight aviation tripling [7]. Together, these trends are expected to significantly increase transport emissions in the next decades [8].

The *World Energy Outlook 2024* report [6] presents three distinct pathways that the energy sector could follow, highlighting the tools available to decision-makers and examining their ef-

1.1. ENVIRONMENTAL CHALLENGES

fects on energy markets, security, emissions, and societal impacts. The Stated Policies Scenario (STEPS) provides insight into the current trajectory of the energy sector, incorporating the latest market data, technology costs, and in-depth analysis of existing policies worldwide. STEPS also serves as a baseline for evaluating outcomes in both optimistic and conservative sensitivity cases. The Announced Pledges Scenario (APS) investigates the effects of fully achieving all national energy and climate commitments on time. Meanwhile, the Net Zero Emissions by 2050 (NZE) Scenario outlines a progressively narrower pathway to achieve net-zero emissions by mid-century.

Figure 1.2 shows the total CO₂ emissions by end-use sector and scenario for 2023, 2030, and 2050. The data reflect a significant reduction in emissions across all end-use sectors, with the transport sector requiring particularly substantial declines in the coming decades to align with NZE or even APS targets. Emissions in the transport sector would need to decrease by more than half under the Announced Pledges Scenario and by over tenfold to meet the Net Zero Emissions by 2050 target.

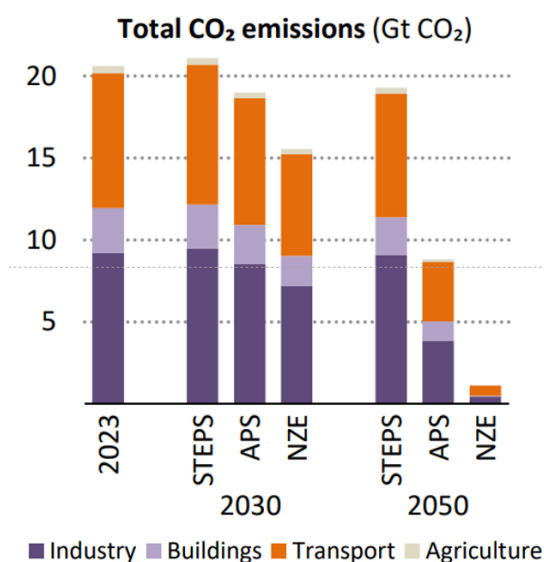


Figure 1.2: CO₂ emissions by end-use sector and scenario, 2023, 2030 and 2050 [6].

The report further outlines the energy consumption pathways by fuel type needed to achieve each scenario, as shown in Figure 1.3. Both the APS and NZE scenarios require substantial reductions in energy consumption from coal, oil, natural gas, and other fossil fuels, coupled with a significant increase in low-emissions electricity, hydrogen, and renewables. Achieving these critical shifts in energy consumption will require focused research and development of new sustainable fuels and rapid advancements in this field, important for timely implementation to align with the NZE scenario.

1.1.2 Sustainable alternatives

In this context, developing sustainable alternative energy sources is essential. Battery electric vehicles (BEVs) are currently among the leading decarbonization solutions for light-duty transport [6]. However, BEV technology does not fully meet all the challenges of the transport sector, especially in applications such as long-distance freight, urban trucks, non-road vehi-

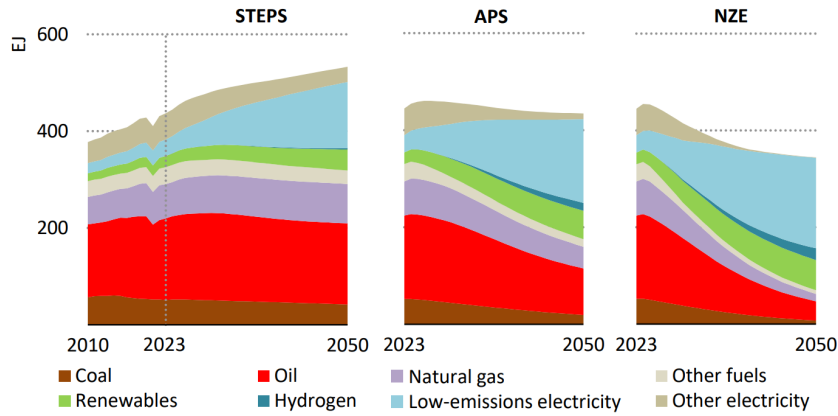


Figure 1.3: Total final consumption by fuel and scenario, 2023-2050 [6].

cles, and large passenger services (e.g., buses, taxis). Issues like limited range, the weight of onboard energy storage, and the need for fast, efficient charging limit BEV use in these areas [9]. Hydrogen-powered vehicles present a compelling alternative for these cases, offering longer ranges than BEVs and refueling times comparable to traditional liquid-fueled vehicles, typically just a few minutes [10]. Decarbonized hydrogen, therefore, emerges as a promising energy vector in efforts to reduce CO₂ emissions across the transport sector, with close-to-zero emissions when used in a fuel cell (FC) or an internal combustion engine (ICE) [11, 12].

Additionally, e-fuels and biofuels play a valuable role in the decarbonization landscape, providing partial CO₂ reductions and addressing the needs of hard-to-electrify sectors, such as aviation and maritime transport, where hydrogen may be less practical. European legislation is actively promoting these alternative fuels in these sectors [13, 14]. In line with these strategies, the 2050 Net Zero Emissions scenario envisions that around 80% of the transport sector will be powered by electricity, hydrogen, and hydrogen-based fuels, as illustrated in Figure 1.4. These technologies are not only being explored for transportation but also to manage renewable energy intermittency and reduce industrial sector emissions [15].

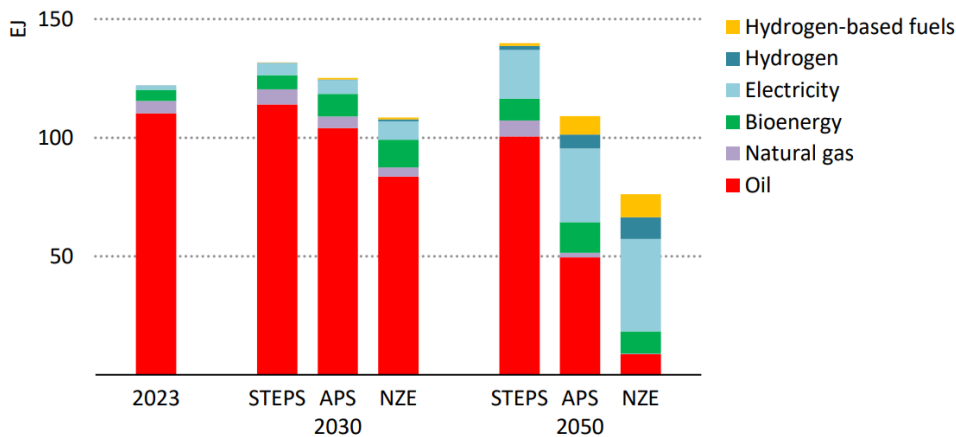


Figure 1.4: Energy demand in transport by fuel and scenario, 2023-2050 [6].

The primary industrial uses of hydrogen today include ammonia and methanol production and as a refining reagent in the oil industry. The transport sector, however, utilizes hydrogen in limited ways, primarily in fuel cell vehicles like buses and taxis. High-CO₂-emitting industries

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such as metallurgy and glassmaking, alongside hydrogen's potential for energy storage from renewable sources, reflect its evolving role in reducing greenhouse gas emissions. Currently, hydrogen sits at the center of plans to decarbonize industry, storing intermittent renewable energy, which is crucial for achieving a future sustainable energy mix [16].

Hydrogen production involves several processes with varying environmental impacts. Common methods include gasification of organic matter (producing a CO and H₂ mix) and steam reforming of natural gas, where the latter dominates the market but has a high carbon footprint, generating CO₂ alongside hydrogen. Pyrolysis, or thermal decomposition without oxygen, also produces hydrogen and can yield carbon black, a valuable by-product. Electrolysis, which splits water into hydrogen and oxygen using electricity, requires significant energy but produces hydrogen with little or no direct CO₂ emissions if powered by renewable energy sources. Based on the primary energy source and carbon emissions, hydrogen is categorized into seven "colors", ranging from *gray* (fossil-derived, high emissions) to *green* (renewably-sourced, low emissions) and others like *turquoise* and *white*, each with distinct production characteristics and environmental impacts, as described in Table 1.1.

Global hydrogen production in 2020 amounted to 75 million tonnes, contributing to about 2% of global CO₂ emissions, similar to the aviation sector. Presently, 73% of global hydrogen is derived from steam reforming, producing gray hydrogen at an economical rate of approximately €3 per kilogram, although it has a high carbon cost. Alternatives include *blue* hydrogen, where CO₂ from natural gas reforming is captured and stored, though at a higher production cost, and *green* hydrogen via electrolysis, which, while less carbon-intensive, remains cost-sensitive due to electricity expenses. The *turquoise* hydrogen process, involving methane pyrolysis, has gained attention as it produces no CO₂ and yields solid carbon black, beneficial in other industrial applications. *White* hydrogen, or naturally occurring hydrogen, presents low CO₂ emissions, though resource and transport feasibility remain under study [9].

However, hydrogen's widespread adoption in mobility faces obstacles, including high production costs, limited refueling infrastructure, and safety concerns related to its handling and storage [12, 11, 16]. Nonetheless, life cycle assessments show that green hydrogen use can reduce CO₂ emissions by around 80% for heavy-duty vehicles compared to diesel, with comparable reductions achieved by both fuel cells and internal combustion engines [17]. Yet, each technology has its specific challenges: fuel cells need to lower their GHG footprint from cell production [18], while hydrogen-fueled ICEs focus on efficiency improvements to reduce hydrogen consumption and the assurance of close-to-zero tail-pipe emissions [12]. Like any internal combustion engine, with high combustion temperatures, nitrogen oxides can be formed. Nitrogen oxides (NO_x) are a group of highly reactive gases composed of nitrogen and oxygen, including nitric oxide (NO) and nitrogen dioxide (NO₂). These emissions are a significant environmental concern due to their role in air pollution and adverse health effects. NO_x contributes to the formation of ground-level ozone and fine particulate matter, both of which are harmful to respiratory health. It is also a precursor to acid rain and can lead to the eutrophication of aquatic systems. Furthermore, NO_x emissions exacerbate global warming by promoting the production of tropospheric ozone, a potent greenhouse gas [19, 20].

The primary mechanisms for NO_x production are:

1. **Thermal NO_x:** This is the dominant form of NO_x in most combustion systems, particularly under high-temperature conditions. Thermal NO_x forms through the Zeldovich mechanism, where molecular nitrogen (N₂) reacts with oxygen radicals (O) at temperatures typically above 1,800 K.

Table 1.1: Definition and characteristics of the seven colors of hydrogen [9]

H ₂ Color	Primary Energy and Material	Industrial Process	Products	CO ₂ Emissions (kg/kg H ₂)	Production Cost (€/kg H ₂)	Water Consumption (L/kg H ₂)
Black/Gray (Carbon H ₂)	Coal/oil + heat	Gasification	H ₂ + CO ₂	20	> 3	10
	Natural gas + heat	Steam reforming	H ₂ + CO ₂	11	3 €	7
Blue (Low-Carbon H ₂)	Coal/oil + Heat	Gasification + CCS (CO ₂ storage)	H ₂ + CO ₂	4	4.5	7
	Natural gas + Heat	Steam reforming	H ₂ + CO ₂	4	4.5	7
Turquoise (Low-Carbon H ₂)	Natural gas + Heat	Pyrolysis	H ₂ + C (carbon black)	4	5	2
Yellow (Low-Carbon H ₂)	Water + Mix Elect.	Electrolysis	H ₂ + O ₂	3	6	22
Pink (Low-Carbon H ₂)	Water + Nuclear Elect.	Electrolysis	H ₂ + O ₂	< 1	5	22
Green (Renewable H ₂)	Water + Renewable Elect.	Electrolysis	H ₂ + O ₂	< 2	4	20
	Biomass	Gasification + CCS	H ₂ + CO ₂	3	6	7
	Biomethane	Steam reforming + CCS	H ₂ + CO ₂	< 3	?	?
	Biomass/Biomethane	Pyrolysis	H ₂ + C (carbon black)	< 3	?	?
	Bio-waste	Biological processes	H ₂ + C	0	6	7

2. **Prompt NO_x**: This mechanism occurs at lower temperatures and is driven by hydrocarbon radicals interacting with molecular nitrogen early in the combustion process. Prompt NO_x is usually less significant in spark-ignition engines compared to thermal NO_x but can be relevant in rich mixtures where hydrocarbon radicals are abundant.
3. **Fuel NO_x**: When fuels containing nitrogen compounds are combusted, the nitrogen in the fuel can contribute directly to NO_x formation. This mechanism is less relevant for hydrogen or natural gas but significant for fossil fuels like coal and heavy oils or ammonia (NH₃).

In internal combustion engines, high-temperature zones and local stoichiometry variations influence NO_x formation. During combustion, flame temperatures often exceed the threshold for significant thermal NO_x production, particularly in lean or stoichiometric mixtures. Strategies such as exhaust gas recirculation (EGR) and after-treatment systems (e.g., selective catalytic reduction, SCR) are used to reduce NO_x emissions [19].

Fuel cell technology remains costly and requires significant infrastructure expansion [18]. Conversely, hydrogen-fueled internal combustion engines (H₂ICEs) are built on mature, robust technology principles that handle varying external conditions such as temperature shifts, vibrations, dust, and variable hydrogen quality. While fuel cells require high-purity hydrogen (99.9%+ with <1 ppm moisture), which can degrade performance when impure, ICEs can operate with lower-purity, more economical hydrogen [21]. The availability of industrial tools for H₂ICEs provides additional economic incentives [12]. Ultimately, it appears that both fuel cells and ICEs will coexist, with the choice of technology shaped by specific use cases. Factors such as urban versus fleet operation, application requirements, and environmental conditions will play a decisive role in selecting the optimal technology [9, 12].

Hydrogen combustion have emerged as a vital technology in the evolving landscape of sustainable mobility, thanks to their potential for zero emissions. As a complement to electrified options like battery-powered or fuel-cell electric vehicles, hydrogen combustion engines offer several advantages. These include the use of well-established and reliable technologies, competitive manufacturing costs, straightforward raw material supply logistics similar to those of fossil fuels, and the ability to utilize existing industrial infrastructure globally [9].

However, the development and optimization of hydrogen combustion engines are not without challenges. Hydrogen's unique combustion properties, which differ significantly from those of traditional fossil fuels, involve modifications in engine design to achieve optimal performance. This requires a deeper understanding of hydrogen combustion phenomena under internal combustion engine conditions [12].

The primary advantages of hydrogen-powered heat engines for mobility include storage density, extended range, and rapid energy recharging – comparable to conventional liquid fuels. These benefits enhance usability and improve resilience under various ambient conditions. Although strategies for implementing this technology may vary significantly among manufacturers, the key segments considering hydrogen combustion engines are [22]:

- Freight transport, encompassing everything from long-haul heavy goods vehicles to utility vehicles [23];
- Construction site vehicles and equipment, service vehicles, and agricultural machinery [24];

- Applications requiring high instantaneous power, such as motorsports [25].

Further investigations are essential to understand the flame properties of hydrogen in internal combustion engines, enabling a deeper comprehension of this decarbonized fuel and the development of industry-suitable technologies. The following section addresses specific characteristics of hydrogen as a fuel in internal combustion engines.

1.2 Hydrogen as a fuel

Assessing the properties of hydrogen and how they differ from those of conventional fuels is essential to understand its suitability as a decarbonized fuel for ICEs. The key characteristics of hydrogen, in terms of physical and chemical properties are discussed in this section.

1.2.1 Physical properties

Before addressing combustion, it is essential to review the physical properties of hydrogen relative to other common fuels, displayed in Table 1.2, highlighting its distinctive physical features as a fuel in internal combustion engines.

Table 1.2: Physical properties of hydrogen compared to isooctane, propane and methane at 300 K and 1 bar*.

	Isooctane [26]	Propane [27]	Methane [28]	Hydrogen [29]
Formula (-)	C_8H_{18}	C_3H_8	CH_4	H_2
Molecular mass ($g \cdot mol^{-1}$)	114	44	16	2
Density ($kg \cdot m^{-3}$)	692 (l)	1.79	0.65	0.08
Mass diffusivity in air ($cm^2 \cdot s^{-1}$)	0.07	0.11	0.22	0.78
LHV ($MJ \cdot kg^{-1}$)	45	46	50	120
LHV ($MJ \cdot m^{-3}$)	32,000 (l)	82.3	32.6	9.6
AFR _{st} (-)	15.0	15.6	17.1	34.2

*Values calculated using Cantera software [30].

(l) = Liquid phase

Hydrogen has a low molecular mass of about 2 g/mol, which is over 50 times lighter than isooctane, which represents gasoline, with a molecular weight of around 114 g/mol, and eight times lighter than methane, the main component of natural gas, at 16 g/mol. This means that, under Normal Pressure and Temperature (NPT) conditions, hydrogen has significantly lower mass per volume. For example, its volumetric density of 0.08 kg/m³ is 22 times lower than propane's at NTP and over 8,000 times lower than liquid-phase (l) isooctane. Additionally, hydrogen's mass diffusivity in air is 0.78 cm²/s, enabling it to mix 3 to 7 times faster in air than propane or methane, respectively.

Hydrogen also has a high mass energy density, with a lower heating value (LHV) of around 120 MJ/kg – approximately 2.5 times that of isooctane. However, due to its low density, hydrogen's volumetric energy density is about 9.6 MJ/m³, which is over a thousand times lower than the energy density of liquid-phase isooctane at 32,000 MJ/m³ and three times lower than methane's. Consequently, for a given volume under the same pressure and temperature, the energy released from hydrogen combustion is significantly lower than that of isooctane, propane, or methane. Lastly, hydrogen's stoichiometric air-fuel ratio – about 34.2, compared to 14 to 17

1.2. HYDROGEN AS A FUEL

for other fuels – means that the mass of air required for complete combustion must be much greater than the mass of hydrogen, which aligns with hydrogen’s much lower density compared to other fuels.

1.2.2 Chemical properties

For three different hydrogen/air conditions, the fuel/air chemical properties are presented in Table 1.3 and compared with isooctane, propane, and methane as reference fuels.

Table 1.3: Fuel-air mixture chemical properties at 1 bar and 300 K*.

	C ₈ H ₁₈ /air [26] ($\phi = 1.00$)	C ₃ H ₈ /air [27] ($\phi = 1.00$)	CH ₄ /air [28] ($\phi = 1.00$)	($\phi = 1.00$)	H ₂ /air [29] ($\phi = 0.50$)	($\phi = 0.25$)
LFL → UFL (ϕ) [31]	0.66 → 3.85	0.5 → 2.53	0.5 → 1.68		0.1 → 7.1	
LFL → UFL (% _v)	1.1 → 6	2.1 → 9.6	5 → 15		4 → 75	
x_F (% _v)	1.7	4.0	9.5	29.6	17.4	9.5
y_F (% _m)	6.2	6.0	5.5	2.9	1.4	0.7
$D_{F,Air}$ (cm ² ·s ⁻¹)	0.07	0.11	0.22	0.78	0.78	0.78
α_u (cm ² ·s ⁻¹)	0.20	0.20	0.22	0.44	0.34	0.28
ν_u (cm ² ·s ⁻¹)	0.14	0.15	0.16	0.22	0.19	0.17
s_L^0 (cm/s)	36	46	38	230	52	< 5
δ_L (mm)	0.06	0.04	0.06	0.02	0.07	> 10
T_b (K)	2,309	2,371	2,226	2,383	1,627	1,058
d_q (mm) [32]	2.2	1.7	2.4	0.8	2.6	> 100
MIE (mJ) [33, 34]	0.23	0.25	0.28	0.02	0.05	0.20
$\sigma = \rho_u/\rho_b$ (-)	8.21	8.25	7.48	6.83	4.95	3.36
Le_D (-)	2.86	1.82	1.00	0.56	0.44	0.36

*Values calculated using Cantera software [30].

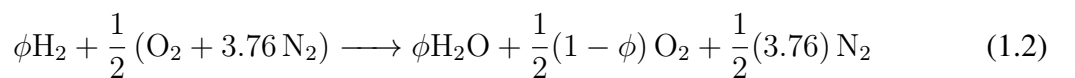
Overall reaction equation

Combustion is an exothermic chemical reaction in which a fuel reacts with an oxidizer, releasing energy in the form of heat. This process requires an initial energy source, such as a spark or heat, to initiate and involves a complex series of elementary reactions. For practical purposes, this complex reaction sequence is often simplified to a global reaction of the form:



where F and O represent the fuel and oxidizer (unburned gas), P represents the combustion products (burned gas), Q is the heat released, and α and β are the stoichiometric coefficients. This simplified, one-step reaction provides a basic material balance but does not capture the full complexity of the actual combustion mechanism.

For specificity, the overall hydrogen/air reaction can be expressed as:



where ϕ represents the fuel-air equivalence ratio, which is the ratio of the actual fuel-to-air ratio to the stoichiometric fuel-to-air ratio. This parameter indicates whether a mixture is rich ($\phi > 1$), lean ($\phi < 1$), or stoichiometric ($\phi = 1$).

Equation 1.1 emphasizes the exothermic nature of the combustion reaction, where chemical energy stored in the fuel is converted into heat. The rate at which this chemical reaction proceeds, termed the reaction rate, is defined as the rate of change of concentration of a reactant or product per unit time. In combustion, the overall reaction comprises a series of elementary reactions, each with its specific reaction rate, governed by factors such as temperature, pressure, and chemical kinetics. The dynamics of flame propagation are intrinsically linked to the reaction rates of these elementary processes. The overall reaction rate, representing the combined effects of all individual reactions, directly determines the rate of heat release.

Laminar flames

Once a flame is established, combustion is sustained by balancing heat transfer from burned gases to unburned gases with the chemical energy supplied by reactive species flowing from the unburned mixture to the burned gases [35]. Figure 1.5 shows a schematic of an unstretched laminar flame propagating from burned to unburned gases. The fresh and burned gases are separated by a thin reaction zone known as the flame front. As the reactive mixture nears the flame front, it gradually heats up, activating chemical reactions that release substantial energy. This energy then transfers to the surrounding unburned mixture, creating a feedback loop that allows the flame to propagate and continuously consume the reactive species. According to Mallard and Le Châtelier's theory [36], the intermediate zone between fresh and burned gases can be divided into two regions: the preheat zone and the reaction zone. Heat flux from the burned gases raises the temperature of the fresh gases upstream, over a thickness δ_{th} . In this preheat zone, chemical reactions are negligible compared to thermal diffusion effects. Within the reaction zone, of thickness δ_r , the peak heat release occurs, due to chemical reactions.

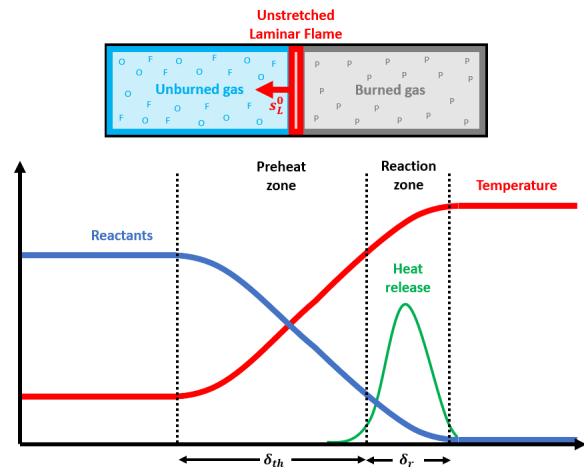


Figure 1.5: Schematics of a premixed laminar plane flame.

Several parameters characterize the laminar flame [35, 37]:

- **Laminar flame speed, s_L :** This parameter represents the rate at which the flame front moves through a flammable mixture relative to the unburned reactants. Factors like fuel type, air-fuel ratio, pressure, reactant temperature, and flame front stretching affect this speed.

- **Laminar flame thickness**, δ_L or δ_S : This thickness is the distance over which temperature and concentration gradients exist within a laminar flame, encompassing both preheat and reaction zones. Common approaches to defining flame thickness include the Zeldovich thickness (δ_L), which is defined as a thermal balance within the flame, and the Spalding thickness (δ_S), calculated as the temperature difference from fresh to burned gases divided by the maximum temperature gradient.
- **Adiabatic flame temperature**, T_b : This temperature is the maximum achievable by combustion of a fuel-oxidizer mix without any heat loss. It depends on fuel type, oxidizer, and initial mixture conditions.

Regarding flame speed, multiple definitions exist, along with various experimental measurement techniques. Here, two definitions proposed by Poinot and Veynante [38] are used. The laminar flame speed is a global measure associated with the consumption rate of fresh gases in a planar flame, representing the speed at which reactants are burned. The absolute speed (or propagation speed) is defined locally as the normal speed of the flame front in the laboratory reference frame. At a given point on an isothermal surface of the flame front, the normal vector $\vec{n}$ to the flame front points towards the fresh gases. The vector $\vec{w}$ represents the flame front's speed relative to the laboratory frame, while $\vec{u}_g$ is the speed of the fresh gases approaching the flame front. By definition, the laminar flame speed, s_L , is perpendicular to the flame front, allowing the vector relationship:

$$\vec{w} = s_L \vec{n} + \vec{u}_g \quad (1.3)$$

In the case of a flat or spherical flame, $s_L \vec{n}$ and $\vec{u}_g$ are collinear with the normal vector $\vec{n}$. The propagation speed, $v_L = \vec{w} \cdot \vec{n}$, is then directly related to both the speed at which the reactive mixture is consumed and the speed of the fresh gases ahead of the flame front.

These laminar flame properties are fundamental to understanding and optimizing the combustion process in internal combustion engines. The laminar flame speed influences how quickly fuel burns in the cylinder. Faster flame speeds typically improve efficiency by allowing fuel to burn more rapidly, generating higher peak pressures closer to the piston's top dead center, maximizing engine power. Slow flame speeds can lead to incomplete combustion, decreasing efficiency and increasing emissions due to unburned fuel. Flame thickness, which represents heat and mass transfer between unburned and burned gases, influences temperature gradients and consumption speed; thinner flames generally produce higher flame temperatures and quicker combustion. The adiabatic flame temperature sets an upper limit on thermal efficiency and helps predict exhaust gas temperatures. High adiabatic temperatures correlate with increased energy output but may cause engine damage and higher thermal NOx emissions.

For hydrogen, laminar flame properties vary significantly with the equivalence ratio, as displayed in Table 1.3. A stoichiometric hydrogen/air flame at ambient conditions has a flame speed of 230 cm/s – over five times faster than other fuels. At $\phi = 0.50$, flame speed drops by fourfold, aligning with stoichiometric propane/air flames. In the ultra-lean region ($\phi < 0.50$), flame speed falls below 5 cm/s, potentially prohibitive for ICEs. Hydrogen/air flames at stoichiometry exhibit a third of the thickness of isooctane and methane, highlighting rapid development. At $\phi = 0.50$, thickness is comparable to other fuels, and at $\phi = 0.25$, thickness exceeds 10 cm, as observed in 0D/1D Cantera simulations, which poses questions. Finally, the adiabatic flame temperature of stoichiometric hydrogen/air mixtures, between 2,300 and 2,400 K, is similar to other fuels; however, it declines substantially to around 1,600 K at $\phi = 0.50$ and

1,000 K at $\phi = 0.25$. This low-temperature combustion, while reducing maximum indicated efficiency, may yield higher absolute efficiency due to reduced heat loss and significantly lower NOx emissions, as formation rates drop with flame temperatures below 1,800 K.

Flammability limits, minimum ignition energy and quenching distance

The presence of fuel and an oxidizer in the same location is not sufficient to form a flame. For combustion to occur, the fuel concentration must fall within specific limits: the Lower Flammability Limit (LFL), below which the mixture is too lean to ignite, and the Upper Flammability Limit (UFL), above which the mixture is too rich. These limits vary based on the fuel-oxidizer mixture and pressure. Additionally, the temperature of the fresh gases must exceed the mixture's ignition temperature, achievable by heating or a spark. The Minimum Ignition Energy (MIE) indicates the mixture's ease of ignition and is defined as the smallest electrical energy required to ignite the fuel-air mixture across a spark plug gap under specific conditions. This energy, typically supplied by an electric spark, must be sufficient to raise the mixture's temperature locally, ensuring sustained combustion. MIE varies with fuel type, concentration, temperature, and pressure; a lower MIE signifies easier ignition, a crucial factor for safety and ignition system design.

The quenching distance, denoted as d_q , is the minimum distance from a wall or surface at which a flame can propagate before being extinguished due to heat loss. As a flame approaches a surface, heat rapidly transfers to it, cooling the flame front and reducing the reacting gases' temperature below the combustion threshold. At this critical distance, thermal losses to the wall exceed the heat generated by the reaction, extinguishing the flame. Factors influencing the quenching distance include fuel type, mixture composition, pressure, and temperature. The quenching distance can be estimated using the model by Jarosinski et al. [32], which demonstrated that the Peclet number, based on the critical distance from the wall relative to the Zeldovich flame thickness, remains constant for various fuels and equivalence ratios. This relationship enables estimating the quenching distance with the laminar flame speed and thermal diffusivity of the unburned mixture, α_u , by the following equation:

$$Pe_L = \frac{d_q}{\delta_L} = \frac{d_q s_L}{\alpha_u} \approx 40 \quad (1.4)$$

Table 1.3 compares hydrogen's flammability and ignition properties to those of isooctane, propane, and methane. Notably, hydrogen exhibits a broad flammability range in equivalence ratios (0.1 to 7.1) and volume percentages (4% to 75%), unlike the other fuels, which do not burn below a 0.5 or above a 4 equivalence ratio. This extensive range is advantageous for internal combustion engines, as hydrogen can ignite in mixtures diluted with air or exhaust gas recirculation (EGR), improving engine efficiency and reducing NOx emissions [39]. For practical application, a minimum equivalence ratio of around 0.20 is needed for stable hydrogen flame propagation in engines [40, 41]. Additionally, hydrogen's LFL of 4% poses specific safety considerations, given its wide flammability limits compared to other fuels [33].

Hydrogen's high flammability and ease of ignition make it suitable for use with spark plugs, requiring only about one-tenth of the ignition energy necessary for the other fuels at stoichiometry. At $\phi = 0.50$, hydrogen's MIE remains four times lower than that of other fuels, and at $\phi = 0.25$, it is still marginally lower, in the tenths of μJ , even with a slower and thicker flame. Furthermore, hydrogen's quenching distance at stoichiometry is approximately 0.8 mm, much shorter than the 2.2 mm observed for isooctane, propane, and methane flames. This shorter

quenching distance benefits hydrogen engines by allowing flame propagation into the engine's dead volumes, reducing unburned fuel residues [12]. However, closer proximity to walls may increase heat losses, potentially affecting efficiency. Under lean mixtures ($\phi = 0.50$), hydrogen's quenching distance resembles that of other fuels but increases substantially under leaner conditions (ultra-lean), where the low flame speed further influences it. Under these lean conditions, Jarosinski's model with Burke's kinetic mechanism estimates a quenching distance greater than 10 cm, indicating that the flame may quench sooner near the cylinder wall at lower equivalence ratios, which could significantly impact combustion efficiency.

Flame Instabilities

Combustion instabilities are diverse and result from the interaction of multiple physical phenomena. These instabilities can be related either to the properties of the system or to mechanisms intrinsic to flame front propagation. They affect the local equilibrium of thermodynamic parameters and species concentrations, which leads to flame front deformation.

Darrieus and Landau [42, 43] identified hydrodynamic (HD) effects on a laminar flame front while neglecting diffusive effects. The Darrieus-Landau instabilities are purely HD in nature and do not account for modifications to the internal structure of the infinitely thin flame front. An initially flat flame front subjected to a small-amplitude disturbance will develop folds characterized by their curvatures: negative in concave regions (relative to the fresh gases) and positive in convex zones. Combustion instabilities can arise due to the deflection of streamlines at the flame front. A reactive flow is marked by a sharp variation in density between fresh and burned gases, represented by the expansion ratio, $\sigma = \rho_u / \rho_b$.

In convex zones, streamlines diverge to conserve mass, resulting in a local decrease in flow velocity. Conversely, in concave zones, streamlines converge, causing an increase in flow velocity, while the unstretched laminar combustion velocity remains unchanged. This results in the continuous amplification of any initial disturbance, meaning the flame front is intrinsically unstable. These instabilities become more pronounced as the laminar flame thickness decreases (i.e., as the density gradient increases), which occurs at higher pressures. These instabilities lead to the formation of large cells at the flame front. For high-pressure spherical flames, such as those in ICEs, these instabilities develop earlier during flame propagation, limiting the duration for which the flame remains laminar.

Unlike HD instabilities, thermodiffusive (TD) instabilities are inherent to combustion mechanisms. During flame propagation, the behavior of the flame front is influenced by the development of mass and heat diffusive fluxes directed tangentially to the flame front. TD instabilities arise from the competition between molecular diffusion (mass flux) and thermal diffusion (heat flux), which can either stabilize the flame or promote the formation of cellular structures. These effects are characterized by the Lewis number, which is defined here as the ratio of thermal diffusivity to molecular diffusivity of the deficient reactant, calculated as follows [35, 44]:

$$Le_D = \frac{\alpha_u}{D_{i,j}} \quad (1.5)$$

where α_u represents the thermal diffusivity of the unburned air-fuel mixture, and $D_{i,j}$ is the mass diffusivity of the deficient reactant i relative to j at the freestream reactant temperature. In a rich flame, oxygen is the limiting reactant, whereas in a lean flame, fuel is the deficient reactant. Given the relative scarcity of reactants compared to nitrogen, j represents N_2 , and $D_{i,j}$ is

therefore considered as the binary diffusion of the deficient reactant towards N_2 due to its abundance [44]. In Table 1.3, the deficient reactant is taken to be the fuel, even at stoichiometric conditions. Based on the Lewis number, different scenarios may arise [35]:

- **Le = 1:** When mass and thermal diffusion effects are balanced, the flame front stabilizes, maintaining a constant flame speed. This situation is typical for stoichiometric methane/air mixtures.
 $\phi = 1.00$: $Le_D^{CH_4/air} = 1.00$ (data from Table 1.3).
- **Le > 1:** Here, thermal diffusion dominates over mass diffusion of the limiting reactant. In convex flame regions, heat diffuses into the fresh gases, slowing the flame speed. In concave regions, heat flows from the burned gases into the reaction zone, increasing flame speed. The flame front stabilizes, as seen in hydrocarbon flames, which remain relatively stable and spherical (thermodiffusively stable flames).
 $\phi = 1.00$: $Le_D^{C_8H_{18}/air} = 2.86$.
 $\phi = 1.00$: $Le_D^{C_3H_8/air} = 1.82$.
- **Le < 1:** In this case, mass diffusion of fresh gases surpasses thermal diffusion. When the flame front is disturbed, fuel accumulates quickly in convex areas, causing them to accelerate. The concave areas, with less fuel, slow down, leading to increased wrinkling of the flame front. This scenario, typical of lean hydrogen flames, amplifies instabilities, increasing the flame surface and altering flame propagation speed.
 $\phi = 1.00$: $Le_D^{H_2/air} = 0.56$.
 $\phi = 0.50$: $Le_D^{H_2/air} = 0.44$.
 $\phi = 0.25$: $Le_D^{H_2/air} = 0.36$.

Figure 1.6 shows Schlieren visualizations of hydrogen/air flame instabilities [45]. The images depict laminar H_2 /air flames with $\phi = 0.80$ at 360 K under varying initial pressures (1 to 5 bar). Initially, the lean H_2 /air flame starts as a smooth, spherical structure but rapidly evolves into a highly wrinkled, cellular form, highly sensitive to initial pressure. This can be attributed to the growth of HD instabilities, which increase with the expansion ratio and pressure [42, 43, 46]. Initial perturbations amplify TD instabilities, further wrinkling the flame front. This disruption in flame stability increases the flame surface area, thereby enhancing flame propagation speed [47, 48].

The two parameters, σ and Le_D , both influence hydrogen flame stability. The expansion ratio of hydrogen/air flames at the tested equivalence ratios is lower than that of stoichiometric isooctane, propane, and methane, indicating a slower growth rate of HD instabilities. However, since the Lewis number is below one for lean hydrogen/air mixtures, the flame is inherently unstable under these conditions. In contrast, the Lewis number for other fuels is at unity (methane/air) or higher (isooctane/air, propane/air), stabilizing these flames. Therefore, while hydrogen HD instability growth is slower, it still triggers cellular structures in the flame front. The resulting laminar flame exhibits characteristic wrinkling that self-accelerates, increasing the laminar flame speed. In internal combustion engines, this effect is further modified by turbulence [49, 41, 47, 50, 51].

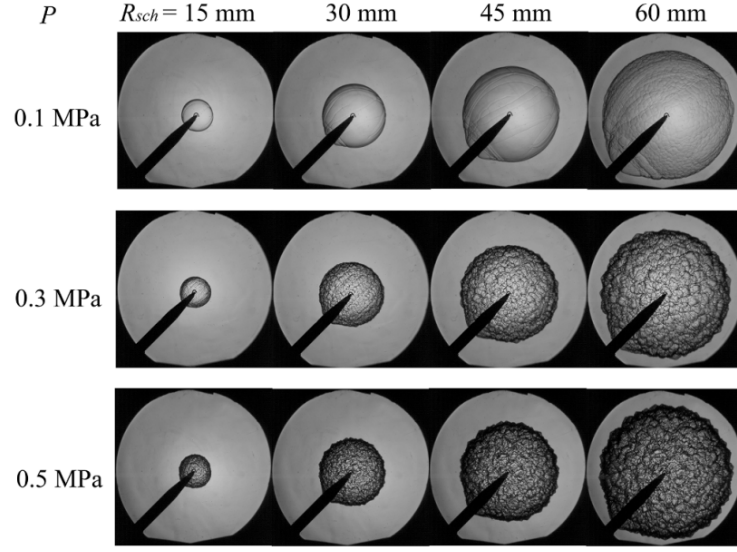


Figure 1.6: Schlieren images showing the impact of initial pressure, P_i , on the expanding hydrogen/air flames at $P_i = 0.1, 0.3$ and 0.5 MPa, $T_i = 360$ K, and $\phi = 0.80$ [45].

Premixed turbulent flames

To qualitatively characterize turbulent flames, it is helpful to compare the various spatial and temporal scales of the two primary phenomena involved: turbulence and combustion. Using dimensionless numbers, turbulent combustion diagrams can be established, allowing for the classification of flames across different regimes.

The main dimensionless numbers used for comparing these scales are:

- **Turbulent Reynolds Number** (Re_t): This number compares turbulence intensity to viscous forces, indicating whether the flow is laminar or turbulent. If $Re_t < 1$, the flow is laminar, while $Re_t > 1$ signifies a turbulent flow.

$$Re_t = \frac{u' L_T}{\nu} \quad (1.6)$$

where u' is the turbulent intensity, L_T is the integral turbulence scale, and ν is the kinematic viscosity.

- **Damköhler Number** (Da): This number compares the characteristic timescales of turbulence to those of combustion chemistry.

$$Da = \frac{\tau_t}{\tau_c} = \frac{L_T}{\delta_L} \cdot \frac{s_L}{u'} \quad (1.7)$$

- **Karlovitz Number** (Ka): This number compares the characteristic time of the smallest turbulent scales (Kolmogorov scales) to the chemical timescale. Assuming homogeneous isotropic turbulence, it is expressed as:

$$Ka = \frac{\tau_c}{\tau_\eta} = \frac{\delta_L}{s_L} \left(\frac{\eta}{u'_\eta} \right)^{-1} = \left(\frac{L_T}{\delta_L} \right)^{-1/2} \left(\frac{u'}{s_L} \right)^{3/2} \quad (1.8)$$

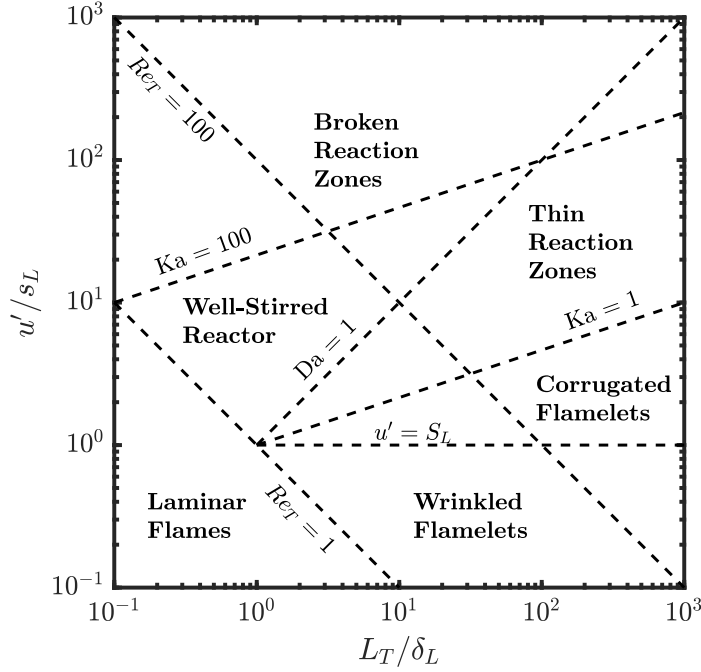


Figure 1.7: Peters-Borghi Diagram [35], which shows the speed ratio as a function of the spatial scale ratio, and defines multiple premixed turbulent combustion regimes.

These three numbers collectively define various premixed turbulent combustion regimes, as illustrated in Figure 1.7, which shows the speed ratio as a function of the length scale ratio.

Borghi's combustion diagram [52] demonstrates that the flamelet regime, as defined by Peters [53], occurs when $Ka < 1$ and $Da > 1$. This condition implies that the flame thickness is smaller than the smallest turbulence scales and thus negligible compared to the largest turbulent structures, which cannot penetrate the flame front. In this regime, the flame consists of multiple thin interfaces with local laminar flame properties that are transported by flow structures. The flamelet regime described by Peters can be subdivided into two further sub-regimes:

- **Wrinkled Flamelets Regime** ($u'/s_L < 1$): In this regime, the flame interacts weakly with turbulence, and wrinkling is minimal, meaning laminar propagation dominates.
- **Corrugated Flamelets Regime** ($u'/s_L > 1$): Here, large turbulence structures have sufficient energy to wrinkle the flame significantly, creating pockets of fresh or burnt gases. While flame fronts may interact, the reaction zone remains a thin interface.

However, flamelets are not strictly limited to $Ka = 1$. As Driscoll [54] noted, flamelets may exist even at Karlovitz numbers greater than 10, as observed in studies by Shepherd et al. [55], Buschmann et al. [56], Dinkelacker et al. [57], and Chen and Bilger [58]. These studies reveal that preheating zone thicknesses can be less than or equal to those of a laminar flame at $Ka > 10$. Thus, flamelets may exist in the Thickened-Wrinkled Flames Regime, which is bounded by $Ka = 1$ (Klimov-Williams) and $Ka = 100$, as proposed by Peters [59]. In this regime ($1 < Ka < 100$), turbulent structures become small enough to penetrate the preheating zone, enhancing mixing without disturbing the reaction zone. The $Ka = 100$ criterion is crucial for studying flamelets as it distinguishes the Thickened-Wrinkled Flames Regime from

the Broken/Distributed Reaction Zones. Within the Thickened-Wrinkled Flames Regime, two sub-zones are present:

- **Well-Stirred Reactor Regime** ($Da < 1$): Here, chemical timescales are much longer than turbulence timescales. All turbulence structures can penetrate the flame front as they are small compared to its thickness, resulting in slow chemical reactions but significant mixing within the flame.
- **Thin Reaction Zones Regime** ($Da > 1$): In this regime, chemical reactions occur faster than turbulence timescales. The reaction rate is primarily influenced by turbulence, and the flame front remains largely impermeable to turbulence structures, which are too large to penetrate it. The turbulence causes the flame front to fold, forming structures similar to laminar flamelets, so this part of the diagram can also be considered part of the flamelet regime.

Direct numerical simulations by Poinso et al. [60] of a flat laminar flame interacting with two swirls confirm that Peters' $Ka = 100$ criterion better defines the flamelet region in the diagram. For Karlovitz numbers above 100, Kolmogorov scales become smaller than the reaction zone thickness, allowing them to penetrate and cause significant disturbances. The two regimes – specifically, the Flamelet Regime and the Thickened-Wrinkled Flames Regime – are standard for premixed combustion in spark-ignition engines [61, 49].

The flames presented in Table 1.3 under NTP conditions are plotted on a Peters-Borghi diagram to compare premixed turbulent combustion regimes for different fuels in Figure 1.8. To create this graph, turbulent intensity and integral length scales from a 0.5 L spark-ignition engine [49] are applied to all mixtures (1.43 m/s and 1.4 mm, respectively). Stoichiometric flames of isooctane, propane, and methane are located in the Thin Reaction Zones Regime near the $Ka = 1$ condition. The hydrogen/air mixture at an equivalence ratio of 0.50 also falls within this regime, indicating a similar turbulent flame behavior. However, under both stoichiometric and ultra-lean conditions ($\phi = 0.25$), hydrogen flames are situated in distinct regions of this diagram, specifically in the Wrinkled Flamelets Region (near the $u' = s_L$ condition) and further in the Broken Reaction Zone Region, where combustion is typically suppressed due to thick reaction zones and smaller turbulent eddies.

A turbulent flow can alter the flame front structure due to velocity gradients in the plane tangent to the flame front. Conversely, the flame affects the flow through gas propagation and expansion, as well as changes in density and viscosity. Turbulence primarily impacts flame behavior in three key ways:

- Increasing flame speed;
- Wrinkling the flame surface due to turbulence;
- Enhancing mixing between fresh and burned gases through increased turbulent diffusivity.

These effects are described in the conservation equations for mass, momentum, energy, and species. However, this system of equations remains incomplete and requires modeling for certain quantities, such as the average reaction rate. For example, in flame surface density models commonly used in engine applications, the average reaction rate of a premixed turbulent flame is expressed as follows:

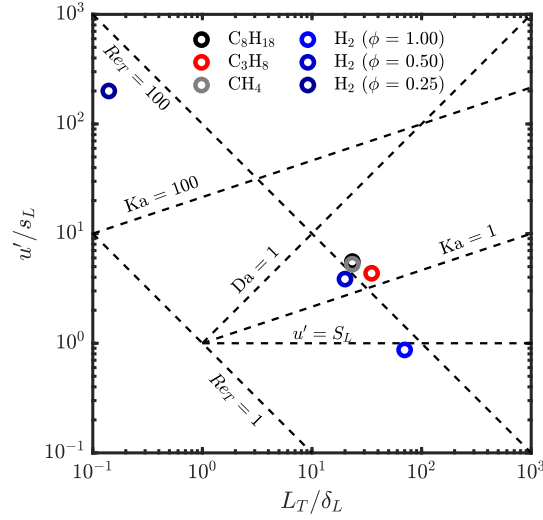


Figure 1.8: Peters-Borghi Diagram for different fuels at NTP and engine-like turbulent conditions.

$$\bar{\dot{\omega}} = \rho_u \cdot \langle s_C \rangle_S \cdot \Sigma \quad (1.9)$$

where ρ_u is the density of fresh gases, $\langle s_C \rangle_S$ represents the average consumption rate of reactants across the flame surface, and Σ denotes the flame surface density.

In the flamelet regime hypothesis (frequently used in modeling), the turbulent flame can be visualized as a series of flamelets possessing characteristics similar to a laminar flame, forming a thin, wrinkled interface shaped by the flow. A turbulent flame front, characterized by a turbulent flame surface area, A_T , turbulent flame speed, s_T , and turbulent flame thickness, δ_T , implies that the mass of reactants crossing the laminar flame surface, A , is equal to that crossing the turbulent surface A_T , as illustrated in Figure 1.9. This relationship is represented by the following equation:

$$\rho_u \cdot A \cdot s_T = \rho_u \cdot A_T \cdot \langle s_C \rangle_S \quad (1.10)$$

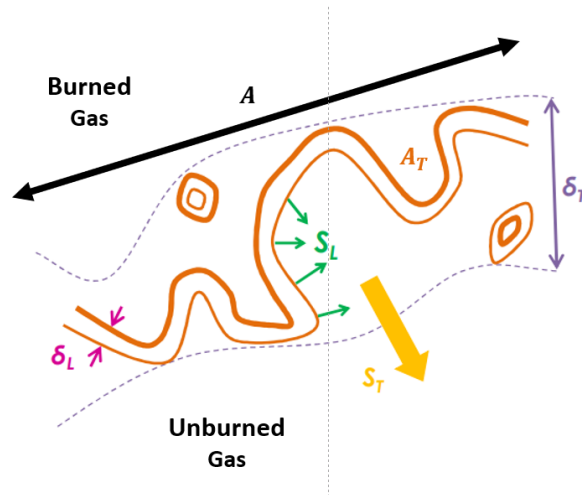


Figure 1.9: Schematic of a premixed turbulent flame [62].

Equating these mass flow rates, as shown by Driscoll [54], it follows:

$$\frac{s_T}{\langle s_C \rangle_S} = \frac{A_T}{A} \quad (1.11)$$

The development of a spherical laminar flame results in a variation in the flame surface over time, causing the flame to stretch. The flame stretch rate, K , is calculated by the surface derivative with respect to time, normalized by the flame surface area, as $K = A^{-1}dA/dt$. The stretch influences the flame speed, leading to the definition of the unstretched laminar flame speed, s_L^0 , which relates to the average consumption rate of reactants, as shown in Equation 1.12. Here, I_0 represents the average stretch factor, which quantifies the effect of the flame's stretching and accounts for both the local flame curvature and flow effects, as defined by Bray [63].

$$\langle s_C \rangle_S = s_L^0 \cdot I_0 \quad (1.12)$$

Thus, when the flame front is curved (i.e., not flat), the stretch factor modifies the laminar flame speed depending on the local curvature and the properties of the mixture. Finally, a relationship between the unstretched laminar flame speed and the turbulent flame speed can be established, as shown by Driscoll et al. [54]:

$$s_T = s_L^0 \cdot \frac{A_T}{A} \cdot I_0 = s_L^0 \cdot \Xi \cdot I_0 \quad (1.13)$$

This equation demonstrates that deviations of the turbulent flame speed from the unstretched laminar flame speed can occur due to an increased flame surface area from wrinkling or variations in the local burning rate relative to an unstretched flamelet. This complex phenomenon is especially significant under internal combustion engine conditions and must be addressed in hydrogen flames to advance this technology, particularly under lean and ultra-lean conditions, where modeling challenges may appear, such as flame instabilities [47, 64, 50].

1.3 Hydrogen-fueled internal combustion engines

The development of hydrogen-fueled internal combustion engines dates back nearly as far as the internal combustion engine itself, with advancements spanning over two centuries. François Isaac de Rivaz pioneered the concept in 1807 by creating the first combustion engine car powered by a hydrogen-oxygen mixture. In 1860, Jean Joseph Etienne Lenoir developed a two-stroke engine fueled by hydrogen generated via electrolysis, marking the first commercially viable internal combustion engine [12]. Throughout the 20th century, H₂ICE technology continued to evolve, with notable innovations such as Norsk Hydro's 1933 onboard ammonia reforming system for hydrogen production and the Musashi Institute of Technology's high-pressure hydrogen storage vehicle, Musashi 1, introduced in 1974. By the 1970s, manufacturers like BMW and Mazda began exploring hydrogen as an alternative fuel. By the early 2000s, this led to models like the BMW Hydrogen 7 and Mazda RX-8 Hydrogen RE, which showcased significant advancements in engine design and hydrogen storage.

Between 2000 and 2018, automakers such as Ford, Quantum, and others made further strides in developing hydrogen-specific vehicles. They introduced improvements in hydrogen storage, direct injection systems, and emissions control to meet increasingly stringent environmental

standards. European and Japanese projects, including HyICE (2004–2007) and NTSEL’s research (2005–2010), significantly pushed the limits of H₂ICE efficiency and power output, laying the foundation for contemporary hydrogen engines [65]. More recently, Alpine, Solution F, and Ligier have introduced H₂ICE racing vehicle demonstrators, highlighting the growing interest in hydrogen engines as a zero-emission solution [25].

Hydrogen-fueled vehicles can be classified by several key characteristics. As Verhelst and Wallner [12] describe, they may be either conversion or dedicated vehicles, depending on whether they were adapted for hydrogen operation by an aftermarket supplier or purpose-built for hydrogen. H₂ICEs are further categorized as mono-fuel or bi-fuel: mono-fuel vehicles run exclusively on hydrogen, whereas bi-fuel vehicles have the option to use hydrogen or an additional fuel. The two main methods for hydrogen storage in H₂ICEs are compressed hydrogen and cryogenic liquid hydrogen, and the engines are typically either reciprocating internal combustion engines or rotary engines.

In some applications, hydrogen acts as a combustion enhancer, combined with another fuel as either a hydrogen blend or in dual-fuel setups. Hydrogen blends often involve hydrogen mixed with natural gas or biogas, while dual-fuel systems simultaneously use hydrogen and another fuel, such as diesel or biodiesel. Most H₂ICE studies focus on spark-ignition engines utilizing either port fuel injection (PFI) or direct injection (DI). Compression ignition engines with direct hydrogen injection or glow-plug ignition are also viable configurations for H₂ICEs. Additionally, hydrogen combustion has been studied across different engine types – spark ignition (SI) and compression ignition (CI) – each offering unique large-scale aerodynamic structures and turbulence levels that influence turbulent flame development and combustion characteristics [65, 66, 16].

The properties of hydrogen significantly affect key ICE phases, including intake, mixture formation, ignition, and combustion [12]. The operation of H₂ICEs and their associated challenges related to mixture formation strategies, abnormal combustion events, and engine performance will be discussed in the following sections. This overall analysis aims to assess the implications of using hydrogen as a fuel in a baseline gasoline four-stroke SI reciprocating engine operating on pure hydrogen from compressed hydrogen storage.

1.3.1 Mixture formation strategies

The low volumetric energy density of hydrogen has significant implications for hydrogen storage on vehicles. For example, at a storage pressure of 350 bar, 1 kg of hydrogen occupies 40 liters; at 700 bar, it occupies 25 liters. Hydrogen can also be stored in liquid form by cooling it to its condensation temperature at atmospheric pressure, which is $-253\text{ }^{\circ}\text{C}$. However, this process is highly energy-costly, though it increases the density to 70.9 kg/m^3 , resulting in an energy density of about $8,510\text{ MJ/m}^3$. Additionally, it is important to consider the mass and volume proportions of the fuel and oxidant within the engine. In terms of mass, it takes 34.2 g of air to completely burn 1 g of hydrogen at stoichiometry – twice as much air as needed for methane – resulting in a mixture of 2.9% hydrogen and 97.1% air by mass, as displayed in Table 1.3. However, in terms of volume, hydrogen occupies 29.6% of the mixture, with air making up the remaining 70.4%. This is 15 times more than isooctane and three times more than methane by volume. Thus, to release the same amount of energy, hydrogen occupies a significantly larger volume in the combustion chamber – three times more than methane, for example. This means that the air supply circuit for a hydrogen combustion engine operating

with a lean mixture must be designed to accommodate 1.5 to 3 times the volume of air required by a gasoline engine for a similar power output.

The use of diluted mixtures is a strategy that helps the mitigation of abnormal combustion events like knocking [67] and lowers combustion temperatures. As an example, Table 1.3 shows the difference in terms of adiabatic flame temperature (T_b) between a stoichiometric hydrogen/air flame of about 2400 K and a ultra-lean hydrogen/air flame, which is about 1100 K, more than 1000 K colder. This low temperature flame reduces thermal NOx formation and can enhance efficiency due to less heat loss [19]. Three main types of dilution can be employed:

1) Dilution by Air:

This method involves reducing the fuel-air equivalence ratio by adding more air, which hydrogen's wide flammability range and low ignition energy make possible. Hydrogen engines can operate at very low equivalence ratio, down to 0.2 [41], and aim to avoid exceeding 0.5 [39, 68], as illustrated in Figure 1.10. Operating at these low equivalence ratios can significantly reduce NOx emissions, potentially achieving near-zero emissions in certain operating conditions. Achieving such high dilution levels requires an efficient supercharging technology to handle the increased air flow rates [12].

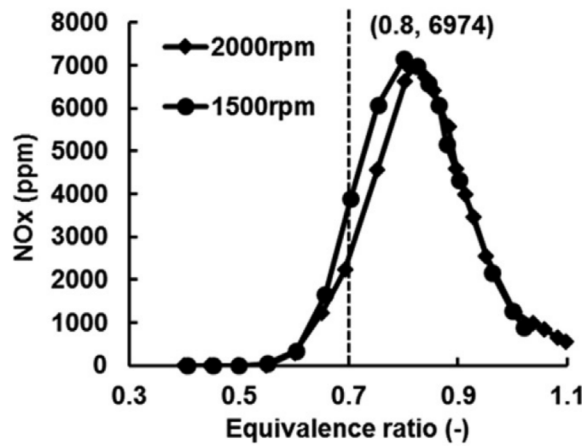


Figure 1.10: NOx emissions as a function of the equivalence ratio for two engine speed in a spark-ignition port-fuel injection H_2 ICE [68].

2) Dilution by Exhaust Gas Recirculation:

EGR strategies involve recirculating a portion of the exhaust gases back into the intake system. This method is widely used in diesel engines and requires a dedicated circuit in the engine's air loop [19]. The exhaust gases, which contain high levels of water due to hydrogen combustion, must be cooled with a heat exchanger to optimize the EGR system's efficiency [12]. Moreover, the presence of NOx in exhaust gases, and consequently in the EGR, can influence the auto-ignition properties of the mixture, as observed in [69].

3) Dilution by Water Injection:

Water injection is another dilution method that involves directly injecting water into the combustion chamber. This method allow for the use of a higher equivalence ratio mixture since the water injection, acting as an inert gas, decreases the adiabatic flame temperature and NOx emissions. It also reduces the need of bigger supercharging systems since higher equivalence ratios are used. However, this strategy requires the installation of a dedicated system, including a tank, pump, pressurized circuit, injectors, and a control system [70].

Hydrogen presents a very high diffusion coefficient in air, approximately 10 times faster than isooctane (see Table 1.3). Consequently, the air-hydrogen mixing process in a combustion engine is theoretically much faster. This quick mixing would lead to a more homogeneous air-fuel mixture, which is advantageous in terms of emissions. Avoiding locally rich fuel areas reduces the risk of high energy release zones associated with elevated flame temperatures, decreasing nitrogen oxide (NO_x) emissions [39]. Additionally, homogenizing limits variations in mixture properties and engine performance [71, 47]. However, some studies by Saudreau et al. [72, 73] have shown that strong baroclinic effects can occur in hydrogen jets within a pulsed cross-flow, significantly impacting mixture preparation.

1.3.2 Abnormal combustion events

Hydrogen's broad flammability range and low ignition energy make it prone to abnormal combustion phenomena such as pre-ignition, knocking, and backfire [12]. These issues are critical in the design of hydrogen combustion engines, as they can significantly impact engine performance and longevity [19].

1) **Pre-Ignition:**

In a typical engine cycle, the air-fuel mixture is compressed within the combustion chamber by the rising piston. Combustion is then initiated by the spark plug, typically a few degrees before or after the Top Dead Center (TDC). Pre-ignition occurs when combustion starts prematurely, before the spark plug fires. This can happen as early as the Bottom Dead Center (BDC), at the beginning of the compression phase when the intake valves have just closed [9]. The exact causes of pre-ignition are currently under investigation. The work by Guo et al. [74] suggests that pre-ignition in hydrogen internal combustion engines results from a complex interaction of multiple factors. Possible causes include hot spots within the combustion chamber, such as exhaust valves, spark plug electrodes, and piston heads, as well as incandescent particles from engine oil combustion and reactive compounds from engine oil degradation [75]. Another possibility is that parasitic sparks, especially when hydrogen is present at the spark plug terminals under low-pressure conditions, may trigger pre-ignition [76].

2) **Backfire:**

Backfire occurs when the air-hydrogen mixture ignites while the intake valves are still open. This leads to combustion and a pressure increase in the intake manifold, which can damage or destroy the intake system. Due to the lower ignition energy, the likelihood of backfiring increases as mixtures approach stoichiometry [12]. It is particularly relevant to engines with port-fuel injection systems, where hydrogen is introduced through the intake ducts before entering the combustion chamber [76]. This phenomenon presents a significant challenge in H₂ICEs, underscoring the need for precise control in engine design and operation [77].

3) **Knock:**

Knock is another abnormal combustion phenomenon that occurs when the fuel mixture ignites prematurely in one or more locations within the combustion chamber, before the flame has fully propagated. This premature ignition happens when the temperature in the unburned gas zone exceeds the auto-ignition temperature of the mixture. Knock is characterized by high-frequency, high-amplitude pressure oscillations caused by the sudden energy release from the self-igniting unburned gases [19]. Hydrogen has a high Research Octane Number (RON $\approx$ 130) [12]. Thus, one might assume that it would be resistant to knocking. However, hydrogen does not align well with the traditional definitions of octane number. While it has a very high RON, it has a much

lower Motor Octane Number (MON) [78]. MON was intended as a more accurate measure of how a fuel behaves under load, as the testing involves a similar engine to that used in RON testing, but with a preheated fuel mixture, higher engine speed, and variable ignition timing to further challenge the fuel's knock resistance [79]. Figure 1.11 illustrates abnormal combustion events of lean hydrogen/air mixtures in an internal combustion engine.

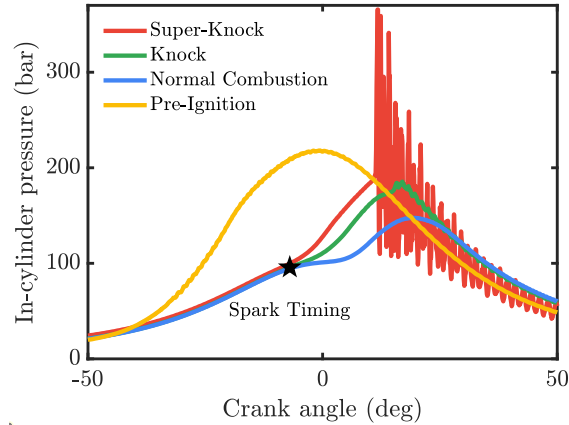


Figure 1.11: Abnormal combustion behaviors of a hydrogen/air mixture in a light-duty diesel baseline engine. Experiments conducted at PRISME Laboratory, University of Orléans. Conditions: $N = 900$ rpm, $IMEP = 7$ bar, $\phi = 0.50$.

1.3.3 Engine performance

The performance of an engine is closely tied to its efficiency, the power it can deliver (which depends on the amount of energy introduced into the engine), and its emissions.

1) Efficiency and power

Hydrogen-fueled ICEs present a challenge in terms of power output due to H_2 's low volumetric energy density. The key is injecting the necessary quantity of hydrogen into the combustion chamber within the time constraints imposed by the engine cycle [76].

Maximizing the amount of hydrogen injected within the limited time frame depends on both the static flow rate of the injector and the injection pressure. Higher injection pressure increases the static flow rate, allowing more hydrogen to be injected in less time. However, the injection pressure must be balanced carefully. It must be lower than the hydrogen tank's pressure and should ideally be minimized to make efficient use of the hydrogen stored in the tank. This approach maximizes the vehicle's range by avoiding the need for additional compression systems [12]. To manage the air required for combustion, supercharging technologies are considered, particularly for engines operating with excess of air. The most suitable supercharging technologies for hydrogen engines are those used in engines that function under high intake pressures, such as: dual-stage supercharging, mechanical compressors or electrically assisted supercharging [9].

The combustion characteristics of hydrogen, combined with the need for technologies that require high supercharging rates, impose significant mechanical stresses on the engine [12]. These stresses are more akin to those experienced by diesel engines than by gasoline engines [19]. To mitigate these stresses and improve power output, one possible strategy is to increase

engine displacement, a process known as up-sizing. This involves designing engines with larger displacements to handle higher loads without increasing mechanical stress [9].

2) Emissions

In addition to dilution techniques, controlling NO_x emissions can be achieved through aftertreatment devices such as Selective Catalytic Reduction (SCR) systems, commonly used in diesel engines. However, these systems must be adapted to the specific NO_x emission levels and conditions of hydrogen engines since they generally produce significantly lower NO_x emissions compared to diesel engines due to their lower equivalence ratio operation. Additionally, because the SCR process requires precise control of the ammonia injection rate, insufficient injection leads to unacceptably low NO_x conversion, while excessive injection causes the undesirable release of ammonia into the atmosphere [12].

While the need for NO_x post-treatment is reduced in hydrogen engines, it remains necessary, particularly during transient phases of speed and torque, where momentary increases in NO_x emissions can occur [9]. The lower exhaust gas temperatures and higher water content of hydrogen engines require post-treatment systems to be optimized for hydrogen combustion. Current research is focused on adapting these systems to hydrogen engines and minimizing the consumption of reductants. There is also potential for using hydrogen itself as a NO_x reductant, which could eliminate the need for carrying AdBlue, a mixture of water and urea used in SCR systems for diesel engines [80, 81].

1.3.4 Engine adaptation

H₂ICEs, considered primarily with a spark-ignition combustion technique [12], require some adaptations to accommodate the distinct properties of this alternative fuel. The geometry of the combustion chamber (cylinder head, intake and exhaust ducts, piston) and its components (spark plug, injector), are crucial for optimizing engine efficiency and emissions. One of the primary challenges in achieving high performance and efficiency is controlling abnormal combustion phenomena, such as pre-ignition and backfire [76]. This can be achieved by modifying the combustion chamber design to manage hot spots, adjusting the thermal conductivity of materials, and improving spark plug and coil technology to avoid parasitic sparks [9].

The optimization of internal aerodynamics and injection strategies is also important to minimize rich pockets of hydrogen. Introducing hydrogen at the optimal moment in relation to air movement by adjusting the timing of fuel injection facilitates thorough mixing between the gases. Direct injection is an effective method to prevent backfire, reducing notably the likelihood of having a flammable mixture in the intake ducts [12]. However, this approach introduces the challenge of managing a more heterogeneous mixture, making combustion emissions more difficult to control [82]. Additionally, the internal aerodynamics are optimized by designing intake ducts that influence the movement and speed of gases entering the cylinder. It also impacts the combustion process as the flame is in a turbulent environment and the interplay between them can significantly change the flame development [37, 41]. Finally, the compression ratio (CR) in H₂ICEs also needs adjustments. Currently, the CRs for hydrogen engines are optimized in the range of 10 to 12:1, which is similar to those used in gasoline or gas engines [12].

1.4 State of the art in in-cylinder hydrogen/air flames

Most experimental studies on hydrogen flames have been conducted under atmospheric conditions, which differ significantly from the high temperature and pressure conditions within an engine's combustion chamber [9, 12]. One of the pioneering studies investigating in-cylinder hydrogen/air flames in an optical engine was conducted by Heywood and Vilchis in 1984 [83]. Their objective was to compare the flame characteristics of propane and hydrogen in a spark ignition engine using high-speed Schlieren imaging. Both fuels were examined under stoichiometric mixtures and part-load conditions, with an intake pressure of 0.5 bar. Hydrogen exhibited significantly faster and spherical flames with reduced combustion variability and smaller flame thickness compared to propane. Moreover, due to the much higher flame speed of hydrogen under these conditions compared to in-cylinder turbulence, its flame development was primarily driven by laminar flame speed. In contrast, turbulence played a more substantial role in propane flame development.

Subsequently, Meier et al. [84] explored the impact of mixture formation on hydrogen combustion. They investigated two injection systems (port-fuel and direct injection) using high-speed Schlieren photography to observe flame propagation behavior in an optical side chamber. The results indicated that flame speeds decreased with decreasing equivalence ratio at a given engine speed. Additionally, the behavior of flame speed as a function of crank angle was found to be highly dependent on both equivalence ratio and engine speed. Measurements of turbulent flame speeds revealed a linear increase with turbulence intensity. Furthermore, ultra-lean mixtures exhibited nearly constant flame speed over the crank angle during the early flame growth period.

White [85] investigated mixture formation in a direct injection engine and the characteristics of hydrogen/air flame propagation, varying equivalence ratios from 0.45 to 0.95. Different injection strategies and pressures were assessed. Pre- and post-IVC (Intake Valve Closing) injections showed distinct combustion development, attributed to differences in mixing and resulting homogeneity. Generally, homogeneous mixtures exhibited reduced cycle-to-cycle variations (CCVs) and nearly constant expansion speeds across measured crank angles. Kirchweyer et al. [86] also examined the impact of mixture formation on combustion processes in direct injection hydrogen-fueled engines. They utilized Planar Laser-Induced Fluorescence (PLIF) measurements to analyze mixture formation, and evaluated flame propagation velocity under various configurations. Equivalence ratio effects were explored from 0.5 to 1.0. For the tested conditions, flame velocity also remained constant during the cycle. Roy et al. [87] were similarly interested in the influence of mixture composition on in-cylinder hydrogen/air flame characteristics. They investigated the effects of injection pressure and timing on flame behavior using chemiluminescence and concluded that injection timing has major impact on mixture formation and flame development.

Salazar and Kaiser [88] investigated the impact of flow field on flame speed of ultra-lean mixtures with high-speed Schlieren imaging. They demonstrated a correlation between in-cylinder pressure variations and flame patterns on a single-cycle basis. In their experimental setup, the flow field notably influenced flame shape and convective displacement. Additionally, a higher tumble ratio was found to increase flame speed during the early flame development phase. In a separate study, Aleiferis and Rosati [89] examined in-cylinder hydrogen/air flames using chemiluminescence and Laser-induced Fluorescence (LIF) of OH, with equivalence ratios ranging from 0.50 to 0.83 at 1000 rpm, employing both Port Fuel Injection and Direct

Injection strategies. Their findings revealed symmetrical flame growth on a macro-scale for both injection strategies. Notably, flames in PFI operation were considerably slower compared to those in DI operation. Furthermore, fewer cyclic combustion variabilities were observed in hydrogen flames compared to gasoline flames. The same authors also analyzed the autoignition of hydrogen/air mixtures with equivalence ratios varying from 0.40 to 0.63 through chemiluminescence and OH PLIF, examining in-cylinder flame behavior, including flame expansion, motion, and the effects of single and double injection strategies [79]. Findings indicated that higher intake temperatures had a limited effect on initial flame timing, but hydrogen's autoignition differed significantly from hydrocarbon HCCI, displaying a swirling motion influenced by fuel-air interactions and stratification. Double injection led to earlier, more symmetrical combustion with less swirling, while leaner mixtures showed fragmented and distorted combustion patterns. Overall, autoignition was slower and deflagrative, resembling propagation more than typical HCCI. In combined spark ignition and HCCI, a secondary flame front formed, reducing the tendency for knocking combustion common in hydrocarbon fuels.

More recently, Welch et al. [90] investigated the impact of thermodiffusive and hydrodynamic instabilities on the initial propagation of lean hydrogen flames in a spark-ignition engine. Using high-speed PLIF with SO_2 tracer gas, the researchers analyzed flame front development in an optically accessible engine at 800 RPM and intake pressures of 0.4 and 0.95 bar, as illustrated in Figure 1.12. When comparing lean hydrogen/air flames to stoichiometric methane/air flames, the study found minimal differences in flame surface density under identical conditions. This suggests that turbulence and dynamic confinement within the engine environment may counteract flame instabilities more than in traditional experimental setups like bomb calorimeters, where such instabilities are more apparent. Despite this attenuation, the study observed that extremely lean hydrogen mixtures increase flame surface density, indicating that flame instabilities become more pronounced under these conditions. The findings suggest that turbulence and flame-wall interactions significantly influence hydrogen combustion in engines, highlighting the importance of further research to fully understand how flame instabilities impact hydrogen-fueled engine performance, especially in low-turbulence or high-optical-resolution scenarios.

1.5 Enhanced data for augmented prediction in ICEs numerical simulations

1.5.1 The need for enhanced data

To meet today's stringent emission standards and improve combustion efficiency in internal combustion engines, various advanced combustion strategies have been proposed. These include EGR, homogeneous charge compression ignition (HCCI), highly dilute spark-ignition, ultra-lean spark-ignition combustion [91], stratified combustion, and engine downsizing. However, implementing such strategies intensifies the sensitivity of the combustion process to in-cylinder flow dynamics, leading to cycle-to-cycle variability.

To accurately simulate engine performance and capture variability, high-fidelity data is essential for numerical simulations, such as Large-Eddy Simulations (LES). Advanced data enables better modeling of complex interactions within the combustion chamber, which is critical for accurately predicting combustion behavior and outcomes. CCV is a central challenge in ICE performance, as it restricts the engine's operational range and can contribute to increased noise

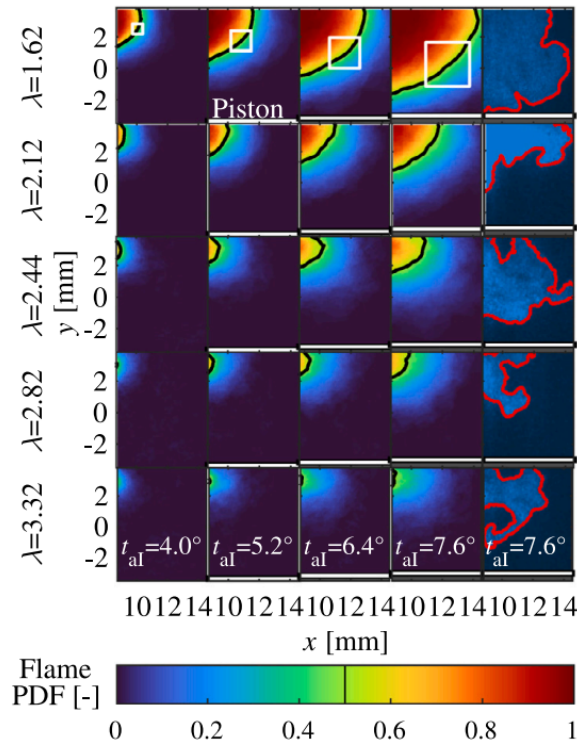


Figure 1.12: Early flame PDF and instantaneous flame images with varying λ for lean hydrogen/air flames [90].

and emissions, including the risk of engine knock. Improved data-driven models are needed to correctly represent CCV's impact on combustion and efficiency, especially as CCV's influence is heightened in the case of alternative fuels like hydrogen [92, 93].

Hydrogen's broad flammability range allows for ultra-lean combustion operation, which helps to reduce NOx emissions. However, it also increases the sensitivity to in-cylinder flow variations, largely due to hydrogen's lower laminar flame speeds, which in turn contributes to CCV. For instance, hydrogen's laminar flame speed at an equivalence ratio of 0.25 is comparable to that of lean gasoline-air mixtures at a ratio of 0.6, demonstrating its slower combustion response under lean conditions. Additionally, hydrogen's wide flammability range and low ignition energy pose risks for pre-ignition or knock due to locally richer mixture zones or hot spots within the combustion chamber, as well as backfiring in the intake manifold in engines with port-fuel injection, as discussed before.

To mitigate such abnormal combustion phenomena, optimizing mixture preparation through precise control of injection parameters and internal aerodynamics is essential. Yet, models that comprehensively capture turbulent combustion interactions under engine conditions are lacking. Recent studies [94, 47, 95] underscore the importance of understanding thermodiffusive and stretch effects on flame behavior with hydrogen and hydrogen-based fuels to account for trends observed in real engine operations. Given hydrogen's unique properties, a significant redesign of ICEs has been recommended [96] to support hydrogen applications effectively.

1.5.2 Cycle-to-cycle variations

To reduce pollutant emissions and enhance engine efficiency, cyclic variability is a critical research area in optimized internal combustion engines [97]. Studies suggest that reducing cycle-to-cycle variations could increase engine power output by up to 10% without additional fuel consumption [98], underscoring the importance of understanding these variations in ICEs. CCVs, which arise from fluctuations in the combustion process, are influenced by inconsistencies in charge composition (air, fuel, and residual gases), fluid motion (both large-scale and small-scale turbulence), mixture inhomogeneity (in composition and temperature), and spark discharge characteristics across cycles [99].

Studies show that CCVs are more pronounced in lean and highly diluted mixtures, as well as under low-load conditions (such as during idling) [98, 99, 100, 101]. Hinze and Cheng [99] experimentally demonstrated the influence of multiple factors on CCVs in gasoline SI engines at idle, showing that fluctuations in indicated mean effective pressure (IMEP) are primarily driven by flow field variations and charge inhomogeneity (54%) and by residual gas mass variation (approximately 33%). Meanwhile, combustion duration variations were mostly attributed to the flow field (around 80%).

Truffin et al. [71] explored the causes of cyclic variability in both experiments and large eddy simulation of a propane-fueled ICE. Their findings revealed that CCVs increase with diluted and lean mixtures. A multivariate analysis evaluated the impacts of various parameters on the early flame and main propagation phases for both mixtures, comparing these results with the experiments of Ozdor et al. [98]. For the lean mixture, the most influential factor for cyclic variability in the early flame phase was flow field fluctuation, followed by global dilution and equivalence ratio disparity, aligning with Ozdor et al.'s conclusions. However, flow field and global dilution showed only moderate correlation in the diluted mixture. In the main propagation phase, global dilution and equivalence ratio had moderate effects on in-cylinder charge.

Recent studies by Ding et al. [92, 93] utilized LES to investigate in-cylinder flow dynamics and CCVs in gasoline SI engines. The first study linked large-scale tumble flow patterns and intake valve jet interactions to combustion variability, suggesting that central flow region dynamics strongly impact flame propagation and combustion speed. The second study focused on the compression phase, revealing that local velocity fields near the spark plug influence flame kernel growth and early flame spread, with faster propagation aided by higher velocities along specific axes. Both studies emphasize that variability in the tumble structure during compression is a primary contributor to CCV.

Because combustion duration in an engine is linked to flame speed, the mixture equivalence ratio has a substantial impact on combustion events [76, 102]. Hydrogen flame speed is primarily influenced by three factors: laminar flame speed, flow field turbulence, and flame instabilities [47, 50]. Several studies, primarily from a decade ago, investigated CCVs in hydrogen-fueled internal combustion engines with both direct-injection and port fuel injection systems [103, 104, 105, 106]. These studies were largely conducted on gasoline-based engines with near-stoichiometric mixtures and examined the effects of hydrogen/air equivalence ratio, engine speed, and load on CCVs in H_2 ICEs retrofitted from gasoline engines. Kim et al. [103] concluded that increased CCVs at lower equivalence ratios are primarily associated with the flame initiation process. Ma et al. [104] observed greater instabilities at lower loads, while Chen [105] found that hydrogen injection timing minimally affected CCVs in port fuel injection hydrogen engines at idle. Sun et al. [106] demonstrated that ignition timing strongly influences CCVs, especially at low equivalence ratios, with minimum variability occurring at

the maximum brake torque (MBT) operating condition. Further research is essential to understand the influence of hydrogen's unique properties on engine parameters, especially under lean and ultra-lean conditions. Thus, optimizing H₂ICE performance relies on a high-fidelity understanding of in-cylinder flow characteristics and flame dynamics.

1.6 Objectives and outline of the thesis

1.6.1 Objectives, novelty and contribution

For the successful application of hydrogen in internal combustion engines, experimental investigations are essential, especially given the specific properties and challenges associated with hydrogen use in ICEs, as discussed in previous sections. The limited data on in-cylinder hydrogen/air flames – particularly under ultra-lean conditions – necessitates such research to advance both scientific understanding and industrial applications. Recent advancements in numerical, experimental, and analytical tools have improved our ability to analyze unsteady in-cylinder flows and combustion, with Large-Eddy Simulation emerging as a critical tool for designing robust spark-ignition engines. Despite validation against defined experiments, LES predictions still face significant uncertainties, particularly in turbulent dynamics and combustion. This challenge is even greater in lean hydrogen combustion applications due to hydrogen's unique flame dynamics (such as thermodiffusive instabilities and thicker flame fronts in ultra-lean conditions), which are not yet fully understood.

This thesis aims to develop innovative tools to enhance the prediction and analysis of hydrogen/air turbulent reactive flows in spark-ignition engine operations, focusing on capturing time-resolved events and understanding complex combustion phenomena. Since multiple physical processes interact within the cylinder, it is essential to decouple these to assess each behavior independently; therefore, this work isolates the mixing challenge to focus specifically on turbulent flame dynamics across various conditions. The high-fidelity experimental data produced here will aid the development of lean hydrogen/air combustion models for ICEs and support the reduction of uncertainties in numerical simulations, particularly LES, by improving model parameters and boundary conditions. The combined use of numerical simulations and experimental investigations offers a powerful approach for advancing the application of reactive flows in industry.

1.6.2 Plan of the thesis

The present Ph.D. thesis will be divided in the following 6 chapters:

- **Chapter 2: Experimental setup and methodology**

This chapter details the process of designing the experimental test bench. It also describes the various techniques that are utilized to measure key parameters, such as the heat release during hydrogen combustion, the internal aerodynamics within the engine, and the characteristics of in-cylinder flames. Furthermore, it outlines the various methodologies employed to conduct the experiments and analyze the data for each of the distinct experimental setups used in the study. It provides a detailed description of the experimental procedures, data collection techniques, and analytical tools that are applied to ensure accurate and reliable results.

- **Chapter 3: Heat release analysis**

This chapter presents the key findings from experiments conducted using the all-metal version of the hydrogen-fueled spark-ignition engine developed for this study with the heat release method. It also delves into an analysis of these results, using fundamental parameters of hydrogen flames to better understand and interpret the engine's performance and combustion characteristics.

- **Chapter 4: Internal aerodynamics characterization**

This chapter evaluates the in-cylinder flow characteristics within the optical engine, using statistical analysis to examine the data. It identifies and extracts the key parameters necessary for analyzing the behavior of the in-cylinder turbulent flames in the subsequent investigation.

- **Chapter 5: In-cylinder flame development**

This chapter examines the characteristics of hydrogen/air flames under different operating conditions, linking theoretical aspects of flame behavior with varying levels of turbulence (through engine speed) and in-cylinder thermodynamic conditions and comparing it to stoichiometric propane/air flames.

- **Chapter 6: Cycle-to-cycle variations**

This chapter analyses hydrogen combustion behavior over repeated engine cycles. It examines the key factors that lead to instability in the engine operation and compares these cyclic variations to those observed while using conventional fuels.

- **Chapter 7: Conclusions**

This chapter summarizes the research conducted, highlighting the key analyses performed on in-cylinder hydrogen combustion. It also outlines potential areas for future study, suggesting directions for further investigation to enhance the understanding and optimization of this technology.

Chapter 2

Experimental setup and methodology

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Introduction

This chapter provides a comprehensive description of the experimental setup, methodology, and data processing tools utilized in this thesis. The first section presents a detailed overview of the single-cylinder optical spark-ignition engine, including all auxiliary components used in the experiments. The second section introduces the heat release analysis method developed for this study, utilizing Three Pressure Analysis and a two-zone thermodynamic model to evaluate the performance parameters and characteristics of both the burned and unburned zones within the combustion chamber. The third section focuses on the use of Particle Image Velocimetry (PIV) for characterizing in-cylinder aerodynamics. It also covers the experimental conditions, data processing procedures, and validation studies conducted to justify the selection of specific parameters and ensure the reliability of the methodologies. In the fourth section, the measurement of hydrogen/air flames inside the cylinder is discussed, emphasizing the theory behind chemiluminescence and the associated data processing techniques. The fifth section examines the methodologies used to study cyclic variability, highlighting the unique aspects of hydrogen combustion. Finally, the chapter concludes with a summary of the measurements and a reflection on the research objectives.

2.1 Test bench configuration

The experiments were conducted with an optical spark-ignition engine (PSA EP6DT version). This engine, originally designed to study gasoline direct-injection experiments [107], was adjusted to perform combustion research on hydrogen/air mixtures.

2.1.1 Test bench

The test bench schematics are displayed in Figure 2.1. Intake air is dehumidified and filtered, and its flow is regulated by an Emerson MicroMotion F025S Coriolis flow meter, which has a measurement accuracy of 0.5% of the flow rate and a maximum flow rate of 20 kg/h. The flow of hydrogen is controlled and monitored by a 30 NLPM Brooks 5850S mass flow meter, with an accuracy of 0.2% of the full scale (FS).

The cooling water and oil are maintained at 85 °C. Intake and exhaust temperatures are monitored using low-frequency K-type thermocouples placed in the plenums and pipes. Pressure measurements are taken at points located 200 mm and 160 mm from the intake and exhaust valves, respectively. The intake and exhaust pressure transducers used are Kistler 4075A10 piezoresistive sensors, with an accuracy of 0.1% FS. Additionally, two high-frequency pressure transducers (Kulite XTL-205DC-190-50G, with a maximum differential pressure of 3.5 bar and an accuracy of 0.1% FS) are installed midway along the intake pipe and at the intake plenum as reference for numerical simulations.

In-cylinder pressure is measured using an AVL QH32C piezoelectric transducer, with a precision of 0.2% FS and a sensitivity of 26.82 pC/bar. As a differential transducer, it requires adjustments based on either intake or exhaust pressure to provide an accurate absolute in-cylinder pressure reading. Pegging was performed over 40 crank angles using the intake pressure, starting at 230° bTDC. The TDC reference was set at 0.6° bTDC in a motoring case at 1200 rpm and 0.9 bar of intake pressure.

2.1. TEST BENCH CONFIGURATION

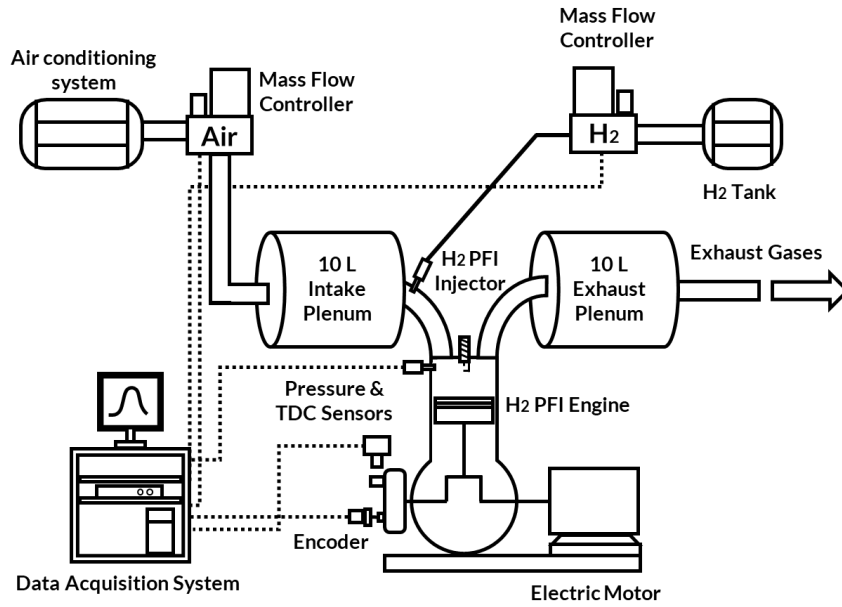


Figure 2.1: Schematic diagram of the test bench.

The engine is coupled with an electric motor-generator, enabling motoring conditions ranging from 600 to 1900 rpm. Recordings are performed at each 0.1 crank angle degree (CAD) by the optical encoder (Kubler 5020). All parameters are stored and controlled by an in-house LabView control system via an Ethernet port to the control computer at the frequency of 10 Hz. In order to guaranty the safety of the installation different alarms are put on the measured data. The test bench is also equipped with hydrogen sensors and a ventilation system is installed to prevent any hydrogen slip to the engine facility.

2.1.2 Optical engine

The EP6 optical engine has a twin-cam, 4 overhead valves and a pent-roof spray-guided cylinder head. The engine's characteristics are summarized in Table 2.1. A transparent liner and a Suprasil quartz glass [108] placed in the cylinder head (with a thickness of 15.00 and 24.25 mm, respectively) were used for the optical measurements, as shown in Figure 2.2.

The optical piston is a Bowditch-type design featuring an extended hollow structure with a 45° cylindrical mirror inside, providing optical access to the combustion chamber. It is specifically designed for direct injection engines and includes a non-symmetrical pent-roof shape with a 41 mm diameter central quartz window. The piston geometry and field of view are shown in Figure 2.3. The piston segments includes two double graphite rings spaced 5 mm apart, positioned 5 mm from the piston head. Throughout this thesis, the reference point is defined at the firing Top Dead Center, where CAD = 0°. The intake and exhaust valve timings are also exhibited in Table 2.1 and will be plotted later in the Three Pressure Analysis subsection.

2.1.3 Intake and exhaust components

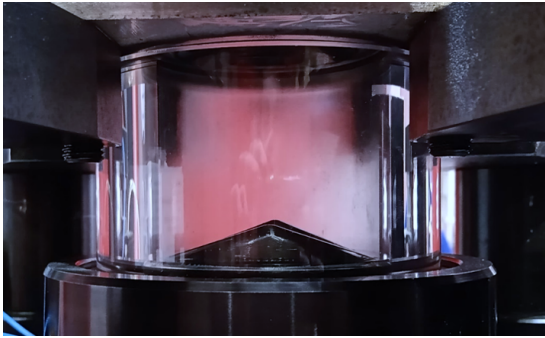
The intake and exhaust ducts, along with plenum volumes, were designed to accommodate the continuous injection of gaseous hydrogen. To highlight the significance of intake plenum

2.1. TEST BENCH CONFIGURATION

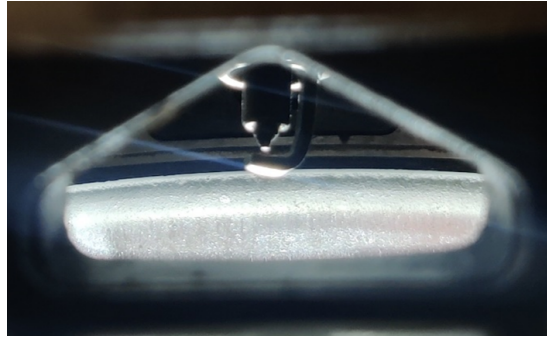
Table 2.1: Engine specifications and operating conditions ($^{\circ}\text{aTDC}$ stands for degrees after firing Top Dead Center). The CAD of valve openings and closures correspond to experimental residual valve lifts of 0.1 mm.

Description (units)	Value
Bore (mm)	85.8
Stroke (mm)	77
Compression ratio (-)	10.0
Connecting rod length	138.5 mm
Piston-to-Crank offset	0.8 mm
Piston geometry	Bowl
Cylinder head type	Pent-roof
IVO ($^{\circ}\text{aTDC}$)	+357
IVC ($^{\circ}\text{aTDC}$)	-122
EVO ($^{\circ}\text{aTDC}$)	+141
EVC ($^{\circ}\text{aTDC}$)	-339
Max. tumble ratio (-)	2.5 [109] ^a

^a At 1 bar and 1200 rpm (-230°aTDC).



(a) Optical liner.



(b) Cylinder head optical window.

Figure 2.2: Optical access points on the engine: liner and spark plug window.

volume and intake duct length, a 0D/1D numerical simulation was conducted in GT Power [110]. The simulation varied the length between the intake plenum and intake valves from 300 to 1100 mm and the intake plenum volume from 0 to 10 L. The intake duct diameter was fixed at 40 mm. Engine speed was varied from 1000 to 2500 rpm to assess its impact on volumetric efficiency (η_V), defined as the ratio of the actual volume of the air-fuel mixture inducted into the cylinders to the theoretical volume the engine could hold, expressed as a percentage [19]. This parameter was used to determine the final intake length and plenum volume for the experimental setup, with the goal of achieving values representative of real conditions across the selected ranges of intake pressure and engine speed. Ultimately, constraints were applied to select the optimal parameters, ensuring they closely align with high-fidelity numerical simulations boundary conditions and can further serve as accurate inputs, especially in Large-Eddy Simulations, as it is shown in Figure 2.4.

2.1. TEST BENCH CONFIGURATION

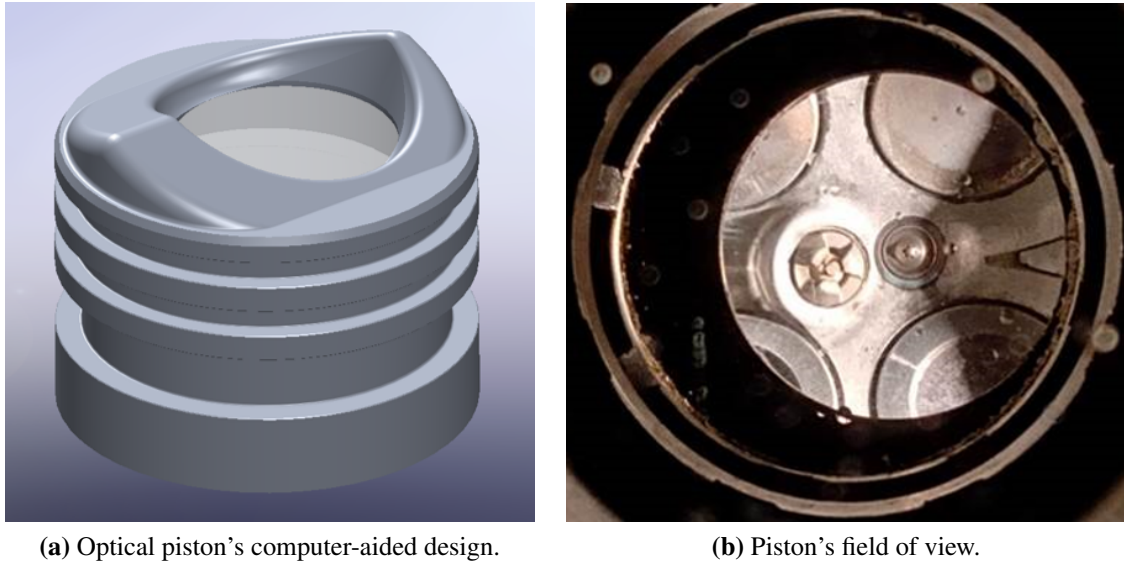


Figure 2.3: Bowditch piston design and field of view.

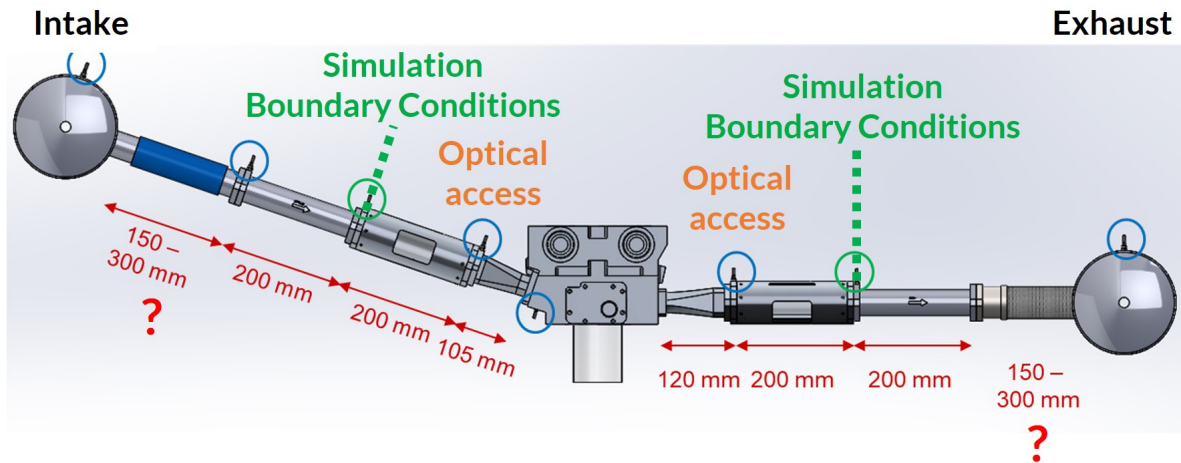


Figure 2.4: Determination of the intake length, exhaust length and plenum volumes. Questions marks are related to the final length adjustments. Final Intake and Exhaust Volumes = 10 L. Final Intake Length = 700 mm. Final Exhaust Length = 750 mm.

2.1.4 Hydrogen injection

Once the intake and exhaust geometries were defined, a study was made to establish the hydrogen injection position. Hydrogen was injected continuously with a tube of 6 and 8 mm of inner and outer diameters, respectively. This tube was centered to the 40 mm intake duct. The experiments aimed at determining the injection configuration resulting in the most homogeneous mixture. Thus, injection is carried out continuously at four different positions: 1) Near Cylinder Head, 2) Half-Intake Pipe, 3) Near Intake Plenum, and 4) Inside Intake Plenum, located 200, 500, 700, and 1000 mm away from the intake valves, respectively, as depicted in Figure 2.5.

To achieve this, the equivalence ratio is varied while maintaining a constant IMEP of 3

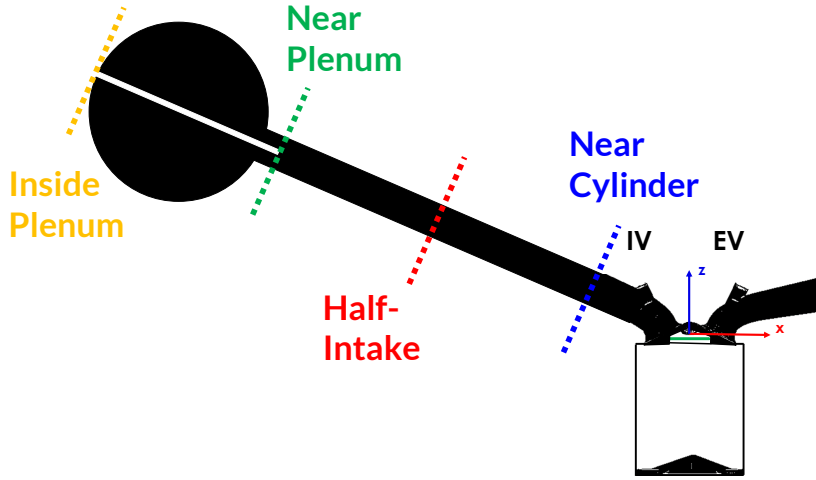


Figure 2.5: Schematics of the investigation into hydrogen injection positions.

bar. The hydrogen and air mass flow controllers set a specific fuel-air equivalence ratio in the intake manifold, defined as ϕ_{int} , which is varied from 0.20 to 0.55. The in-cylinder equivalence ratio, ϕ_{cyl} , which is the one used to assess combustion parameters, is lower since unburned air (due to lean combustion) remains as a residual in the combustion chamber. The spark timing is adjusted for each condition to target the crankshaft angle at which 50% of the total fuel mass in the cylinder has been burned during the combustion process (CA50) at 8 °aTDC (after firing Top Dead Center). To identify the optimal mixing strategy, histograms of both CA10 (Crank Angle at 10% Mass Fraction Burned) and CA50 are analyzed (calculated with the apparent heat release rate, discussed further in this chapter), as displayed for the CA10 in one specific condition in Figure 2.6. The strategy with the lowest overall standard deviation in both combustion timings, indicated by the narrower CA probability density function (pdf), is selected for the subsequent tests, since it corresponds to less fluctuations due to mixture heterogeneity.

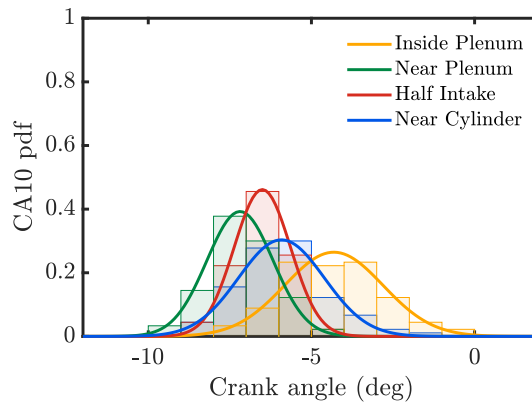


Figure 2.6: Methodology for selecting the most homogeneous injection position for a CA10 probability histogram at an equivalence ratio of 0.35 over 100 cycles.

2.1.5 Spark plug

Due to the distinct combustion properties of hydrogen, including its low minimum ignition energy and wide flammability limits, as well as the increased susceptibility of hydrogen/air mixtures to abnormal combustion events, a study is conducted to identify the most suitable spark plug. The goal is to select a spark plug that would ensure stable combustion at low loads while minimizing the risk of abnormal combustion at high loads. To accomplish this, five different spark plugs are tested. The models and specifications of these spark plugs are detailed in Figure 2.7 and Table 2.2.

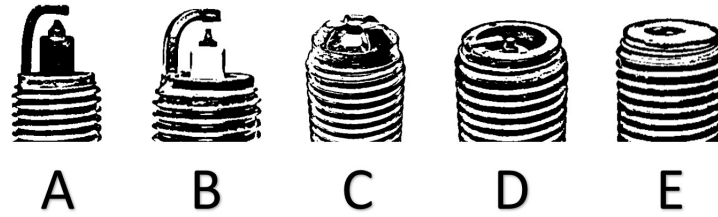


Figure 2.7: Explored spark plug geometries in the study.

Table 2.2: Spark plug models and references.

Reference	Spark plug model	Heat range (NGK)
A	Bosch ZR8TPP15	5
B	NGK PLZKBR7B	7
C	Bosch ZLR07MTE	10
D	Champion Proto-1	10
E	Champion Proto-2	11

In terms of geometry, spark plugs A and B have J-type protruded ground electrodes, spark plug C is equipped with three ground electrodes, spark plug D features a single side-gap non-protruded ground electrode, and spark plug E is of the surface gap type, with no exposed ground electrode.

The effects of the equivalence ratio and various spark plugs on cyclic variations are assessed under low-load conditions in the optical engine. The coefficient of variation of IMEP (CoV_{IMEP}) is used as a measure of engine stability, while the combustion duration ($\Delta\theta$), determined using the heat release rate (HRR) equation, as will be discussed later, is used to analyze the combustion process and flame variability. For high-load conditions, insights are drawn from laboratory experience with other hydrogen engines, particularly those based on diesel architectures, which are capable of withstanding higher in-cylinder pressures and more severe combustion conditions [9, 12].

2.2 Heat release analysis

Once geometry and components are fixed, a first analysis is conducted using a classic pressure-based metric, examining the in-cylinder pressure trace as a function of the crank angle and referred to as heat release analysis. With the in-cylinder pressure and a prediction of the

heat transfer to the cylinder walls, the combustion heat release can be calculated using the conservation of energy equation. This prediction is conducted using a two-zone combustion model in a 0D/1D numerical simulation, allowing for the assessment of unburned and burned zones, presenting distinct properties. The goal is to enhance the accuracy of heat transfer models [111] and consequently the combustion timings (CA2, CA5, CA10, and CA50, which represent the crank angles at which 2%, 5%, 10%, and 50% of the fuel is burned, respectively) and the evaluation of the unburned gas temperature. For the simulation, the Three Pressure Analysis (TPA) within the GT Power software [110] is employed.

2.2.1 Three Pressure Analysis

The TPA model in GT-SUITE software is a widely used method for estimating critical engine performance parameters by analyzing pressure measurements taken at three key engine locations: the intake manifold, the exhaust manifold, and the cylinder. This approach enables the determination of parameters such as volumetric efficiency, residual gas fraction, and in-cylinder heat release rates without necessitating a comprehensive modeling of the entire engine cycle [110].

The process begins by collecting time-resolved pressure data from these three points. The model then applies the principles of mass, momentum, and energy conservation to calculate instantaneous mass flow rates, temperatures, and pressures within the engine system. This method is particularly valuable for analyzing cyclic variations and pinpointing losses in the intake and exhaust systems, as well as within the combustion chamber.

In the simulation, high-speed intake and exhaust pressure curves acquired experimentally are set as input conditions. The TPA model is constructed by incorporating engine components such as ports, runners, valves, the cylinder, and the engine crank train geometry to estimate cylinder conditions. Specific details like valve lifts and discharge coefficients are also required for accurate modeling.

The TPA method is employed in two types of experimental analysis: ensemble-averaged and multiple consecutive cycles. The former is used to examine average operating conditions over 100 cycles, while the latter is utilized to study cycle-to-cycle variations. In both cases, instantaneous pressure trace measurements from the intake and exhaust ports are used as boundary conditions, and the calculated apparent burn rate is fitted to predict combustion parameters.

The engine, along with the intake and exhaust ports, is modeled in the software, as shown in Figure 2.8. The numerical model includes measured intake and exhaust valve lifts and discharge coefficients. Figure 2.9 presents an example of the imposed pressure traces and valve lifts.

Once the pressure inputs and geometry are set, the next step is to define the boundary conditions. Achieving accurate results with the TPA method requires a close alignment between the simulated and measured cylinder pressure traces. To ensure this, the engine's compression ratio and heat transfer within the combustion chamber must be accurately specified. Additionally, the wall temperatures of the intake and exhaust ports, as well as the combustion chamber, are critical for estimating volumetric efficiency and heat transfer.

Given the limited detailed information about the cooling system and heat transfer coefficients for individual components, a model was used to estimate the heat flux absorbed by the cooling water and the wall material. This approach follows a methodology similar to the "Eng-CylTWalSoln" template in GT-SUITE [110], calculating the wall temperatures for the cylinder head, cylinder, and piston. For the intake and exhaust ports, the wall temperature is set equal to

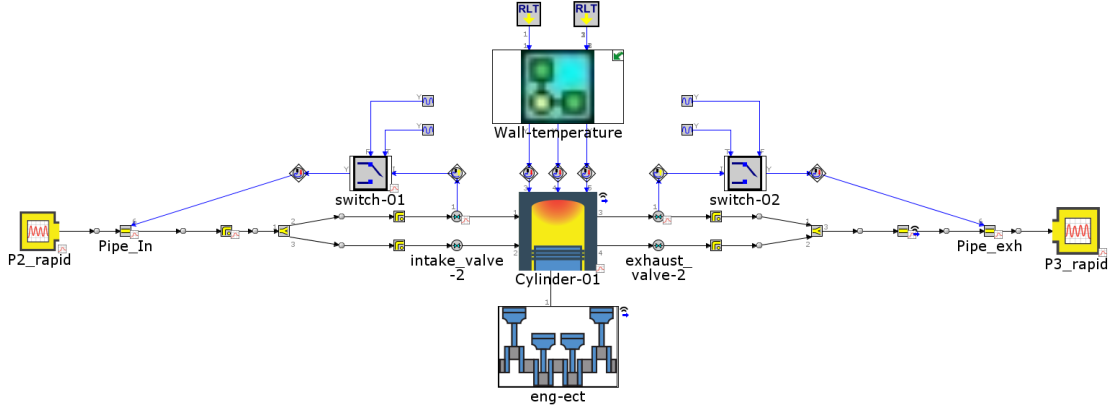


Figure 2.8: Three pressure analysis model developed for the EP6 optical engine.

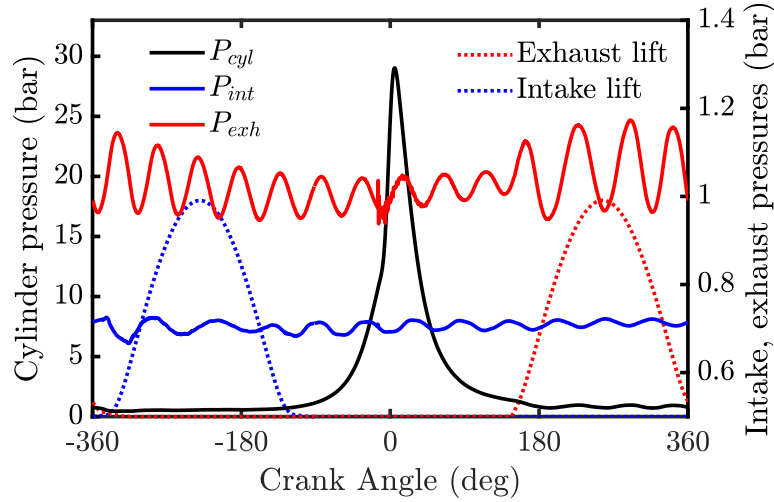


Figure 2.9: An example of ensemble-averaged measured in-cylinder, intake, and exhaust pressures, as well as intake and exhaust valve lifts, operating at $P_{int} = 0.7$ bar, $N = 1200$ rpm, $\phi = 0.55$, and spark timing at 15° bTDC.

that of the cylinder head.

The in-cylinder heat transfer coefficient, h , is calculated using the classic Woschni equation [19], traditionally used to estimate the convective heat transfer coefficient in internal combustion engines, calculated as indicated in Equation 2.1, as a function of the Bore diameter (B), the in-cylinder pressure (p), the in-cylinder temperature (T) and the gas velocity (w) accounting for piston motion and combustion.

$$h = 3.26B^{-0.2}p^{0.8}T^{-0.55}w^{0.8} \quad (2.1)$$

To match the gross indicated mean effective pressure (gIMEP) and the in-cylinder pressure trace, a constant in-cylinder heat transfer coefficient multiplier is adjusted for each operating condition. The GT Direct Optimizer tool is then employed to minimize the relative error between the experimental data and the simulation results, allowing the heat transfer multiplier to vary between 1 and 3 [112].

2.2.2 Performance parameters

In the heat release analysis, some key indicators of engine performance are analyzed: IMEP, combustion timings (e.g. CA2, 5, 10 and 50) and duration, $\Delta\theta$. The Indicated Mean Effective Pressure (IMEP) represents the average pressure exerted on the pistons during the power stroke [19]. It is given by the following equation:

$$\text{IMEP} = \frac{W_{ind}}{V_d} \quad (2.2)$$

where W_{ind} is the indicated work per cycle (in Joules) and V_d is the displacement volume of the cylinder (in cubic meters). The indicated work can be calculated by integrating the in-cylinder pressure, P , over the volume change, dV , during the engine cycle [19]:

$$W_{ind} = - \oint P dV \quad (2.3)$$

The combustion timings and duration are calculated with the mass fraction burned (MFB) parameter. The MFB provides insights into the combustion process by indicating the fraction of fuel that has been burned at any given point in the engine cycle. It is derived from in-cylinder pressure measurements using a thermodynamic analysis approach, specifically from the heat release rate (HRR).

The apparent heat release rate, $dQ_{ap}/d\theta$, is determined from the pressure data using the first law of thermodynamics. The heat release rate is calculated as:

$$\frac{dQ_{ap}}{d\theta} = \frac{\gamma}{\gamma - 1} \cdot P \cdot \frac{dV}{d\theta} + \frac{1}{\gamma - 1} \cdot V \cdot \frac{dP}{d\theta} \quad (2.4)$$

where γ is the ratio of specific heats. The heat transfer heat release, $dQ_{ht}/d\theta$, is then added to the apparent heat release to obtain the chemical energy - or gross heat release, $dQ_{ch}/d\theta$, as follows:

$$\frac{dQ_{ch}}{d\theta} = \frac{dQ_{ap}}{d\theta} + \frac{dQ_{ht}}{d\theta} \quad (2.5)$$

The gross heat release rate is then integrated over the crank angle (from ignition timing, θ_{ign}) to obtain the cumulative gross heat release, Q_{ch} :

$$Q_{ch}(\theta) = \int_{\theta_{ign}}^{\theta} \frac{dQ_{ch}}{d\theta'} d\theta' \quad (2.6)$$

Finally, the mass fraction burned, x_b , is defined as:

$$x_b(\theta) = \frac{Q_{ch}(\theta)}{Q_{total}} \quad (2.7)$$

where Q_{total} is the total heat release, calculated by integrating the heat release over the entire combustion event.

Furthermore, the information of the unburned and burned mixtures over the engine cycle, such as pressure, temperatures, etc., calculated from the two-zone model, can be used to assess the flame properties (e.g. laminar flame speed, adiabatic flame temperature, etc.) at different crank angles with a kinetic mechanism [113].

All of these parameters can be calculated over a cycle basis, meaning that statistical analysis can be made. The main functions used throughout this thesis are: the mean ($\bar{X}$), the standard deviation (σ_X) and the coefficient of variation (CoV_X), which is defined as the ratio between the standard deviation and the mean value and analyzed in percentage. It is used to assess the relative variability or dispersion of a set of data points in relation to the mean of the data set. Mathematically, the CoV_X is calculated as follows:

$$\text{CoV}_X = \frac{\sigma_X}{\bar{X}} \cdot 100\% \quad (2.8)$$

2.2.3 All-metal engine study methodology

A preliminary study is conducted using an all-metal cooled liner, allowing for higher in-cylinder pressure conditions. The objective is to understand hydrogen combustion in engines across different load conditions and equivalence ratios. Load levels ranges from 1 to 4 bar IMEP (with a maximum in-cylinder pressure limited to 50 bar due to mechanical constraints of the quartz window), while the equivalence ratio is varied from 0.20 to 0.55. For each condition, the combustion duration and its variability are analyzed and compared, with a focus on the different phases of flame development. In this thesis, the in-cylinder combustion is divided into three main phases [19]:

1. **Flame Initiation (0 to 10% of Mass Fraction Burned, MFB):** The flame initiation phase starts at the beginning of the spark discharge and continues until 10% of the total fuel mass has been burned. This phase is characterized by the kernel formation and early flame growth, which is critical for establishing a stable combustion process. During this period, the flame front is highly sensitive to ignition energy, turbulence, and the local air-fuel ratio [19].
2. **Flame Propagation (10 to 50% of MFB):** After the flame kernel has formed, the flame propagation phase occurs as the flame front moves rapidly through the combustion chamber, burning the remaining fuel. This stage, between 10% and 50% of MFB, is when the air-fuel mixture is consumed without a great flame-wall interaction. It is directly influenced by the turbulence levels within the chamber. Increased turbulence enhances the rate of flame propagation by wrinkling the flame front, which increases the surface area for combustion. During this phase, the engine achieves its maximum heat release rate, which significantly influences the pressure rise and overall engine performance.
3. **End-Flame (50 to 90% of MFB):** The final phase of combustion, known as the end-flame phase, covers the period from 50% to 90% of MFB. This phase represents the tail end of the combustion process, where the flame front reaches the combustion chamber walls and the remaining unburned fuel is consumed. Although the rate of combustion slows down in this phase, it is essential for achieving complete combustion and increasing combustion efficiency.

This analysis provides an initial understanding of the combustion process and serves as a foundation for interpreting other experimental conditions and measurements conducted with the optical engine. As will be further explored in the chapter on all-metal configuration results, examining the flow structures and characterizing the early stages of flame development emerged

as a key factor in the analysis. Therefore, additional investigations are conducted under similar thermodynamic conditions at the onset of flame kernel formation, as well as using aerodynamic and flame development measurement techniques. The detailed experimental configurations and operating conditions of these measurements are discussed in the following sections.

2.3 Internal aerodynamics characterization

The flame in an internal combustion engine is exposed to stochastic flow fields that can be highly turbulent, significantly influencing flame development. To accurately study the behavior of the turbulent flame, it is essential to thoroughly understand its surrounding environment, particularly flow parameters like mean flow and turbulence scales. To achieve this, a High-speed Particle Image Velocimetry (HS-PIV) analysis is conducted.

2.3.1 Particle Image Velocimetry

Particle Image Velocimetry (PIV) is a non-intrusive technique, first introduced by Pickering and Halliwell [114], and Adrian [115], to measure two velocity components in a two-dimensional space. It is based on the principle of Mie scattering, where particles within a flow are illuminated by a light source, typically a laser sheet. The flow is seeded upstream of the study area with solid or liquid particles small enough (on the order of micrometers) to follow the flow accurately.

The technique involves capturing two instantaneous images at close time intervals and determining the displacement of the *seeding* particles between the two images. Since the time interval is known, the two components of the particle velocity in the (x, y) plane can be calculated using the following relationships:

$$U = \frac{\Delta x}{\Delta t} \text{ and } V = \frac{\Delta y}{\Delta t} \quad (2.9)$$

In these equations, U and V represent the particle velocity components along the x and y axes, respectively, while Δx and Δy represent the displacement, and Δt is the time interval between the two images. This interval is assumed to be sufficiently short so that the velocities calculated can be considered instantaneous.

To handle the displacement of the high concentration of particles, the images are divided into small grids or *interrogation windows* (IW) [116]. For each IW, the displacement of particle patterns between the first and second image is determined using cross-correlation. The cross-correlation function $R(\Delta x, \Delta y)$ between the two windows $f(x, y)$ and $g(x, y)$ is defined as:

$$R(\Delta x, \Delta y) = \sum_{x,y} f(x, y) \cdot g(x + \Delta x, y + \Delta y) \quad (2.10)$$

where $f(x, y)$ and $g(x, y)$ are the intensity distributions in the first and second images, respectively, and $\Delta x, \Delta y$ represent the shifts in the x and y directions.

To efficiently compute the cross-correlation, the Fast Fourier Transform (FFT) is commonly used. The cross-correlation in the spatial domain is equivalent to the product of the Fourier transforms of the images in the frequency domain:

$$R(\Delta x, \Delta y) = \text{FFT}^{-1}[F(u, v) \cdot G^*(u, v)] \quad (2.11)$$

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where $F(u, v)$ and $G(u, v)$ are the Fourier transforms of the images $f(x, y)$ and $g(x, y)$, and $G^*(u, v)$ is the complex conjugate of $G(u, v)$. The inverse FFT (FFT^{-1}) is then applied to return the cross-correlation in the spatial domain.

Typically, the cross-correlation function shows a distinct peak, with its position relative to the center of the window indicating the direction and magnitude of the average displacement of the particles in that interrogation window. By applying this process across all cells in the image, the velocity field of the entire study area is reconstructed, as shown in Figure 2.10

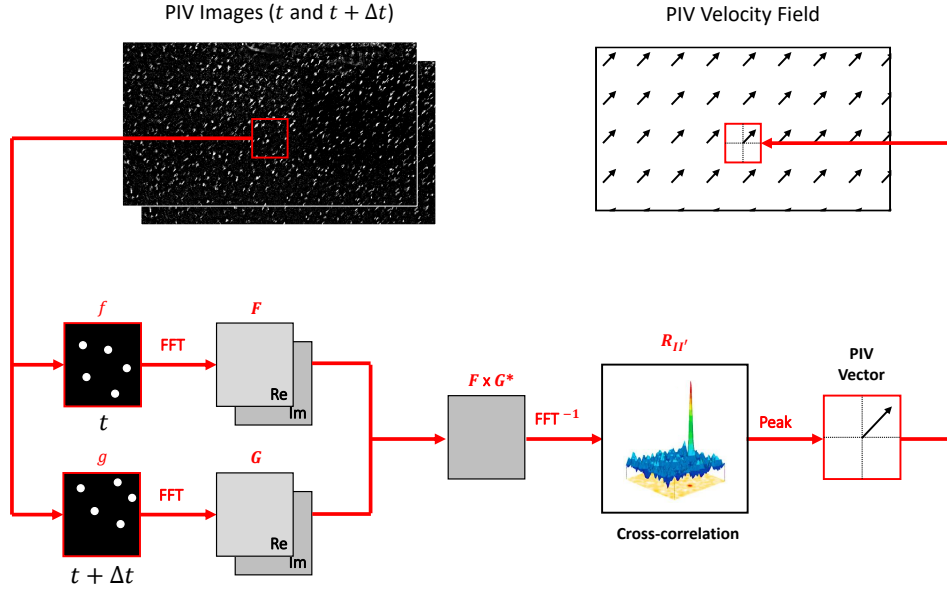


Figure 2.10: Schematic representation of PIV images processing: velocity field determination with interrogation window size and cross-correlation function to track particle displacements.

Choosing the size of the IWs requires balancing the need for high measurement resolution (smaller cell sizes) with the necessity of having a sufficient number of particles in each cell to ensure reliable intercorrelation calculations. The delay Δt between images is selected so that the maximum displacement between the two images corresponds to about one-quarter of the interrogation window size [117]. This criterion offers a good balance between measurement precision and minimizing the risk of losing track of tracer particles from one image to the next. Consequently, this choice directly influences the timing between the two laser pulses.

Limited by the constraints of low-repetition PIV, early studies often captured only a single exposure per cycle, yielding uncorrelated instantaneous velocity fields that were analyzed for cycle-to-cycle variations [115, 118]. Researchers focused on understanding large-scale in-cylinder flow dynamics. For example, Reuss et al. [119] studied high-swirl flows, while Brücker et al. [120] used scanning PIV to investigate the generation of small-scale structures during the compression stroke. Later, Reuss et al. [121] further examined cycle-to-cycle variations and large-scale velocity structures. With advancements in PIV technology, particularly high-speed cameras and lasers, more detailed and time-resolved analyses of in-cylinder flow became possible, enhancing our understanding of flow structure evolution during the engine cycle, as demonstrated in Voisine et al.'s study [122] on the spatio-temporal structure and CCVs of an in-cylinder tumbling flow, and improving the accuracy of Computational Fluid Dynamics (CFD)

models, seen in [123].

In this study, PIV measurements are recorded at various crank angles throughout the engine cycle, producing data at kilohertz-level frequency. This high-speed PIV technique captures time-resolved velocity fields for each cycle, enabling comprehensive comparisons of in-cylinder pressure, flow patterns, and flame development across individual cycles.

2.3.2 PIV Setups

Equipments

PIV experiments are conducted using a high-speed 532 nm Nd:YAG laser (Quantronix Dual Hawk-HP) and two Complementary Metal-Oxide-Semiconductor (CMOS) high-speed cameras (Phantom v1610 and v1611) with a full resolution of 1280x800 pixels² and equipped with either a 100 or 200 mm objective lens (depending on the configuration) and a band-pass filter (Central Wave Length: 532 nm; Full Width to Half Maximum: 10 nm). The crank-angle encoder is used to synchronize laser and camera to the engine via Lavision High Speed Controller. A TDC signal is used as a start input to save simultaneously PIV images and in-cylinder pressure in consecutive cycles. The pulse energy is measured at 11 *mJ* and inter-pulsed time between both laser pulses was optimized from 20 to 30 μs at each condition and the laser a repetition rate was changed up to 8 kHz to obtain a given crank angle resolution, which will be detailed below.

The seeding particles are silicon oil droplets, which are injected upstream of the intake plenum, where a portion of the intake air is diverted to an oil diffuser system [124]. Silicone oil droplets have relatively high evaporation temperatures compared to other liquid droplets and are often selected when optical clarity and good scattering characteristics are desired. The droplets are particularly beneficial for laser illumination, offering strong light scattering while maintaining consistent size distributions in the intake flow [125]. To further validate the chosen particles, the Stokes number, St , is calculated to evaluate if the suspended seeding particles follow the fluid flow [118]. It is defined as:

$$St = \frac{\tau_p}{\tau_f} \quad (2.12)$$

where τ_p is the particle relaxation time, which is the time it takes for a particle to respond to changes in the surrounding fluid flow, and τ_f is the characteristic time scale of the fluid, which could be related to flow features like the eddy turnover time or the time scale of the flow around obstacles [118, 122, 109]. The Stokes number provides insight into how well a particle can follow the fluid motion:

- $St \ll 1$: The particle follows the fluid motion very closely, behaving almost like a fluid element.
- $St \approx 1$: The particle partially follows the fluid motion but may also exhibit some lag or inertia effects.
- $St \gg 1$: The particle is unable to follow the fluid motion and tends to move independently of the fluid flow, dominated by its own inertia.

The particle relaxation time, τ_p , is calculated by Equation 2.13:

$$\tau_p = \frac{\rho_p d_p^2}{18\mu_a} \quad (2.13)$$

where ρ_p is the particle density, d_p is the particle diameter, and μ_a is the dynamic viscosity of the air. This time scale is compared to various fluid time scales to evaluate how well the tracers can follow different scales of in-cylinder fluid motion. Air parameters are calculated using the transport properties from GRI-Mech 3.0 [28] and the silicon oil density was set to 1.04 kg/m^3 .

The evaluated fluid time scales are the following [118]:

1. Engine time scale, τ_e : It represents the time it takes for the fluid to travel the engine stroke. It is calculated as the engine stroke divided by the mean piston speed: $S/\bar{U}_p$.
2. Mean tumble turn-over time scale, τ_T : It represents the tumble motion and is calculated as: $2/(R_t \cdot \omega)$ where R_t is the tumble ratio and ω is the angular velocity of the crankshaft.
3. Turbulent turn-over time scale, τ_{turb} : It is defined by L/u' where L is the size of most energetic eddies and u' an order of magnitude of the rms of the turbulent velocity fluctuation of these eddies. One estimation can be done as function of CAD as proposed by Lumley [118] and presented in Table 2.3, with b , cylinder bore and h , the clearance height.
4. Small eddies turn-over time scale, τ_Δ : It is defined as $\tau_{turb} \cdot (\Delta/L)^{2/3}$, where Δ is the size of the smallest observed turbulent structure which corresponds to the PIV interrogation window, set in this preliminary study at 1 mm.

These different time scales are compared to the particle response times in Table 2.3 for various crank angle degrees (CAD) in the cycle at 1200 rpm, as proposed by Cosadia et al. [126]. It is noticeable that the particle response time is always several orders of magnitude shorter than the fluid time scale within the engine at different CADs, indicating that the seeding particles can follow these fluid scales ($St \ll 1$).

Table 2.3: Calculated in-cylinder flow time scales [126].

CAD (°bTDC)	L	u'	τ_p (s)	τ_e (s)	τ_T (s)	τ_{turb} (s)	τ_Δ (s)
270	$b/6$	$10 \cdot \bar{U}_P$	3.1 E-9	2.5 E-2	6.4 E-3	3.7 E-4	6.1 E-5
180	$b/6$	$\bar{U}_P$	3.1 E-9	2.5 E-2	6.4 E-3	3.7 E-3	6.1 E-4
90	$b/6$	$0.5 \cdot \bar{U}_P$	2.6 E-9	2.5 E-2	6.4 E-3	7.4 E-3	1.2 E-3
0	$h/6$	$0.5 \cdot \bar{U}_P$	1.7 E-9	2.5 E-2	6.4 E-3	1.4 E-3	7.0 E-4

Different PIV configurations are employed to study the flow field characteristics throughout the engine cycle. Three planes are chosen: two vertical and one horizontal. A laser sheet is generated through three cylindrical lenses and is set at the region of interest with a width of approximately 1 mm.

Vertical Cylinder (VC) Configuration

The first configuration is designed to capture the flow field in the tumble plane, positioning the laser sheet in the center of the liner. The v1610 high-speed camera with a 200 mm focal

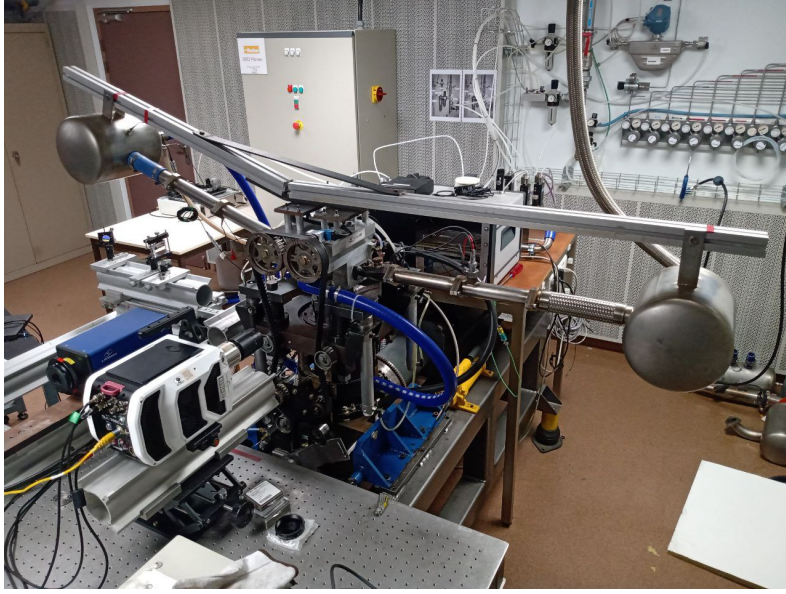


Figure 2.11: Photo of the test bench in the VC configuration.

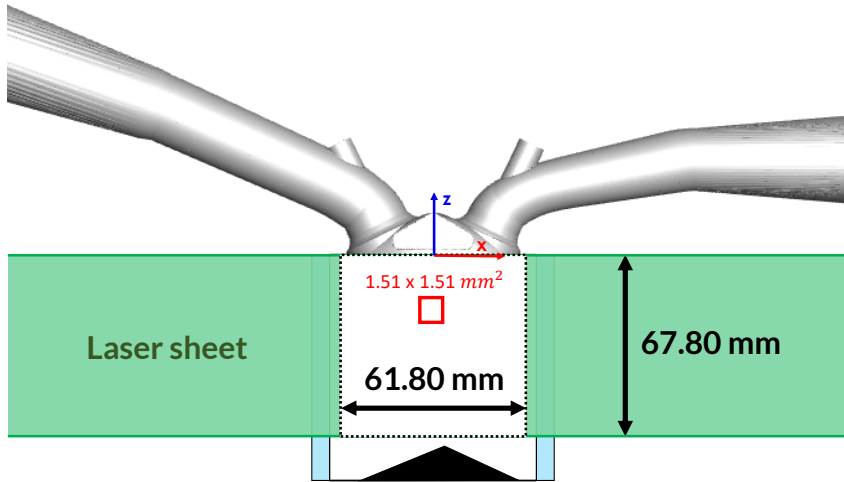


Figure 2.12: Laser sheet and vector density schematic in the VC configuration.

length was positioned facing the quartz liner to capture this large-scale structure. Figure 2.11 illustrates the test bench setup, and Figure 2.12 shows the schematics of the PIV measurements.

In this configuration, the laser sheet has a height of 67.80 mm, creating a FoV of 67.80 x 61.80 mm² with a magnification ratio of 0.090 mm/pixel. The optimal interrogation window was determined to be 32x32 pixels² with a 50% overlap, as will be discussed later. The final vectors are spaced at intervals of 1.50 mm.

The flow fields, which will be presented in the results chapter, are plotted with their origin at the intersection of: 1) the plane between the quartz liner and the cylinder head, $z = 0$, and 2) the line that is coaxial with the liner, as shown in Figure 2.12. Additionally, as the crank angle changes, piston movement alters the FoV due to the obstruction of the laser sheet. Data

2.3. INTERNAL AERODYNAMICS CHARACTERIZATION

is obtained over 150 cycles, with measurements taken every 5 CAD from 315 to 45 °bTDC.

Vertical Combustion Chamber (VCC) Configuration

The second configuration is also vertical, focusing on measuring the 2D flow field within the combustion chamber. In this setup, the laser sheet passes through the optical piston, while the V1611 high-speed camera with a 200 mm objective lens is positioned facing the optical window in the cylinder head. To minimize reflections from the laser sheet within the combustion chamber, particularly around the spark plug, the cylinder head is painted black, and the laser sheet is shifted 7.5 mm away from the center of the spark plug towards the camera.

The schematic of the vertical PIV imaging setup is illustrated in Figure 2.13. In this configuration, the FoV is 30.0 x 15.0 mm², with a magnification ratio of 0.031 mm/pixel, resulting in a vector density of 0.50 mm/vector. The origin is set at the center electrode of the spark plug, as shown in the figure. Piston movement interferes with the flow field measurements at the end of the compression stroke (after 30 °bTDC).

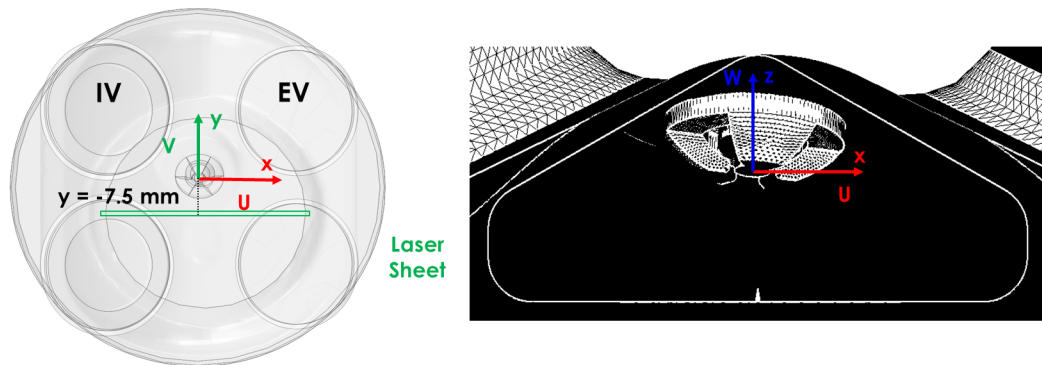


Figure 2.13: Origin, laser sheet positioning, and camera FoV schematic in the VCC configuration..

Horizontal Combustion Chamber (HCC) Configuration

The third and final PIV configuration is horizontal. In this setup, the in-cylinder pressure transducer is replaced by a second optical quartz window so that the laser sheet can pass through it and does not reflect inside the combustion chamber. It is generated 5 mm below the center electrode of the spark plug in the XY plane. The high-speed camera, equipped with a 100 mm objective lens, captures images through the optical piston, as illustrated in Figure 2.14. Velocity fields are measured from 195 to 30 °bTDC at every 5 crank angles. The field of view measures 22.0x40.7 mm², with a pixel size of 0.052 mm.

Finally, Figure 2.15 illustrates the positions of both the horizontal and vertical planes within the combustion chamber.

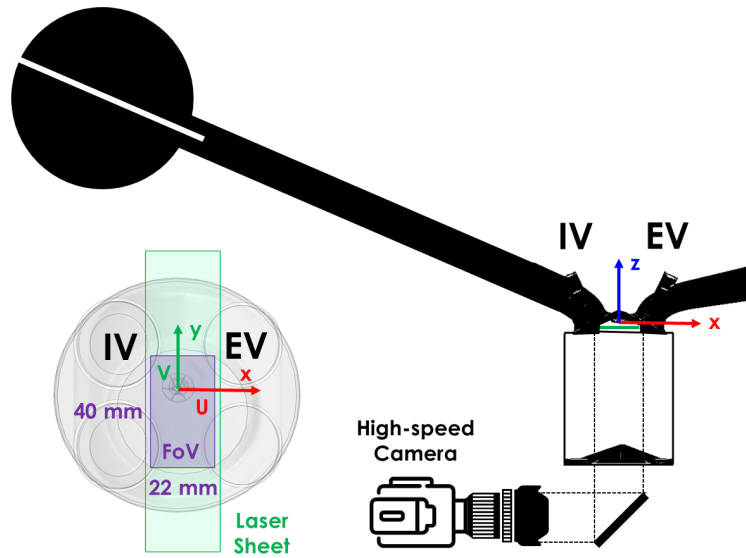


Figure 2.14: Laser sheet and origin positioning in the HCC configuration, with camera placement relative to the Bowditch piston and its FoV.

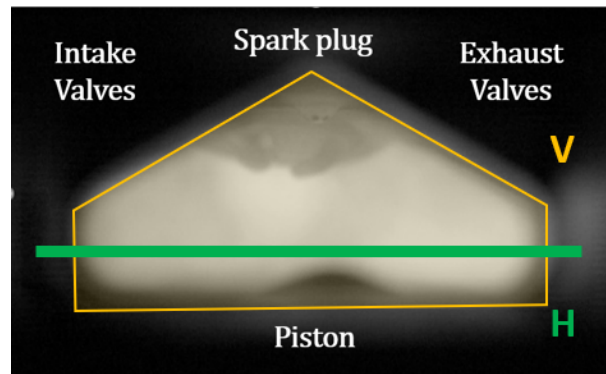


Figure 2.15: Laser sheet placement inside the combustion chamber in both horizontal (H) and vertical (V) configurations.

2.3.3 Experimental conditions

For the three PIV configurations, tests are conducted under motoring conditions at two intake pressures (0.7 and 0.9 bar) and three engine speeds (900, 1200, and 1500 rpm). These conditions allow for the characterization of flow field patterns and turbulence indicators, as well as how they vary with intake pressure and engine speed. Additionally, comparisons between non-reactive and reactive flows under the same conditions are made in the VCC configuration for an equivalence ratio of 0.4.

Table 2.4: Experimental conditions on PIV measurements.

	CAD ($^{\circ}$ aTDC)	FoV (mm ²)	Pixel size (mm)
VC	-315 $\rightarrow$ -45 (per 5)	67.8 x 61.8	0.094
VCC	-90 $\rightarrow$ 0 (per 2)	30.0 x 15.0	0.031
HCC	-190 $\rightarrow$ -30 (per 5)	22.0 x 40.7	0.052

2.3.4 Images processing

Pre-processing methods

First, image pre-processing methods are applied. Contrast-Limited Adaptive Histogram Equalization (CLAHE) of 64×64 pixels² is used to enhance the contrast of the images, particularly in areas where the contrast is low [127]. It equalizes the histogram of the image by dividing it into small regions, meaning that the contrast enhancement is localized and adapted to different parts of the image. Also, the background subtraction (calculated by the mean intensity) is employed to reduce image noise, enhance particle visibility and mitigate static background interference [128].

PIV parameters

The velocity fields are obtained using DaVis software (LaVision). The selection of interrogation window size and overlap parameters is performed by varying both under the same experimental condition and comparing the resulting velocity field maps and statistical values. As previously mentioned, the size of the interrogation window depends on the number of particles within the window and the need for high-resolution data. This means that the interrogation window should be as small as possible while still ensuring reliable data from the cross-correlation function. Additionally, increasing the overlap between interrogation windows can enhance flow field resolution without reducing the number of particles per interrogation area. Figure 2.16 illustrates the sensitivity study made of a PIV field in the HCC configuration in relation to interrogation window size and overlap value.

Figure 2.16a shows the mean velocity field over 150 cycles for three different interrogation window sizes, all with a 50% overlap: 64×64 , 32×32 , and 16×16 pixels². Since each area generates only one cross-correlation function, and one vector, the 32×32 pixels² interrogation windows have four times more PIV vectors than the 64×64 windows, and four times fewer than the 16×16 . More vectors provide higher resolution and more information, however, smaller windows contain fewer particles, potentially leading to unreliable cross-correlation functions. The 16×16 PIV velocity field displays some unphysical flow structures, particularly near the spark plug ($x = y = 0$). This can be attributed, for instance, to a small reflection near the spark plug that affects the vector field processing when the interrogation window size is too small.

A similar trade-off occurs when varying the overlap parameter. Lower overlap values result in a low-resolution velocity field, while higher values increase computational load and may introduce noise and spurious vectors [129]. Figure 2.16b illustrates the effect of the overlap parameter for an IW of 32×32 pixels². The reduction in vector density with decreased overlap is evident. However, at 75% overlap, the number of spurious vectors increases, particularly at the image borders.

The impact of both parameters is also analyzed in terms of statistical properties. Figure 2.17

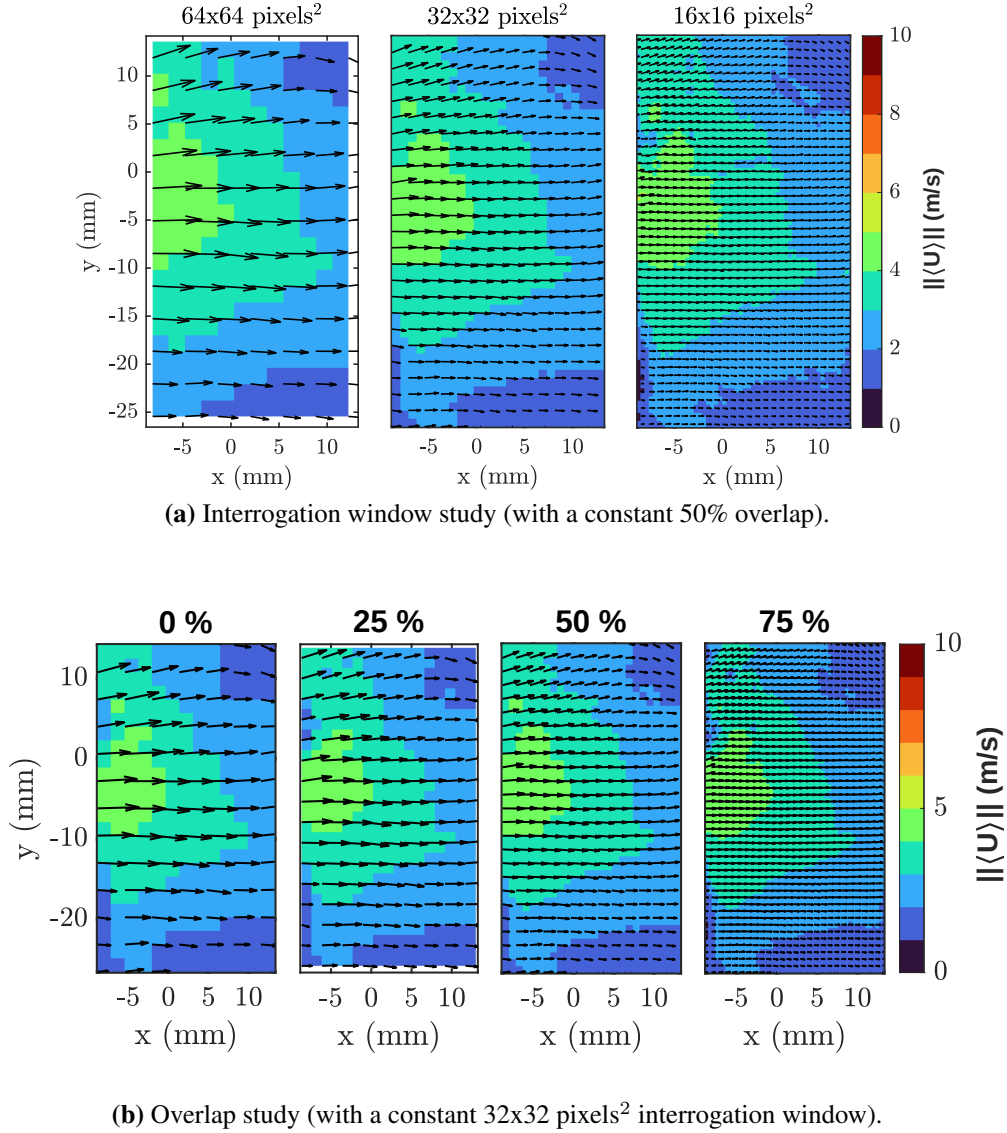


Figure 2.16: Sensitivity analysis of interrogation window size and overlap value in the HCC configuration at an intake pressure of 0.7 bar and 1200 rpm at 90 °bTDC.

shows the effect of IW size on the standard deviation of the flow velocity in the x and y directions, u' and v' , respectively. The differences in these parameters are within the measurement uncertainty [130], with the relative difference between the 16x16 and 64x64 sizes being less than 10% across all CAD. Therefore, an interrogation window size of 32x32 pixels² is chosen for all configurations. Consequently, a moderate overlap of 50% is selected as a compromise between accuracy and noise.

The number of cycles required for statistical convergence is also examined. Figure 2.18 shows the ratio between the mean values of the U and V components of the velocity at the center of the velocity field for a given number of cycles, compared to the values obtained with 250 cycles, as a function of the number of cycles (left). The same comparison is made for the standard deviation values (right). These calculations are performed using the same configuration and condition as the IW tests described earlier. As expected, both the mean and standard

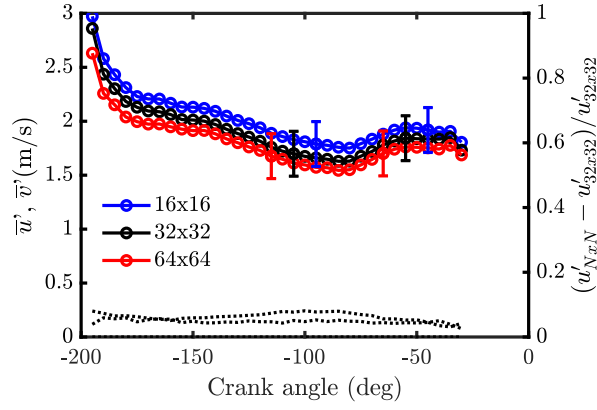


Figure 2.17: Sensitivity analysis of interrogation window size on turbulent intensity, u' .

deviation values approach 1 at 250 cycles. However, these values remain within the $\pm 5\%$ range only when the number of cycles exceeds 150.

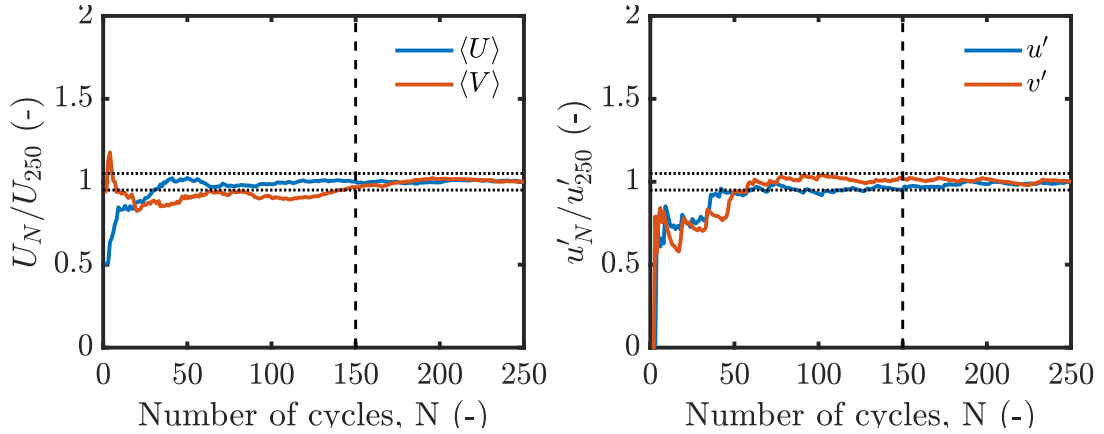


Figure 2.18: Statistical analysis of number of cycles on the convergence of results of both ensemble-averaged velocities and turbulent intensity in x and y directions in the HCC configuration.

The same experiment is conducted under different conditions, yielding consistent results. Therefore, all PIV measurements in this thesis are performed using statistics based on 150 cycles.

Vectors validation

Finally, vector validation techniques are used to enhance the robustness of the PIV analysis and ensure that the velocity fields accurately represent the physical flow within the experimental setup. According to Raffel et al. [129] and Westerweel [117], validation techniques, such as image-based contrast filters and statistical filters (e.g. standard deviation and median) are effective in maintaining the accuracy of the flow field while minimizing the risk of introducing artifacts during processing.

First, image-based filters are applied to potentially remove spurious vectors that can arise from various sources, such as reflections, low particle density, or poor image quality. Thus, a

low and a high contrast filters are used with thresholds of 0.1% and 50%. Additionally, vector validation is performed using a standard deviation filter optimized at 8σ and a local median filter with a 3x3 kernel. The standard deviation filter helps to eliminate vectors that deviate significantly from the mean flow field, while the local median filter addresses isolated erroneous vectors by comparing them to the median value of surrounding vectors.

2.3.5 Decomposition Methods

In order to understand the underlying structure and dynamics of flow fields, including turbulence, coherent structures, and other flow phenomena, decomposition methods are used to separate complex fluid flow patterns into simpler, constituent components that are easier to analyze and interpret. Several decomposition methods are used in the literature, such as:

- Reynolds Decomposition: that separates a turbulent flow into its mean and fluctuating components [118].
- Proper Orthogonal Decomposition: that decomposes a velocity field into a series of orthogonal modes ranked by their energy content. Each mode represents a distinct flow structure, and the sum of these modes can reconstruct the original velocity field [118].
- Fourier Decomposition: that express the velocity field as a sum of sinusoidal functions (Fourier series), each with a specific frequency and amplitude [131].
- Wavelet Decomposition: that provides both spatial and frequency information and can handle non-stationary signals [132].
- Empirical Mode Decomposition: a data-driven method that decomposes a signal into intrinsic mode functions (IMFs), which represent simple oscillatory modes in the data [109].
- Dynamic Mode Decomposition: a method that extracts dynamic information from a sequence of velocity fields, identifying spatial modes associated with specific temporal dynamics [133].

In this thesis, three decomposition methods are employed to analyze the PIV fields: 1) the Reynolds Decomposition, 2) the Empirical Mode Decomposition (EMD), and 3) the Triple Decomposition.

Reynolds Decomposition

Reynolds Decomposition involves splitting the instantaneous velocity field, $\mathbf{U}$, into two parts: the time-averaged or ensemble-averaged component, $\langle \mathbf{U} \rangle$ or $\mathbf{U}_{EA}$, and the fluctuating component, $\mathbf{u}$, that represents the deviation from the mean [19, 118]. The Reynold decomposition is shown in Equation 2.14. It enables the examination of the primary flow field pattern and the in-cylinder turbulence intensity and flow variability across different configurations as a function of crank angle.

$$\mathbf{U} = \langle \mathbf{U} \rangle + \mathbf{u} \quad (2.14)$$

Additionally, the variation in the flow field can be quantified by the root mean square (rms) of the fluctuating component, denoted as u' .

Empirical Mode Decomposition

Empirical Mode Decomposition (EMD) is a data-driven, adaptive signal decomposition technique designed to analyze non-linear and non-stationary time series data. Unlike traditional methods that rely on predefined basis functions, EMD decomposes a signal into a set of Intrinsic Mode Functions (IMFs) derived directly from the data.

The EMD process involves iteratively sifting the original signal to extract these IMFs. Each IMF represents a simple oscillatory mode of the signal, and the sum of all IMFs (along with the residual) reconstructs the original signal [109].

The EMD process works as follows: 1) The algorithm identifies all the local maxima and minima of the signal; 2) Interpolation methods are used to create upper and lower envelopes by connecting the maxima and minima, respectively; 3) The mean of these two envelopes is computed; 4) The mean is subtracted from the original signal to produce a component known as a "proto-IMF." This process is repeated (sifting) until the proto-IMF satisfies the IMF criteria (such as having the same number of zero-crossings and extrema or being within a tolerance); 5) The IMF is separated from the original signal, and the residual is subjected to the same process to extract further IMFs; 6) The process stops when the residual becomes a monotonic function or a function with only one extremum, which means no further IMFs can be extracted. Further details on the Empirical Mode Decomposition are provided in Appendix A.

EMD has increasingly been used to analyze in-cylinder flow fields in internal combustion engines [134, 135, 136]. These flows are complex and turbulent, exhibiting a wide range of temporal and spatial scales. Traditional analysis methods may struggle to capture the intricate dynamics, especially when dealing with the non-linearities and non-stationarities inherent in such flows. EMD provides a robust framework to address these challenges [134].

For instance, Sadeghi et al. applied EMD to the in-cylinder velocity field, creating low-frequency (LF) and high-frequency (HF) components, denoted as U_{LF} and u_{HF} , respectively [134], as shown in Equation 2.15.

$$U = U_{LF} + u_{HF} \quad (2.15)$$

The LF signal is defined as the sum of the residual and the last IMF. Consequently, the HF signal was derived as the sum of all other IMFs, as well as in [136]. This approach allows for a more precise characterization of the high-frequency component, as the fluctuating velocity in the Reynolds Decomposition results from the variability of both high-frequency and low-frequency components.

Triple Decomposition

The variability of the low-frequency (LF) velocity can be used to define a new velocity component. The U_{LF} component is divided into two parts: the ensemble average component, $\langle U_{LF} \rangle$, and the cyclic variation component, u_{CCV} , as shown in Equation 2.16.

$$U_{LF} = \langle U_{LF} \rangle + u_{CCV} \quad (2.16)$$

Consequently, the instantaneous velocity field can be divided into three components through Triple Decomposition, as illustrated in Equation 2.17:

$$U = \langle U_{LF} \rangle + u_{CCV} + u_{HF} \quad (2.17)$$

2.4. IN-CYLINDER FLAME MEASUREMENTS

High-frequency variations are generally associated with turbulence, while variability in the low-frequency flow field is linked to engine cycle-to-cycle variations (CCV) [135, 136]. Figure 2.19 presents different velocity components derived from these three decompositions for a velocity field in the HCC configuration at a specific cycle and crank angle. This figure highlights the distinctions between the velocity components and demonstrates how these decompositions can extract different types of data from the same flow field. These analyses will be used in this thesis to characterize in-cylinder aerodynamics and to understand the effects of turbulence on hydrogen in-cylinder flames.

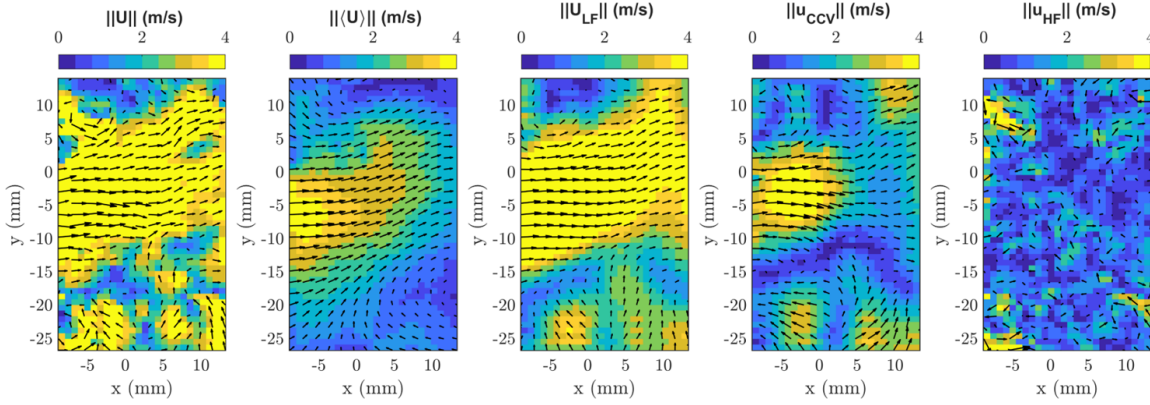


Figure 2.19: Illustration of the decomposition of an instantaneous velocity field ($\mathbf{U}$) into ensemble-averaged ($\langle \mathbf{U} \rangle$), low-frequency ($\mathbf{U}_{LF}$), low-frequency cycle-to-cycle variations ($\mathbf{u}_{CCV}$) and high-frequency fluctuations ($\mathbf{u}_{HF}$).

It is important to note that the parameters used in the EMD analysis are adopted from [109, 137], following an exhaustive sensitivity analysis of these parameters.

2.4 In-cylinder flame measurements

2.4.1 Chemiluminescence Theory

Chemiluminescence refers to the emission of light as a result of a chemical reaction, typically occurring when a molecule returns from an excited electronic state to its ground state, releasing energy in the form of photons. This phenomenon can be utilized as a diagnostic tool in various fields, particularly in the study of combustion processes, such as those occurring within internal combustion engines (ICEs). In the context of combustion diagnostics, chemiluminescence measurements involve capturing and analyzing the light emitted by reactive species like OH^* , CH^* and C_2^* radicals during combustion [138, 139].

These reactive species emit light at specific wavelengths as they transition from excited states to lower energy states. By detecting and quantifying this light, researchers can infer important information about the combustion process, including flame temperature, equivalence ratio, and the distribution of reactive intermediates. The most commonly studied chemiluminescent species in combustion diagnostics are OH^* (around 306–310 nm), CH^* (around 430 nm), and C_2^* (around 516.5 nm), as these species provide valuable insights into the fuel-air mixing, flame structure, and ignition phenomena. In hydrogen/air flames, due to the decarbonized nature of hydrogen, the OH^* species is primarily tracked.

2.4. IN-CYLINDER FLAME MEASUREMENTS

In an internal combustion engine, chemiluminescence measurements are typically performed using high-sensitivity photodetectors, such as photomultiplier tubes (PMTs) or intensified charge-coupled devices (ICCDs). These detectors are capable of capturing the faint light emitted by the radicals in the harsh environment of the engine cylinder. Often, the light is filtered through narrow bandpass filters that isolate the specific wavelengths corresponding to the chemiluminescent species of interest. The intensity of the captured light can then be analyzed to determine the distribution and concentration of the reactive species, which, in turn, helps in understanding the combustion dynamics within the engine.

Chemiluminescence measurements have been extensively employed in the study of combustion processes within internal combustion engines to gain insights into flame behavior, pollutant formation, and overall engine performance. The technique's non-intrusive nature makes it particularly valuable for in-cylinder diagnostics, where traditional measurement methods might disturb the combustion process. As engine technologies evolved, so did the application of flame spectroscopy. One of the significant advancements was the ability to perform time-resolved measurements inside the engine cylinder. This advancement allowed researchers to study the temporal evolution of flame front propagation and the onset of ignition [140].

In recent years, there has been a growing interest in using chemiluminescence to study lean-burn and alternative fuel combustion in internal combustion engines. Lean-burn combustion, which is critical for improving fuel efficiency and reducing emissions, presents challenges in achieving stable combustion. Chemiluminescence measurements of OH^* and CH^* have been used to optimize ignition timing and air-fuel mixing in such engines. While chemiluminescence measurements provide valuable data, they also come with challenges. The harsh environment of an internal combustion engine, characterized by high pressures and temperatures, can affect the accuracy of the measurements. Additionally, the overlap of emission spectra from different species and the fundamental 3D topology of such flames can complicate the 2D analysis. Advances in optical diagnostics, such as the use of ICCDs and advanced filtering techniques, have helped mitigate these challenges, allowing for more precise measurements, specially with the ongoing transition to low-carbon and zero-carbon fuels.

2.4.2 Setup

Chemiluminescence measurements are performed simultaneously with in-cylinder pressure readings using the Bowditch piston. The images were captured by a high-speed camera (Phantom v1610) paired with a high-speed intensifier (La Vision High-speed IRO). This configuration is optimized to detect OH^* emissions, typically ranging from 280 to 350 nm, with a peak at 308 nm [141]. Three different setups are tested: 1) direct chemiluminescence measurements (no filters); 2) a 318 nm band-pass filter (BPF) with a 175 nm full width at half-maximum (FWHM), covering a broad UV spectral range; and 3) a narrow 310 nm BPF (FWHM 10 nm). The third option overly filtered the flame, resulting in a poor signal. Flame images obtained at lower equivalence ratios with no BPF exhibited higher noise levels (e.g. signal-to-noise ratio - SNR - of 2.2 at $\phi = 0.30$) due to increased intensification. Thus, the second measurement configuration is employed to enhance the SNR, particularly under low equivalence ratio conditions ($\phi \leq 0.35$). For instance, at an equivalence ratio of 0.3, the SNR increases fivefold using the filter compared to no filter. Furthermore, the influence of noise on the outcomes can be assessed by examining the variation in flame contour detection with different sizes of median filters. Altering the filter size from 1x1 to 15x15 pixels² can result in equivalent flame radius variations

2.4. IN-CYLINDER FLAME MEASUREMENTS

ranging from 0.2% (at $\phi = 0.5$) to 3.3% (at $\phi = 0.2$).

For the chemiluminescence analysis, the image resolution is 0.092 mm per pixel, and the imaging frequency is set to capture a flame image at every crank angle degree. The intensifier gain and gate settings are configured at 50% and 30 μs at $\phi = 0.55$, gradually increasing to 70% and 80 μs at $\phi = 0.20$.

2.4.3 Experimental conditions

To analyze and compare the propagation of the hydrogen/air flame inside the cylinder under various conditions, the spark timing is set at -15 °aTDC. This ensures similar thermodynamic conditions at the onset of the flame kernel. Consequently, the equivalence ratio ($0.20 \leq \phi \leq 0.55$), engine speed ($900 \leq N \leq 1500$ rpm), intake pressure ($0.6 \leq P_{int} \leq 0.9$ bar), and ignition dwell time ($300 \leq D \leq 2000$ μs) are varied to assess the impact of each parameter on flame development.

Furthermore, propane/air flames are also studied as a comparison. They are studied at the same thermodynamic conditions as the hydrogen-flames. Equivalence ratio ($0.70 \leq \phi \leq 1.50$), engine speed ($900 \leq N \leq 1500$ rpm), intake pressure ($0.4 \leq P_{int} \leq 0.7$ bar), and ignition dwell time ($300 \leq D \leq 2000$ μs) are also varied for the propane flame development investigation.

2.4.4 Flame contour extraction

Chemiluminescence images underwent post-processing, involving several steps: a median filter (7x7 pixels), binarization (with threshold varying from 10 to 20% of the image's maximum pixel intensity depending on the equivalence ratio), and contour detection, as depicted in Figure 2.20.

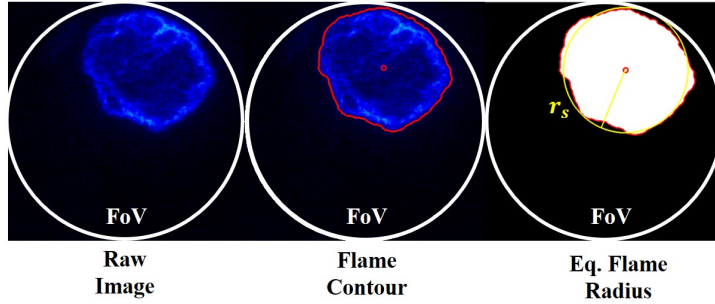


Figure 2.20: Chemiluminescence image processing for a hydrogen/air flame with an equivalence ratio of 0.50. The figure shows the field of view (FoV) through the quartz piston bowl, including the flame contour and the radius, r_s , calculated from the projected flame surface.

Various parameters are then extracted, including the projected surface area, A_{flame}^{proj} , and the equivalent flame radius:

$$r_s = \sqrt{A_{flame}^{proj}/\pi} \quad (2.18)$$

This analysis is performed across the engine cycle, spanning from -15 to +16 degrees aTDC, and concludes upon the flame contour trans-passing the piston window boundary. An additional significant parameter that can be computed is the equivalent flame propagation speed, denoted as v_T . This is defined as the change in the equivalent flame surface radius over the time interval

between two crank angles: $v_T = \frac{dr_S}{dt}$. The statistics are only calculated with results of more than 50 cycles at a given crank angle.

2.5 Cycle-to-cycle variations study

As presented in Chapter 1, cycle-to-cycle variability in internal combustion engines is a critical factor affecting performance. Given the distinct properties of ultra-lean hydrogen compared to conventional fuels, a fundamental analysis of CCV as well as its study in numerical simulations is essential for the development of future hydrogen engines.

2.5.1 Setup

Additionally to the experimental setups already presented in the previous sections which are all in multiple cycles and can be studied on a cyclic basis, further investigations are conducted to understand the effect of the velocity field on the combustion phenomena. Thus, simultaneous in-cylinder pressure, chemiluminescence and PIV measurements are conducted to understand the cyclic variability performance of hydrogen flames.

Thus, in the VCC configuration, a second high-speed camera (Phantom v1610) and a short-pass dichroic mirror (Transmission: 300 – 350 nm, Reflection: Visible wavelengths) are integrated to allow for simultaneous chemiluminescence and PIV measurements. The high-speed camera, connected to the high-speed intensifier and band-pass filter, is directed towards the quartz window optical access at the cylinder head to visualize the flame near the spark plug. The experimental bench in this configuration is illustrated in Figure 2.21

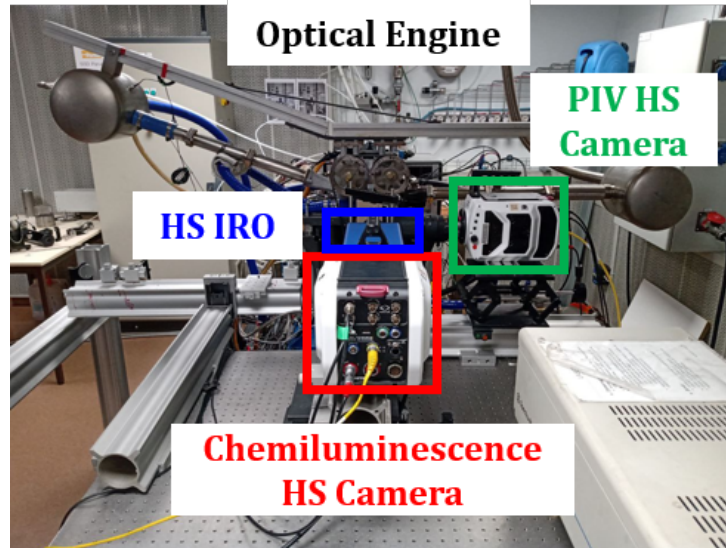


Figure 2.21: Experimental test bench setup for simultaneous HS-PIV and chemiluminescence measurements. The figure illustrates the arrangement of the optical components and measurement systems used in the experiment.

In the vertical chemiluminescence configuration, the magnification factor is 0.044 mm/pixel and images are captured at every 2 crank angle degrees from -90 to 20 °aTDC.

2.5.2 Experimental conditions and methodology

The experimental conditions are similar to those of the horizontal chemiluminescence study of hydrogen/air flames as well as the post-processing analyses.

Conclusion

This chapter has provided a detailed overview of the experimental setup and methodologies used in this thesis, focusing on heat-release, PIV, chemiluminescence, and CCV analyses. The procedures for data acquisition and processing have been carefully outlined to ensure a clear understanding of the approach taken to investigate in-cylinder hydrogen/air ultra-lean combustion.

Multiple configurations were implemented for the different types of measurements to capture relevant information within the engine. Each configuration was specifically tailored to distinct aspects of the engine cycle, resulting in a robust dataset for analyzing the complex phenomena involved. The chapter highlighted the careful selection of parameters, emphasizing their impact on the quality of the results.

Steps taken to ensure the reliability and accuracy of the obtained data were also discussed. The use of advanced techniques, such as Empirical Mode Decomposition to separate different components of the velocity field, are intended to provide deeper insights into high-frequency turbulence and low-frequency cycle-to-cycle variations, adding significant value to the analysis.

The methodologies presented in this chapter establish the foundation for the subsequent analysis of in-cylinder aerodynamics and combustion development. These approaches enable a detailed examination of how flow structures and turbulence interact with hydrogen combustion, contributing valuable data to the understanding of zero-carbon internal combustion engine dynamics. The thoroughness of the experimental setup and data processing ensures that the results discussed in later chapters are both robust and reliable, providing a strong basis for the conclusions drawn from this study. Table 2.5 provides a summary of the key experimental conditions and methods described in this chapter, highlighting the most relevant information for each measurement technique and configuration.

Table 2.5: Summary of experimental conditions and measurement techniques used in this thesis.

Investigation	All-metal	High-speed PIV		Chemil.	Cycle-to-cycle variations	
Configuration	-	VC	VCC	HCC	HCC	VCC
FoV (mm ²)	-	67.8 x 61.8	30.0 x 15.0	$\pi \cdot 20^2$	(Chemil.)	(HS-PIV + Chemil.)
Pixel size (mm)	-	0.094	0.031	0.092	$\pi \cdot 20^2$	30.0 x 15.0
Vector density (mm/vector)	-	1.50	0.50	-	0.092	0.044 and 0.094, resp.
CAD (aTDC)	-360.0 $\rightarrow$ 359.9°	-315 $\rightarrow$ -45°	-90 $\rightarrow$ 0°	-190 $\rightarrow$ -30°	-190 $\rightarrow$ -30°	-90 $\rightarrow$ 0°
Acq. Rate	0.1°	5°	2°	5°	5°	2°
Nb. Cycles	100	150	150	100	100	100
Varying Param.	IMEP, ϕ Spark plug, ϕ P_{int} , N , ϕ	P_{int} , N		P_{int} , N , ϕ , D	P_{int} , N , ϕ , D	P_{int} , N , ϕ

Chapter 3

All-metal engine operation

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Introduction

In this chapter, the detailed results for the all-metal engine configuration will be presented. The first section focuses on the design and setup of the intake and exhaust systems, as well as the selection of the spark plug and hydrogen injection positions. The second section covers the validation of the TPA model, ensuring its accuracy in predicting engine behavior under various operating conditions and the set parameters. Finally, the third section presents and discusses the in-cylinder combustion analysis, with particular emphasis on the performance of ultra-lean hydrogen/air mixtures, highlighting key insights into combustion characteristics, flame development and applied combustion theory.

3.1 Test bench definition

Before starting the in-cylinder hydrogen combustion analysis, the engine components are selected based on the following criteria: 1) ensuring a safe test facility; 2) replicating real engine operating conditions; and 3) providing controllable and well-defined boundary conditions. While the engine cylinder and piston were chosen due to availability, the intake and exhaust systems, spark plug geometry, and hydrogen injection position were determined to align with the goals of this thesis.

3.1.1 Intake and exhaust systems

For the intake and exhaust systems, the main objectives are to establish proper boundary conditions (BCs) sufficiently distant from the intake and exhaust valves (more than 400 mm, as shown in Figure 2.4), for high-fidelity simulations, while replicating real engine-like conditions. This information is important for high-fidelity numerical simulations. Two long pipes are considered for this purpose. A preliminary study is conducted using GT-SUITE software, where the combustion chamber, intake and exhaust valves, and manifolds are modeled. A series of 0D/1D numerical simulations are then carried out to assess the impact of intake pipe length and plenum volume on the engine's volumetric efficiency. Figure 3.1 shows the volumetric efficiency as a function of intake length (ranging from 300 to 1100 mm) for two plenum configurations: no intake plenum (left) and a 10 L intake plenum (right), across four engine speeds (1000 to 2500 rpm) with $\phi = 0.40$.

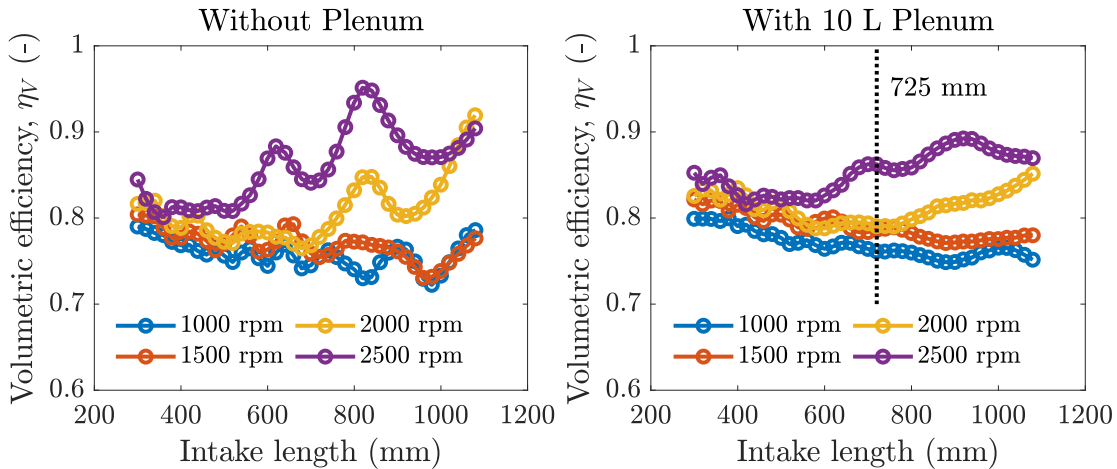


Figure 3.1: Impact of intake length on volumetric efficiency: Without intake plenum (left); With a 10 L intake plenum (right). Intake length varies from 300 to 1100 mm and engine speed ranges from 1000 to 2500 rpm.

The results without intake plenum indicate that, regardless of engine speed, longer intake lengths lead to greater variations in volumetric efficiency, likely due to acoustic effects within the intake duct. This effect becomes more pronounced at higher engine speeds. For instance, at 2500 rpm, increasing the intake length by 700 to 800 mm significantly boosts volumetric efficiency from 0.85 to 0.95. While lower engine speeds reduce the magnitude of these variations, they do not eliminate them. Thus, an engine without an intake plenum experiences volumetric efficiency that varies considerably based on intake length and engine speed.

Given that the goal of the experimental bench is to maintain consistent and well-defined conditions, and that small changes in intake length can cause significant differences in trapped cylinder mass, a strategy is developed to mitigate the acoustic effects caused by the intake and exhaust valve motion. Drawing from both laboratory experience and literature [123], it is known that installing plenum volumes upstream and downstream of the engine helps reduce these acoustic fluctuations. The larger the plenum volume, the greater the attenuation. However, since the hydrogen injection position is still under study, safety concerns required limiting the plenum volume to reduce the risk of explosion in the intake ducts. Consequently, a 10 L plenum is selected for low frequency attenuation, and its effectiveness is validated in the numerical simulations.

The right-hand side of Figure 3.1 demonstrates the effectiveness of the 10 L plenum in mitigating variability. The amplitude of volumetric efficiency oscillations decreased, as did the differences between engine speeds. Therefore, a 10 L noise-reduction plenum is selected for both the intake and exhaust systems. The intake length is chosen to be long enough to accommodate various testing elements (including the possibility to include an optical window for PIV measurements) but short enough to minimize acoustic variability and large changes across engine speeds. Ultimately, an intake length of 725 mm between the intake valves and the plenum is selected.

3.1.2 Hydrogen injection

Once the intake and exhaust systems are defined, designed, and manufactured, an experimental study on hydrogen injection positions is conducted. Figure 3.2 links the mixture homogeneity to the combustion timing variations. The standard deviations of CA10 (3.2a) and CA50 (3.2b) over 100 cycles are plotted against the fuel-air equivalence ratio in the intake pipe for the four injection positions. Both Figures illustrate the impact of the equivalence ratio on combustion variability across all configurations. It is clear that as the fuel-air equivalence ratio increases, combustion variability decreases. This can be attributed to faster flame speeds and shorter combustion durations, resulting in reduced operating variability [98, 71].

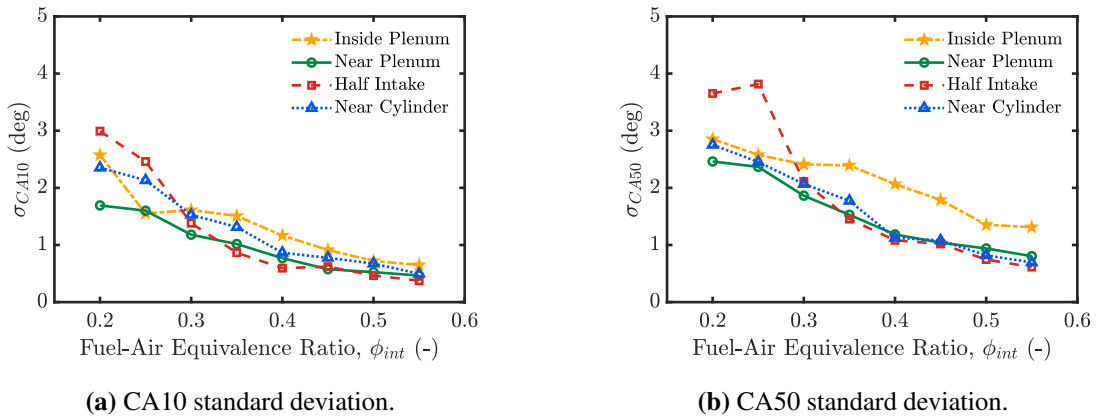


Figure 3.2: The impact of hydrogen injection position on flame variability, illustrated by the standard deviation of a) CA10 and b) CA50, plotted against the fuel-air equivalence ratio.

By comparing fluctuations in combustion phasing at the same equivalence ratio, the mixing quality of different configurations can be evaluated, allowing them to be ranked by their

mixing performance and variability. The injection inside the intake plenum shows the highest instability for both CA10 and CA50, especially at higher equivalence ratios ($\phi > 0.3$). This instability could be caused by increased variability in hydrogen entering the pipe due to acoustic resonances within the plenum. The second most variable configuration involves injection near the cylinder head. While it performs similarly to the other configurations (Half Intake and Near Plenum) in terms of CA50, it is the second most variable for CA10. The third configuration, the half-intake pipe position, shows the most stable combustion phasing at the highest equivalence ratios tested, but exhibits greater variability in both CA10 and CA50 when ϕ is less than 0.3. Therefore, the near intake plenum position is chosen as the preferred configuration for subsequent experiments, due to its lower cyclic variability, indicating superior mixing performance. Additionally, a 3D RANS simulation is also performed to indicate the best mixing configuration. Numerical setup and results are displayed in Appendix B.

3.1.3 Spark plug

The influence of various spark plugs on engine performance – stability, combustion duration, and combustion CCVs – is assessed to determine the best option for hydrogen combustion. As outlined in the "Experimental Setup and Methodology" chapter, an equivalence ratio sweep is conducted using five different spark plugs (Figure 2.7 and Table 2.2), with intake pressure and spark timing adjusted to maintain a targeted IMEP of 2 bar and a constant CA50 at 8 °aTDC, the optimal spark timing, i.e. the Minimum Advance for Maximum Brake Torque (MBT), which leads to the minimal variability.

Figure 3.3 shows the coefficient of variation of IMEP as a function of equivalence ratio for each spark plug. It is notable that all conditions exhibit a similar CoV of around 1% for equivalence ratios above 0.30, but increased instability is observed at equivalence ratios of 0.30 or lower. This rise in operating instability, expected due to higher air dilution [71], is not uniform across all spark plug types. Specifically, colder spark plugs (those with a higher heat range on the NGK chart) show greater instability at low loads and equivalence ratios. The most unstable operation is seen with the coldest spark plug (E), a surface gap type, which has a CoV_{IMEP} of 16%. In contrast, the hottest spark plug (A), with a highly protruding ground electrode, exhibits much less instability, with a coefficient of 6%.

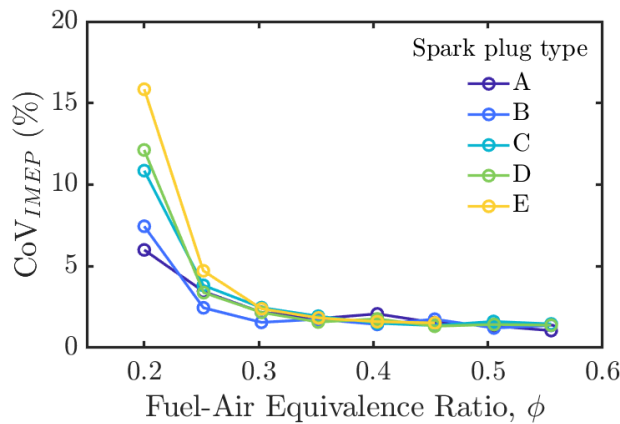


Figure 3.3: Spark plug effect on engine stability.

It is important to note that the engine is considered stable when the CoV_{IMEP} is below 4%.

3.1. TEST BENCH DEFINITION

None of the tested spark plugs provided stable operation at an equivalence ratio of 0.20, though all, except for E, achieved stability at $\phi = 0.25$.

The impact of the spark plug on combustion duration is analyzed in Figure 3.4, which shows the duration in crank angle degrees (CAD) for each combustion phase as a function of the equivalence ratio. At $\phi \geq 0.50$, the flame phases have a similar duration of around 15 CAD. As the mixture becomes leaner (lower equivalence ratio), the combustion duration increases, but the extent of this increase varies across the phases. Both flame propagation (10-50%) and end-flame (50-90%) phases extend by about 5 to 10 CAD in leaner mixtures, whereas the flame initiation phase can extend by up to 30 CAD – representing a 150% increase. This suggests that flame initiation is particularly critical in hydrogen combustion engines.

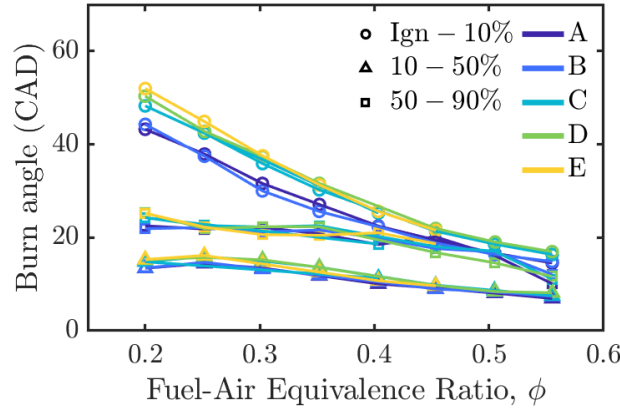


Figure 3.4: Spark plug effect on combustion duration.

The choice of spark plug also affects combustion duration. While flame propagation and the end-flame phases are minimally impacted by spark plug selection, the flame kernel creation and development phases are significantly influenced. Hotter spark plugs result in a faster flame initiation period and shorter overall combustion duration. This difference becomes more pronounced as the air-fuel ratio increases, reaching up to 10 CAD at $\phi = 0.20$. This can be attributed to reduced heat losses with these spark plug geometries, leading to a more robust flame kernel. However, these types of spark plugs are not ideal at high loads, as they can become hot spots for abnormal combustion. In contrast, colder spark plugs, which are preferable at high loads, can cause unstable operation at low loads, resulting in up to three times more instability with the tested spark plugs, as observed before.

Figure 3.5 presents the coefficient of variation (CoV) of the combustion duration as a function of the equivalence ratio. The combustion CCVs exhibit different behaviors depending on the flame phase. For both the flame initiation and propagation phases, the CoV increases as the equivalence ratio decreases, rising from 4% and 5% at $\phi = 0.55$ to approximately 7% and 9% at $\phi = 0.20$, respectively. In contrast, the end-flame phase shows a non-monotonic behavior, with a peak CoV of around 13% at $\phi = 0.50$ and a minimum of approximately 6% at $\phi = 0.35$. This is likely due to the mass fraction burned being calculated using the apparent heat release rate, which does not account for heat transfer in the engine cylinder. Neglecting this aspect makes the final stage of combustion, where the flame interacts with the cylinder walls, less distinct, leading to less reliable results. Consequently, a TPA (Three Pressure Analysis) model will be employed in future analysis to better account for heat transfer and provide more accurate results, since common models are not adapted for hydrogen combustion [111].

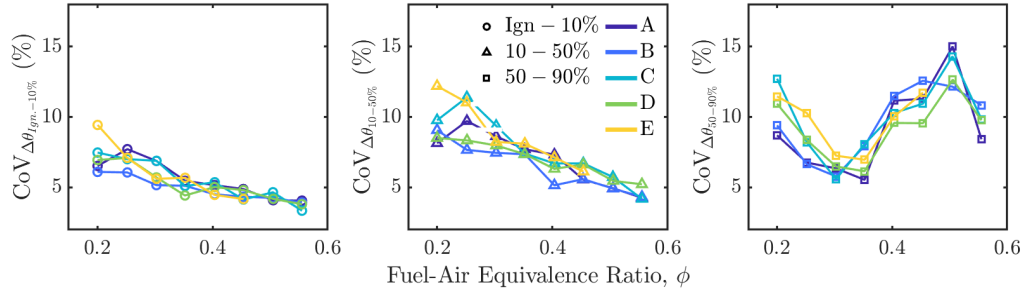


Figure 3.5: Spark plug effect on combustion duration variation for the three combustion phases: flame initiation (left), flame propagation (middle), and end-flame (right).

No significant effect of spark plug choice is observed on the CoV of combustion duration, indicating that the variation in flame timing behaves similarly across different spark plugs. However, while the CoV remains similar, the standard deviation of the combustion durations differs, particularly in the flame initiation phase. Since this phase is strongly influenced by spark plug selection, the standard deviation of flame initiation varies accordingly among the different spark plugs. Consequently, to balance combustion stability and minimize abnormal combustion (based on laboratory observations), spark plug C is used in the experiments going forward.

3.2 TPA Model

The developed Three Pressure Analysis model from GT-SUITE software is employed to evaluate in-cylinder parameters using intake, exhaust, and in-cylinder pressure data, thereby reducing uncertainties related to unknown parameters. This section presents the validation of the model. Additionally, key input and output parameters are analyzed to understand and better define the operating conditions studied throughout this thesis.

3.2.1 Input parameters

The compression ratio is a critical parameter in 0D/1D engine simulations, significantly affecting the accuracy of combustion modeling. To experimentally evaluate it for the selected engine, simulations are conducted under two motoring conditions, as outlined in Table 3.1, using the Woschni heat transfer model [19]. A design of experiments (DoE) approach is employed, based on a geometric compression ratio of 10.0:1. The simulated compression ratio was varied between 9.4:1 and 10.4:1 in 0.2-point increments. The resulting in-cylinder pressure traces for the studied conditions are plotted against the crank angle in Figure 3.6.

Table 3.1: Two motoring reference conditions.

Engine speed	P_{int}	P_{exh}	T_{int}
1200 rpm	0.7 bar	1 bar	23 °C
1200 rpm	0.9 bar	1 bar	23 °C

The comparison reveals that the measured cylinder pressure closely aligns with a compression ratio of 9.6:1 for both motoring conditions. This suggests that a compression ratio of

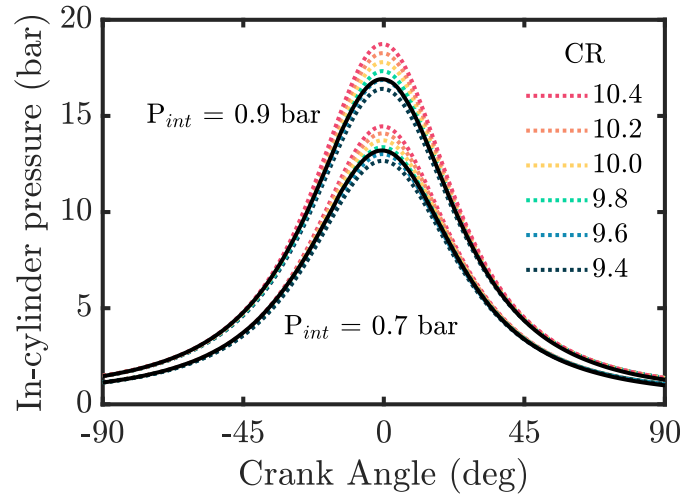


Figure 3.6: Effective compression ratio study for the two motoring reference cases.

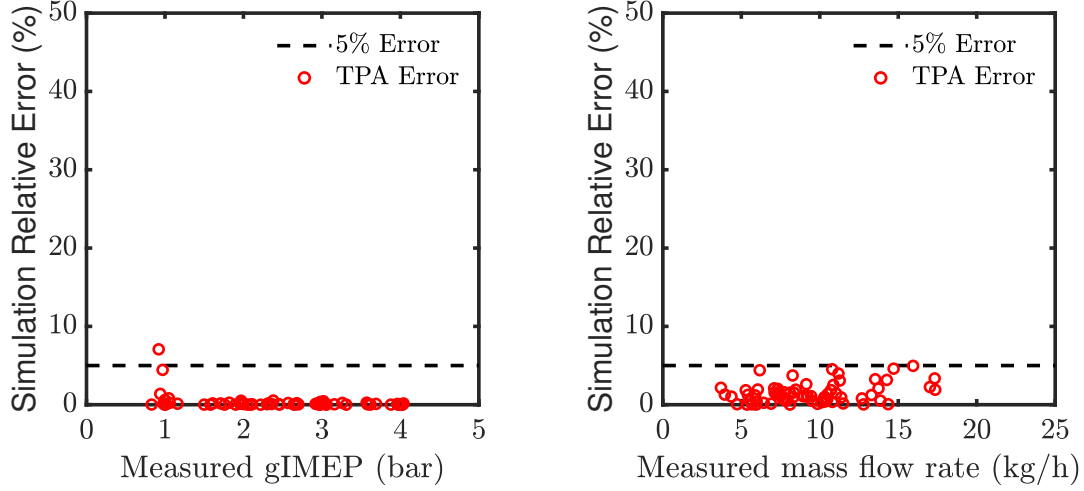
9.6:1 provides the best fit to the experimental data. Therefore, this value was selected and held constant for all subsequent experimental conditions analyzed in this study.

3.2.2 Validation

The model is validated for hydrogen combustion across a range of equivalence ratios (0.25 to 0.55), intake pressures (0.7 and 0.9 bar), spark timings (from -87 to -15 °aTDC), and engine speeds (900, 1200, and 1500 rpm). The validation process compared simulated results with measured values for two key parameters: (a) mass flow rate at the intake, which offers insights into volumetric efficiency and in-cylinder trapped mass, and (b) gIMEP, which reflects the gross work done during the cycle. The relative errors between simulated and measured values were found to be within 1% for gIMEP (over 95% of the simulations) and 5% for the total mass flow rate (over 100% of the simulations), as shown in Figures 3.7a and 3.7b.

Additionally, Figure 3.8 compares ensemble-averaged measured and simulated cylinder pressure traces for two distinct operating conditions: 4 bar IMEP with a spark timing of -45 °aTDC and an equivalence ratio of 0.25, and 3 bar IMEP with a spark timing of -7 °aTDC and an equivalence ratio of 0.55. Despite the experimental conditions exhibiting different pressure traces, the simulation accurately captured the in-cylinder behavior.

Figure 3.9 shows the ensemble-averaged in-cylinder pressure, P_{cyl} , as a function of crank angle for similar thermodynamic conditions at spark timing used in the in-cylinder flame development study. Both the measured and simulated pressure traces are plotted for equivalence ratios ranging from 0.25 to 0.55, in 0.05 increments, as well as for the motored condition. At these conditions, the simulation can not accurately represent the $\phi_{int} = 0.20$ mixture, probably due to a lower combustion efficiency, which will be discussed further. However, above this equivalence ratio, the pressure profiles are consistent across all conditions, indicating that the simulation accurately captures the thermodynamic behavior. This allows for reliable analysis of key outputs such as burned and unburned gas properties throughout the cycle. As an example, the mass fraction burned is plotted alongside the pressure trace, demonstrating the model's ability to provide detailed information on combustion progression. The figure also illustrates how increasing the equivalence ratio leads to higher energy release (reflected in higher peak



(a) Gross Indicated Mean Effective Pressure (gIMEP) relative error between experiment and simulation for all conditions. (b) Mass flow rate (MFR) relative error between experiment and simulation for all conditions.

Figure 3.7: Validation parameters and procedure.

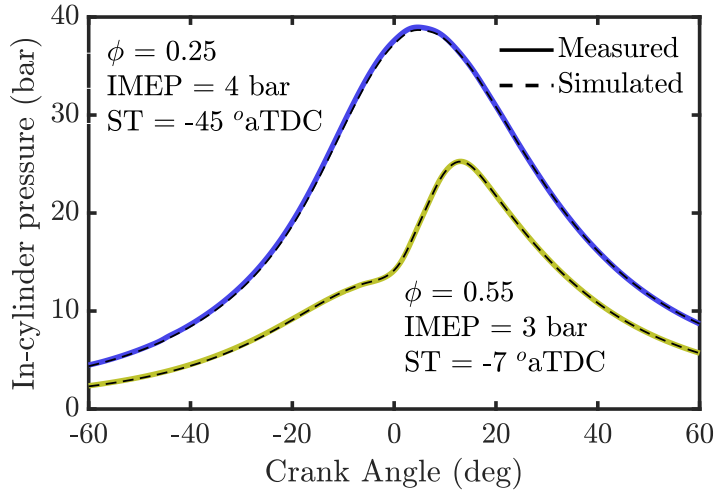


Figure 3.8: Illustration of the simulated and measured ensemble-averaged pressure traces for two distinct experimental conditions.

pressures) and faster combustion, with a shorter duration in crank angle degrees, as expected.

3.2.3 Output parameters

As discussed earlier, hydrogen/air mixtures behave differently from conventional fuels, especially under ultra-lean conditions, making rigorous post-processing of experimental data critical. The heat transfer model, for example, plays a significant role in determining net heat release, which directly impacts the calculation of the mass fraction burned and the subsequent combustion analysis. Therefore, it is essential to thoroughly understand the key parameters influencing flame behavior in the upcoming study.

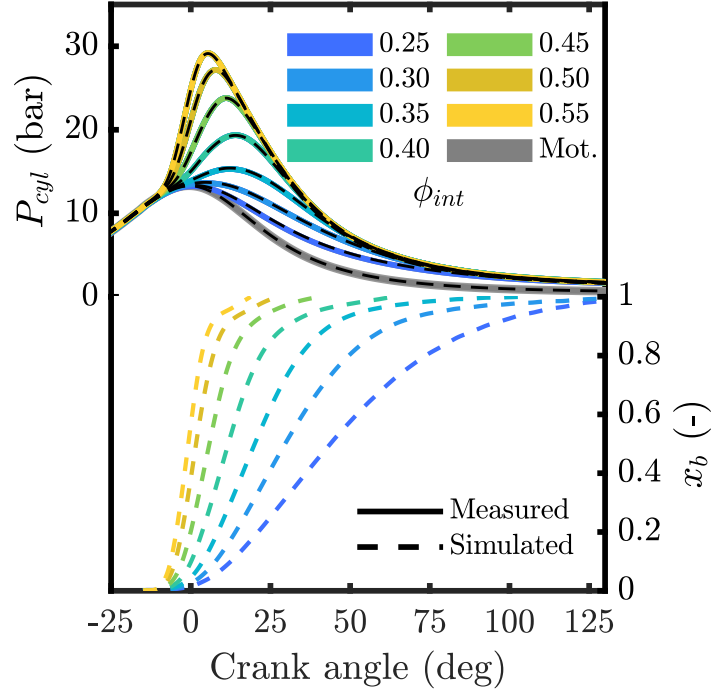


Figure 3.9: Measured and simulated in-cylinder pressure, P_{cyl} , for motored and seven equivalence ratios mixtures, and mass fraction burned, x_b , as a function of the crank angle.

Heat transfer model

The TPA model adjusted the multiplier coefficient of Woschni heat transfer model by varying it from 1 to 3 to match the gIMEP during the combustion phase. Across all tested conditions, the analysis showed that the heat transfer convection multiplier ranged from 1.3 to 2.8, indicating that the Woschni equation generally underestimates heat transfer for hydrogen combustion in engines. Notably, the highest values of the convection multiplier were observed at low equivalence ratios, and as the fuel-air equivalence ratio increased, the values decreased, approaching 1. This suggests that ultra-lean hydrogen combustion deviates more from the Woschni equation than mixtures closer to stoichiometry. This can be attributed to the difference in burned gas temperatures between typical internal combustion engine fuels and ultra-lean hydrogen flames. As shown in the Chapter 1 (Table 1.3), the burned gas temperature of ultra-lean hydrogen/air flames is about half that of stoichiometric isooctane-air mixtures. Since heat transfer depends on the temperature difference between the in-cylinder gas and the engine walls (or ambient), its magnitude is lower than in models for conventional fuels. Consequently, the Woschni heat transfer coefficient is multiplied by a factor greater than 1, meaning the actual heat transfer is more substantial than predicted by the Woschni equation, particularly under higher air dilution, in line with the decrease in burned gas temperature.

Intake and in-cylinder equivalence ratios

As explained previously, the hydrogen and air mass flow controllers set a specific fuel-air equivalence ratio in the intake manifold, ϕ_{int} . The GT-SUITE simulation, using the TPA model, predicts the in-cylinder equivalence ratio, ϕ_{cyl} , accounting for the unburned air in the residual

gas, which varies depending on the experimental conditions. Figure 3.10 shows the relationship between ϕ_{cyl} and ϕ_{int} for a constant engine speed of 1200 rpm and intake pressure of 0.7 bar. The in-cylinder equivalence ratio follows an approximately linear trend with the intake equivalence ratio, showing a consistent global difference of around 0.03. This linear relationship holds true across all tested operating conditions, with a variation of 0.03 ± 0.01 below the equivalence ratio set in the intake pipe. Therefore, moving forward, it will be referred to interchangeably as intake or in-cylinder. Note that all combustion characteristics are calculated based on the in-cylinder equivalence ratio derived from simulation data.

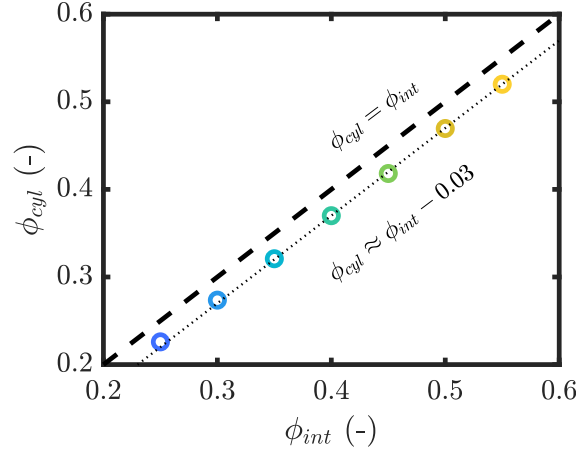


Figure 3.10: In-cylinder equivalence ratio, ϕ_{cyl} , as a function of the intake equivalence ratio, ϕ_{int} .

3.3 Combustion analysis

Two combustion analyses were performed: The IMEP sweep and the equivalence ratio sweep.

3.3.1 Load and Equivalence Ratio Investigation

As explained in the 'Experimental Setup and Methodology' chapter, this analysis examines the effect of the equivalence ratio at four different IMEP levels (1, 2, 3, and 4 bar). To maintain the same load across varying equivalence ratios, the intake pressure and spark timing are adjusted to achieve a CA50 at 8° aTDC, ensuring consistent work output and combustion phasing under all conditions. The objective of this experiment is to understand the impact of the equivalence ratio on hydrogen combustion at a constant work output, which can help define optimal engine control strategies for load, rpm, and spark timing.

First, the coefficient of variation of the IMEP is analyzed. Figure 3.11 shows the relationship between CoV (in percentage) and fuel-air equivalence ratio for all IMEP values. The results indicate that the CoV of IMEP increases as the equivalence ratio decreases, which is expected. However, the increase remains below the stability threshold of 4%. This is noteworthy, as flame properties such as laminar flame speed and adiabatic flame temperature vary significantly across these equivalence ratios. The engine remains stable down to $\phi = 0.2$ ($\lambda = 5$), but misfires occur at leaner mixtures for all loads.

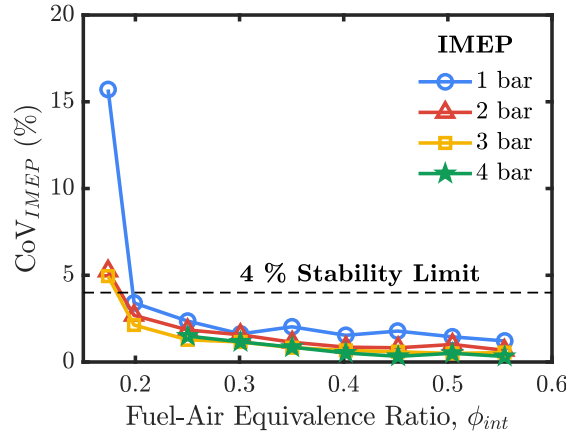


Figure 3.11: Equivalence ratio and load effects on engine stability.

Additionally, it is observed that CCVs increase as the load decreases, consistent with findings in the literature [98, 103]. At the same equivalence ratio, an IMEP of 4 bar can be up to five times more stable than an IMEP of 1 bar (at $\phi = 0.45$). Since idling (IMEP = 1 bar) represents the lowest load expected in an internal combustion engine for transport applications, and low loads are generally associated with higher variability, the absence of high CCV levels in this condition indicates overall stable operation.

To further understand why cyclic variations remain low across this broad range of equivalence ratios, it is important to analyze the combustion durations under these operating conditions. Figure 3.12 illustrates the effect of equivalence ratio and load on the duration of three flame phases: the flame initiation phase, the flame propagation phase, and the end-flame phase (from 50 to 90% MFB). The total combustion duration (from 10 to 90% MFB) is also presented at the bottom.

The flame initiation phase is the most significantly affected by changes in the equivalence ratio, followed by the flame propagation and end-flame phases, respectively. The flame initiation phase exhibits a second-order trend with respect to the equivalence ratio, while the combustion duration from 10 to 50% MFB follows an almost linear trend, and the end-flame phase remains nearly constant at around 30 crank angle degrees. As the equivalence ratio decreases from 0.55 to 0.2, the combustion duration increases by +50% (from 22 to 31 CAD) in the end-flame phase (IMEP = 3 bar), by +211% (from 6.5 to 21.5 CAD) in the flame propagation phase (IMEP = 2 bar), and by +370% (from 9 to 42 CAD) in the flame initiation phase (IMEP = 2 bar). The flame initiation duration is also the most sensitive to load variations (i.e., intake pressure). For instance, an increase in load from 1 to 4 bar (intake pressure from 0.5 to 1.05 bar) accelerates the combustion process by 6 CAD at $\phi = 0.35$ and by more than 10 CAD at $\phi = 0.2$ when IMEP rises from 1 to 3 bar (intake pressure from 0.74 to 1.3 bar). In contrast, the end-flame phase appears largely unaffected by load variations.

The flame initiation phase is identified as critical for flame development and overall performance in hydrogen internal combustion engines, as previously noted in swirl-based geometries [39]. However, it is challenging to draw definitive conclusions from a constant IMEP experiment since key parameters like intake pressure, equivalence ratio, and spark timing are also changing. To gain a deeper understanding of hydrogen combustion physics in an ICE, further experimental analysis is required.

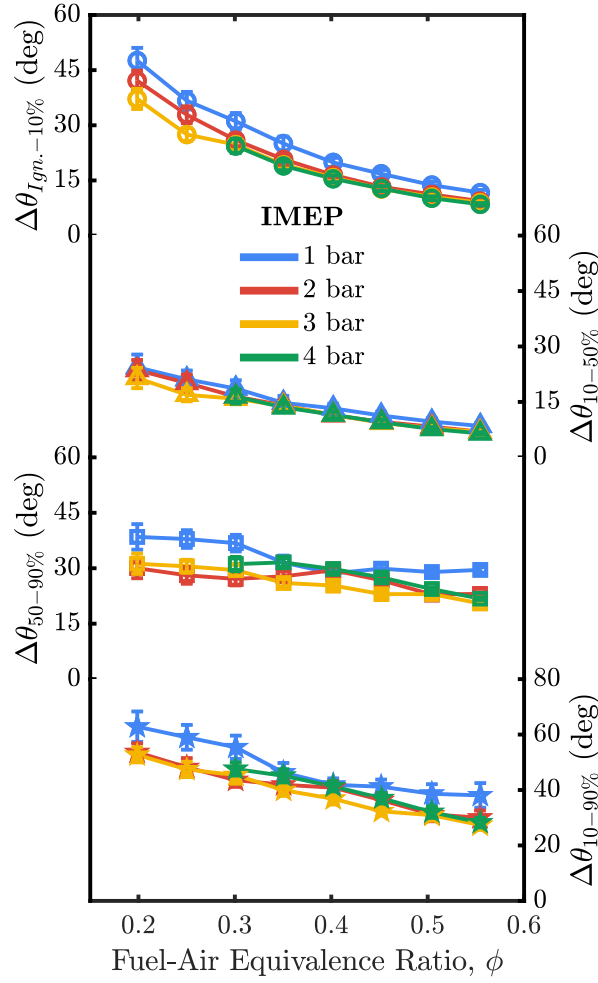


Figure 3.12: Combustion duration of the flame initiation (first on top), flame propagation (second), end-flame (third), and total, 10 to 90% (fourth on bottom), as a function of the equivalence ratio for the ϕ_{int} and IMEP sweep. The error bars represent two times the standard deviation.

3.3.2 Flame Initiation Investigation

To investigate the impact of equivalence ratio, turbulence, and pressure on hydrogen combustion, an analysis is conducted with intake pressure and spark timing held constant to maintain similar thermodynamic conditions at the moment of ignition. The study varies the equivalence ratio, which significantly affects flame properties, and engine speed, which influences turbulence. Figure 3.13 shows the variation in in-cylinder pressure and mass fraction burned as functions of crank angle for different equivalence ratios ($0.25 \leq \phi_{int} \leq 0.55$) and engine speeds ($900 \leq N \leq 1500$ rpm). A total of 21 experimental conditions are tested at two intake pressures (0.7 and 0.9 bar). Given that the flame initiation phase showed the greatest sensitivity in combustion progress parameters, the combustion duration from spark timing to 10% mass fraction burned (MFB) is used to compare the effects of equivalence ratio, engine speed, and intake pressure.

It is important to note that spark timing is not adjusted to optimize burning time. Consequently, the comparison focuses primarily on the flame initiation phase, where the thermody-

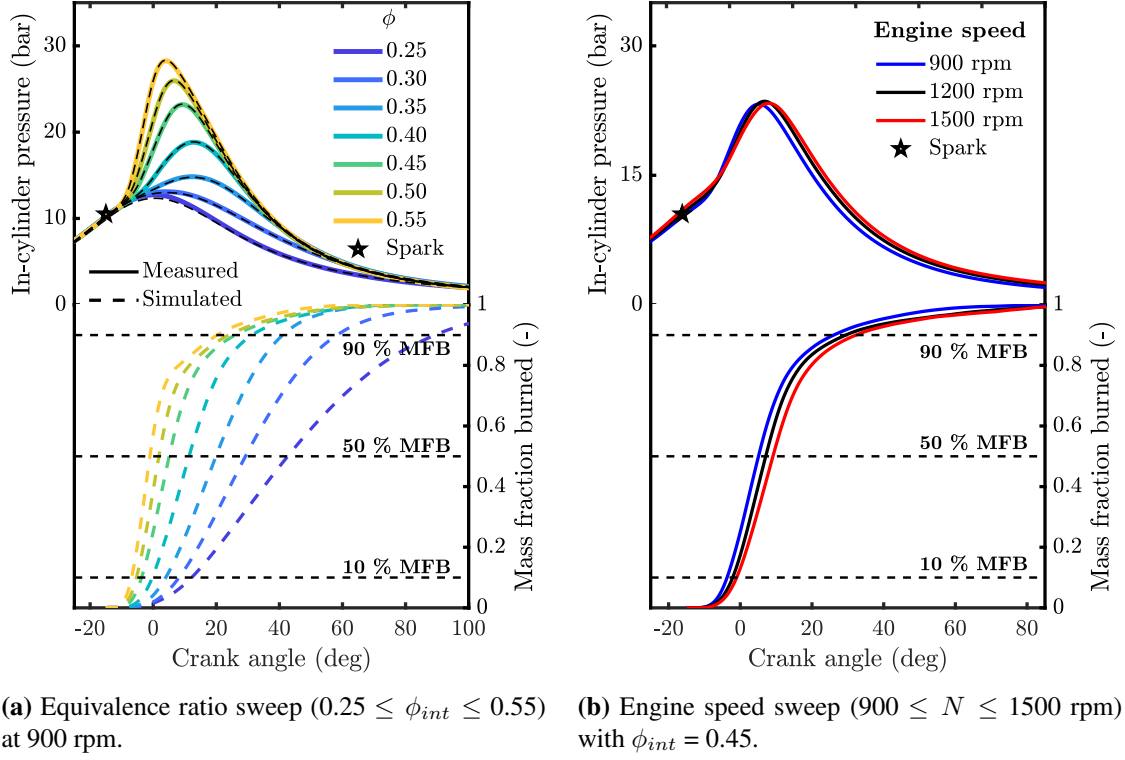


Figure 3.13: In-cylinder pressure and mass fraction burned as a function of the crank angle. The mean intake pressure is 0.7 bar and the spark timing is constant at 15 °bTDC.

dynamic conditions are closer to real engine operation, and combustion phasing is not the primary focus. The differences in flame kernel development due to variations in equivalence ratio and turbulence will be further examined using turbulent flame modeling equations. Figure 3.14 shows this duration for the three engine speeds tested at $P_{int} = 0.7$ bar. The results indicate that the burning angle during the flame initiation phase decreases as the equivalence ratio increases. This can be attributed to the rise in laminar flame speed under these conditions. As the equivalence ratio increased from 0.25 to 0.55, the burning angle reduced from 26.6 (at $\phi = 0.25$ for the three engine speeds) to 8.1 CAD (at 900 rpm), 9.1 CAD (at 1200 rpm), and 10.5 CAD (at 1500 rpm), representing a reduction of up to 69.5%.

Additionally, during the early stages of flame development, the burning angle remains similar across all engine speeds for equivalence ratios below 0.35. While the crank angles may not reflect the same physical time, turbulence influences the flame speed such that the flames burn within the same amount of crankshaft rotation. However, at higher equivalence ratios, the burning time begins to differ. At 900 rpm, combustion occurs over fewer crank angle degrees than at 1500 rpm, suggesting that turbulence has a reduced effect on burning speed at higher equivalence ratios. Instead, the burning speed is predominantly governed by fundamental flame properties, such as laminar flame speed. Since the laminar flame speed remains constant for a given pressure, temperature, and equivalence ratio, a higher engine speed requires more crank angle degrees to complete combustion.

To further analyze flame behavior under these experimental conditions, it is necessary to examine the burning process in terms of physical time. Figure 3.15 presents the same results

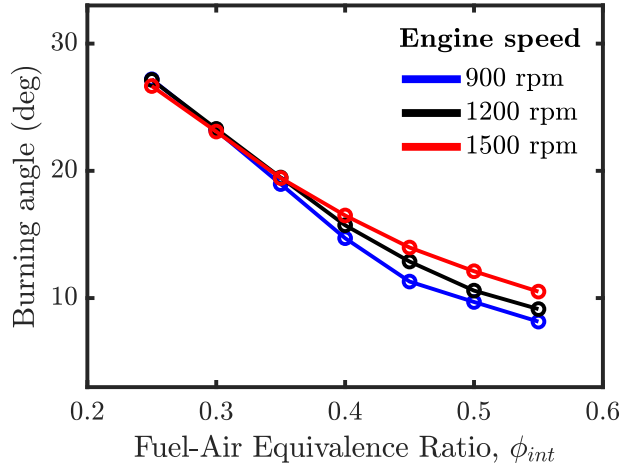


Figure 3.14: Combustion duration for the three engine speeds (in crank angle degrees) as a function of the fuel-air equivalence ratio with $P_{int} = 0.7$ bar.

as Figure 3.14, but with the y-axis showing burning time in milliseconds ($t_{\Delta\theta}$). As expected, the burning time for flame initiation decreases with increasing equivalence ratio for all engine speeds due to the higher laminar flame speed of hydrogen/air mixtures. However, the rate of decrease varies with turbulence conditions. As hypothesized, the burning time for flame kernel development (from spark timing to 10% MFB) becomes increasingly dependent on flame properties as the equivalence ratio rises. This is evident from the convergence of burning times at higher equivalence ratios. Conversely, at lower equivalence ratios, burning time varies noticeably between engine speeds during the initial flame phase, confirming that turbulence significantly influences flame development under these conditions.

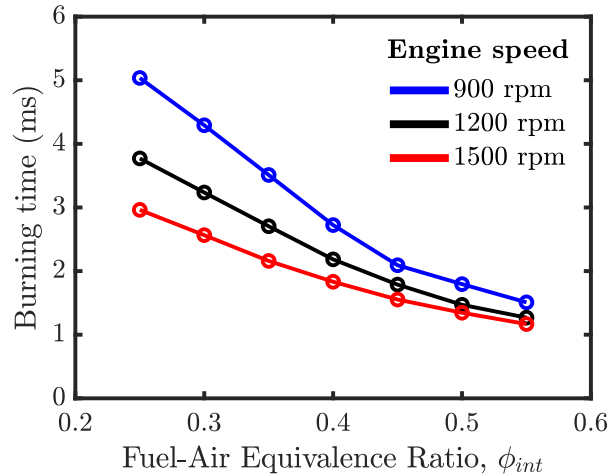


Figure 3.15: Combustion duration (in ms) for the three engine speeds (900, 1200 and 1500 rpm) as a function of the equivalence ratio.

To account for the influence of turbulent intensity and isolate the flame propagation characteristics, an analysis of the burning time relative to laminar flame properties is conducted. A characteristic flame time, denoted as t_f , is introduced, defined as the ratio of the laminar flame

thickness (δ_L) to the laminar flame speed (s_L^0). To calculate these flame properties, simulations are performed using the CONVERGE CFD software [142], incorporating three hydrogen/air kinetic mechanisms: Burke et al. [29], Alekseev et al. [143], and GRI-Mech 3.0 [28], under spark timing conditions.

Figure 3.16 presents the laminar flame speed and thickness obtained from the equivalence ratio sweep at 900 rpm using the specified kinetic mechanism, with pressures and temperatures of approximately 10.5 ± 0.4 bar and 680 ± 5 K for all equivalence ratios and engine speeds. Notably, significant variations in flame speed are observed across different equivalence ratios. For example, at $\phi = 0.55$, the laminar flame speed calculated using the mechanism of Alekseev et al. is 2.99 m/s, while at $\phi = 0.25$, it drops to 3.5 cm/s, a difference of nearly 100 times. Despite this substantial disparity, the difference in combustion duration between these conditions remain relatively small.

It is important to note that while these kinetic mechanisms are validated against experimental data, they may not have been specifically tested at the high pressures and low equivalence ratios relevant to this study. Additionally, hydrogen flames in these conditions may be prone to instabilities, which can significantly affect the measurement and calculation of laminar flame speed [144]. As such, there may be some uncertainty in determining flame speed under these operating conditions. Moreover, the different kinetic mechanisms exhibit notable discrepancies. For instance, GRI-Mech 3.0 underestimates the flame speed by approximately 40% across all equivalence ratios, while overestimating the flame thickness by around 160% compared to the Burke et al. and Alekseev et al. mechanisms. For simplicity and because of its widespread use in commercial CFD software [145], the Burke mechanism is selected for further analysis of flame properties in this thesis.

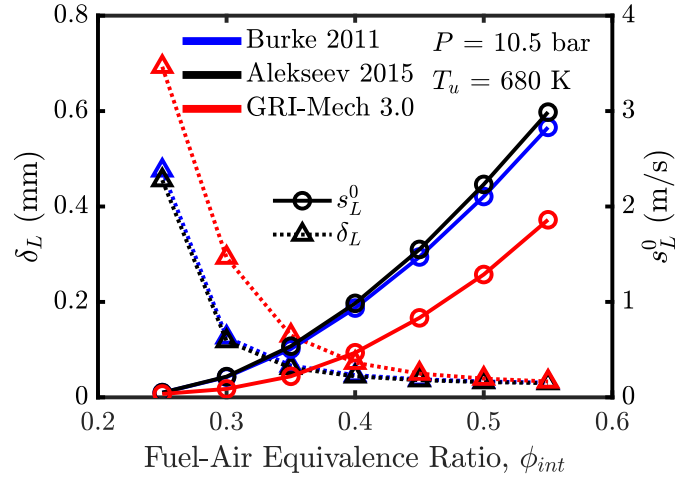


Figure 3.16: Laminar flame speed, s_L^0 , and thickness, δ_L , as a function of the equivalence ratio calculated at the spark timing pressure and temperature conditions for the 900 rpm experiments.

To better analyze burning time in relation to flame properties, a dimensionless time, t^* , is introduced. It is calculated as the ratio of the physical burning time, $t_{\Delta\theta}$ (the time required to burn 10% of the mass after spark timing), to the characteristic flame time, $t_f = \delta_L/s_L^0$ (Equation 3.1). Figure 3.17 shows the dimensionless time as a function of the fuel-air equivalence ratio.

$$t^* = \frac{t_{\Delta\theta}}{t_f} \quad (3.1)$$

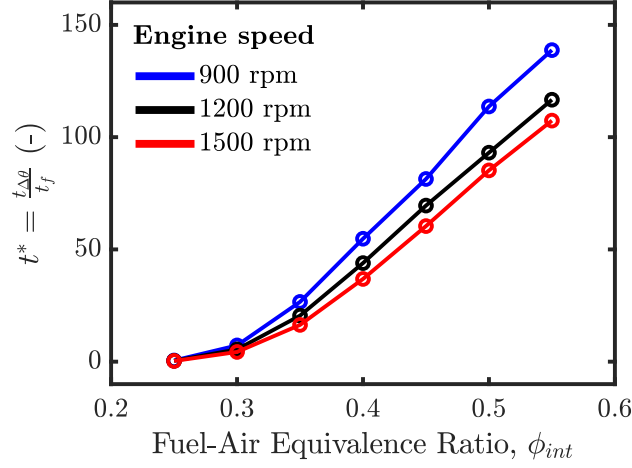


Figure 3.17: Dimensionless time, $t^* = t_{\Delta\theta}/t_f$, as a function of the fuel-air equivalence ratio.

The results reveal a non-linear relationship, with the dimensionless time increasing as the equivalence ratio rises, indicating thinner and faster flames. The influence of turbulence is also apparent, as greater turbulence enhances flame speed and shortens combustion time. This leads to the question: How much does turbulence affect ultra-lean hydrogen flames? To address this, a classical approach based on turbulent intensity is applied to analyze turbulent flames, to be integrated in the characteristic flame timescale. The turbulent flame speed, s_T , is determined using the Damköhler expression [146], where u' represents the characteristic mean turbulent velocity fluctuation.

$$s_T = s_L \left(1 + \frac{u'}{s_L} \right) \quad (3.2)$$

This velocity is estimated for the three engine speeds by considering the mean piston speed, $\overline{S_p}$, as described in [19, 147]. The turbulent velocities for 900, 1200, and 1500 rpm are calculated as 1.29, 1.71, and 2.14 m/s, respectively.

$$u' \approx \frac{\overline{S_p}}{2} \quad (3.3)$$

Figure 3.18 shows the dimensionless time, accounting for the effect of turbulent flame speed, as a function of the equivalence ratio. Notably, the ratio of physical burning time to chemical flame time converges into a single curve for all three engine speeds, indicating that the increase in flame speed due to turbulence is accurately captured by the Damköhler equation. Additionally, the trend appears more linear with respect to the equivalence ratio, as reflected by the improvement in the coefficient of determination, which increases from 97.8% to 98.5% at 900 rpm.

It is well established that the hydrogen/air flame speed is influenced by both turbulence and inherent instabilities, such as thermodiffusive instabilities [47, 64, 148]. The effect of these thermodiffusive instabilities on flame speed depends on factors like equivalence ratio, pressure, and temperature, and various studies have attempted to quantify this influence.

Darrieus and Landau, in their seminal works [42, 43], were among the first to predict the occurrence of unconditional instability in planar flames due to thermal expansion across the

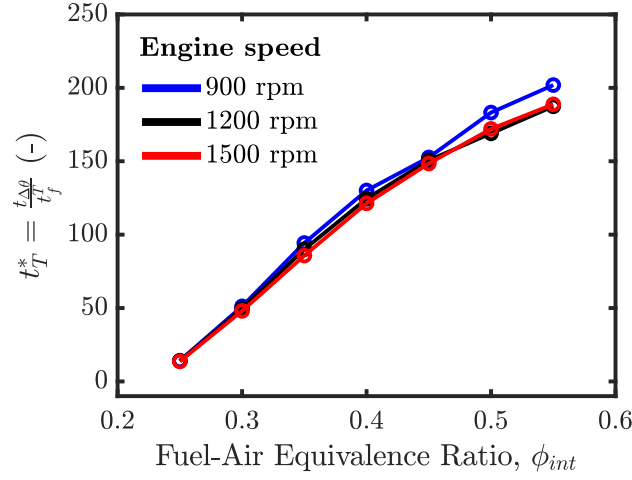


Figure 3.18: Dimensionless time taking into account the turbulent flame speed, $t_T^* = t_{\Delta\theta}/t_f^T$, as a function of the fuel-air equivalence ratio.

flame front. To examine this phenomenon, one can consider a flame surface propagating at a speed of s_L with a characteristic thickness of δ_L . The flame surface, F , can be described by:

$$F(x, t) = A \exp(\omega t + i k x) \quad (3.4)$$

In this formulation, ω represents the instability growth rate, and k is the wavenumber. The normalized growth rate, commonly referred to as the Darrieus-Landau expression, is provided by [46]:

$$\tilde{\omega} = \omega \frac{\delta_L}{s_L} = \frac{1}{\sigma + 1} \left(\sqrt{\sigma^3 + \sigma^2 - \sigma} - \sigma \right) \tilde{k} = \omega_{DL} \tilde{k} \quad (3.5)$$

In this equation, σ represents the ratio of the densities of unburned to burned gas (ρ_u/ρ_b), and the wavenumber is normalized by the flame thickness ($\tilde{k} = k\delta_L$). Typically, in combustion scenarios, σ is greater than 1, leading to a positive growth rate ω , which suggests that the flame is unstable across all wavenumbers.

However, experimental observations have shown that this unconditional instability predicted by the Darrieus-Landau expression does not occur. To address the stabilizing and destabilizing effects of diffusion across the flame, further research has been conducted [149, 150, 151]. This has led to the development of a new model that includes a second-order term in $\tilde{k}$, as described by [152]:

$$\tilde{\omega} = \omega_{DL} \tilde{k} - [B_1 + B_2 \beta (Le_{eff} - 1) B_3 Pr] \tilde{k}^2 = \omega_{DL} \tilde{k} + \omega_2 \tilde{k}^2 \quad (3.6)$$

Here, B_i are constants dependent on the density ratio σ and thermal conductivity. The parameter β represents the Zel'dovich number of the reaction, and Pr denotes the Prandtl number. The coefficient ω_2 reflects the impact of the second-order term. A negative ω_2 signifies a stabilizing effect, resulting in a finite wavenumber beyond which flame waves are suppressed (thermodiffusive stability). Conversely, a positive ω_2 indicates flame instability (thermodiffusive instability).

Recent studies have calculated the ω_2 parameter across a wide range of equivalence ratios, pressures, and temperatures [153, 48, 148]. Figure 3.19 presents contour plots from Hernandez

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et al. [148] (using the Burke et al. [29] mechanism) that illustrate how ω_2 varies with different equivalence ratios and pressures at a temperature of 750 K, which approximates the in-cylinder conditions at spark timing.

The contour map of ω_2 shows that higher positive values occur at lower equivalence ratios ($0.20 < \phi < 0.50$) and within a pressure range of 0.5 to 6 MPa. In contrast, ω_2 becomes negative (indicating flame stabilization) at higher equivalence ratios and lower pressures. The white stars on the map indicate the in-cylinder conditions for experiments conducted at 900 rpm, highlighting variations in flame acceleration under engine operating conditions. For example, at an equivalence ratio of 0.25, ω_2 exceeds 6, while at an equivalence ratio of 0.55, ω_2 approaches 0 under the same pressure and temperature conditions.

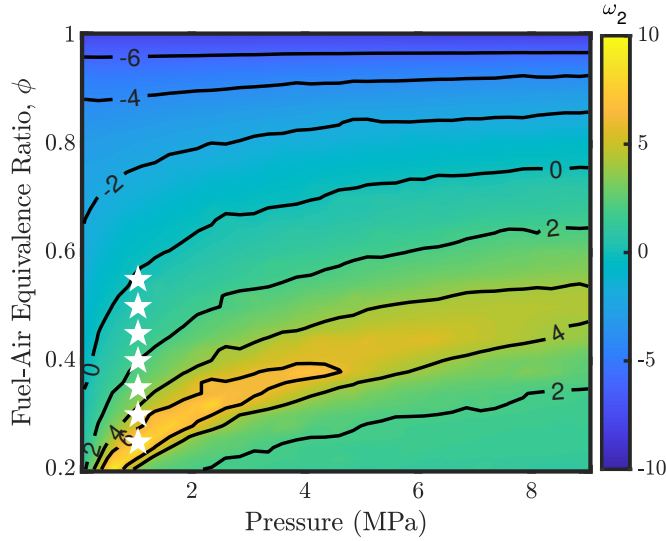


Figure 3.19: Map of the ω_2 variable over pressure and equivalence ratio for $T = 750$ K [148]. The white stars represent the cylinder conditions at spark timing for the 900 rpm experiments.

Equations 3.7 and 3.8 provide a method for estimating flame speed enhancement and variations in flame thickness based on the instability parameter ω_2 [148, 48]:

$$\frac{s_F}{s_L} = \begin{cases} \exp(0.08\omega_2) & \text{if } P < \Pi_c \\ 1 + 0.47\omega_2 & \text{otherwise} \end{cases} \quad (3.7)$$

$$\frac{\delta_F}{\delta_L} = \begin{cases} \exp(-0.06\omega_2) & \text{if } P < \Pi_c \\ \frac{1}{1+0.26\omega_2} & \text{otherwise} \end{cases} \quad (3.8)$$

In this expression, s_F and δ_F represent the flame speed and thickness considering instability effects, while s_L and δ_L are the laminar flame speed and thickness, respectively. The pressure criterion Π_c is calculated according to Equation 3.9 [153], where Θ is the ratio between the unburned gas temperature and a reference temperature, T_{ref} , set at 300 K.

$$\Pi_c = \left(\frac{20\phi}{7 - 2\Theta} \right)^{150/(21+10\Theta)} \quad (3.9)$$

By accounting for the flame modifications due to thermodiffusive instabilities and applying the Damköhler expression for turbulent combustion, it becomes possible to better understand

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and correlate the engine's burning time with hydrogen flame properties. Figure 3.20 compares the dimensionless time, considering both thermodiffusive instabilities and turbulence, with the scenario where only turbulence is factored in. This comparison provides insights into the combined influence of these effects on the combustion process.

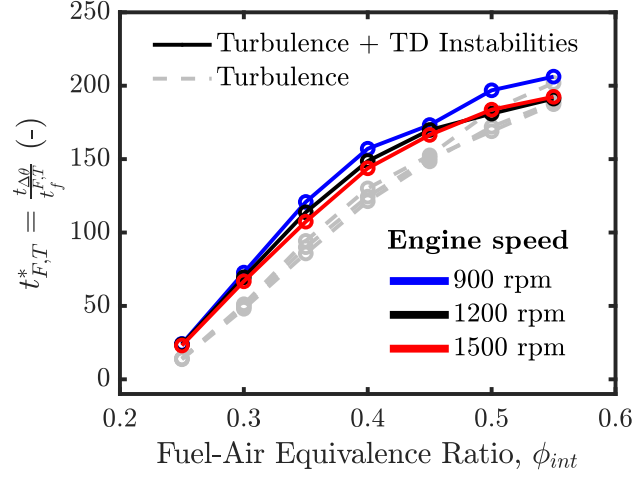


Figure 3.20: Dimensionless time accounting for the hydrogen flame acceleration due to thermodiffusive instabilities, $t_{F,T}^* = t_{\Delta\theta}/t_f^{F,T}$, as a function of the fuel-air equivalence ratio.

As anticipated, thermodiffusive instabilities reduce chemical reaction time, resulting in an increase in the dimensionless time compared to the curve that neglects these instabilities (especially at low equivalence ratios). However, the relationship between the physical burning time and the flame's chemical characteristic time is non-linear. Between equivalence ratios of 0.25 and 0.4, the trend appears linear, but beyond this range, the dimensionless time increases less significantly relative to the equivalence ratio. This suggests an interdependence between turbulence and thermodiffusive instabilities that should be considered for a comprehensive understanding of their combined impact on the combustion process.

As discussed previously, caution must be exercised when interpreting laminar flame speeds at high pressures and low equivalence ratios, as well as the results that involve these parameters, such as u'/s_L and s_F/s_L . To provide clarity, Figure 3.21 illustrates u'/s_L , which quantifies the flame speed increase due to turbulence according to the Damköhler expression, and s_F/s_L , representing the flame speed enhancement due to thermodiffusive instabilities.

The ratio u'/s_L shows exponential growth as the equivalence ratio decreases, reaching values between 30 and 40 at $\phi = 0.25$. Such a variation is uncommon with conventional fuels, which exhibit minimal changes in laminar flame speed across different equivalence ratios compared to hydrogen. Additionally, flame speed enhancement from TD instabilities ranges from 1.01 to 1.10 at high equivalence ratios ($\phi = 0.55$ and 0.45), and from 1.94 to 1.46 at lower equivalence ratios ($\phi = 0.25$ and 0.3). These values offer quantitative insight into the roles of turbulence and instabilities in flame behavior within internal combustion engines, especially at low load conditions.

Figure 3.22 shows the dimensionless time for three engine speeds as a function of equivalence ratio at two intake pressures ($P_{int} = 0.7$ and 0.9 bar). At higher intake pressures, combustion duration slightly decreases, indicating faster combustion. Moreover, the laminar flame speed increases with intake pressure, causing the dimensionless time to rise, particularly at

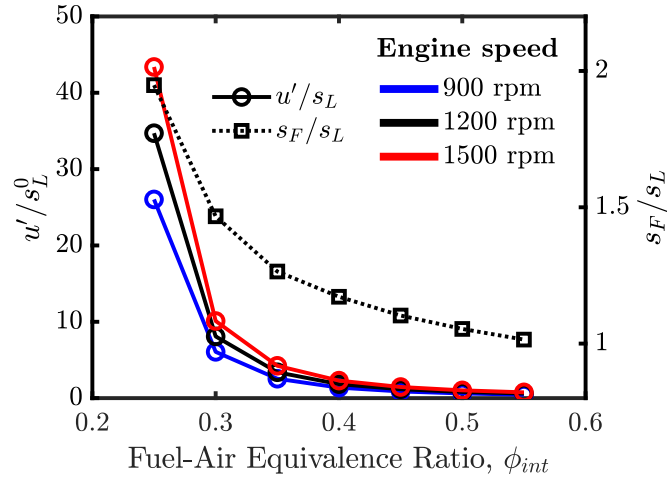


Figure 3.21: u'/s_L and s_F/s_L as a function of the equivalence ratio for the three engine speeds at 0.7 bar of intake pressure.

higher equivalence ratios. This trend approaches linearity, suggesting a more direct correlation between physical burning time and the flame's chemical characteristic time. However, equivalence ratios beyond 0.4 start to deviate from this linear trend.

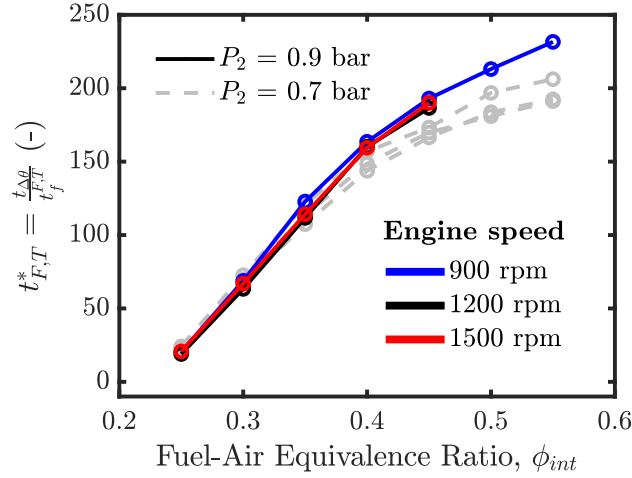


Figure 3.22: Dimensionless time accounting for the hydrogen flame acceleration due to thermodiffusive instabilities and turbulence for two intake pressures ($P_{int} = 0.7$ and 0.9 bar) as a function of the fuel-air equivalence ratio.

The analysis also shows that the point of maximum instability shifts with varying equivalence ratios, particularly under different pressures at the time of spark. Figure 3.19 reveals that higher pressures lead to maximum instability at higher equivalence ratios. This is well reflected in Figure 3.22, where the curve bends after a linear trend at lower equivalence ratios, with the deviation occurring at a higher equivalence ratio ($\phi = 0.45$). For higher values, this bending suggests that other factors or phenomena not included in the current model may influence combustion behavior under these conditions. Further investigation and refinement of the flame model may be needed to accurately capture the combustion characteristics at higher

equivalence ratios, particularly for precise prediction of the laminar flame speed.

3.3.3 Turbulent flame regime

As seen in the previous analysis, varying the equivalence ratio of the hydrogen/air mixture and the engine speed causes the flame properties to deviate from those of a laminar flame. Given that the in-cylinder conditions are primarily turbulent, an analysis of flames in a turbulent regime is necessary to better understand their behavior. To this end, the Peters-Borghi premixed turbulent combustion diagram for the tested conditions at spark timing is evaluated. To plot the experimental conditions on this diagram, certain assumptions are made. First, the turbulent intensity, u' , and integral length scale, L_T , are estimated using in-cylinder flow measurements from a similar engine architecture [49]. Turbulent intensity values for 900, 1200, and 1500 rpm are provided in the previous section, while the integral length scale is assumed to remain constant across varying engine speeds and intake pressures, with a value of 1.4 mm. The in-cylinder pressure and temperature at spark timing are defined as 10.5 bar and 700 K for all conditions with an intake pressure of 0.7 bar, and 13.5 bar and 750 K for conditions with an intake pressure of 0.9 bar. The laminar flame speed is calculated as previously described, using the Burke et al. kinetic mechanism, and the Zeldovich flame thickness definition [35]. Figure 3.23 presents the 21 experimental conditions for the intake pressure of 0.7 bar, along with the experimental conditions for the extreme equivalence ratios at the intake pressure of 0.9 bar (three engine speeds for each equivalence ratio), totaling 27 points.

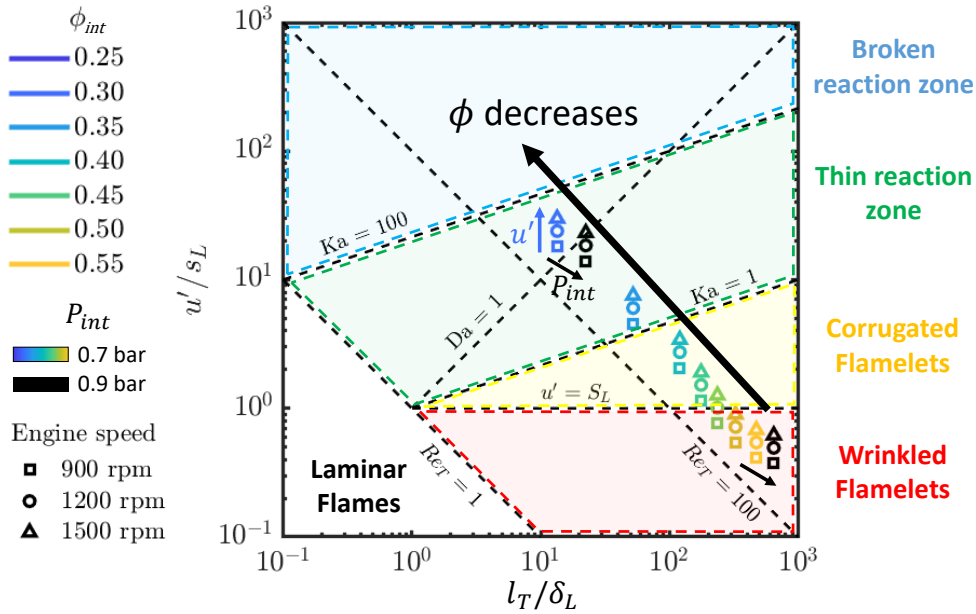


Figure 3.23: Turbulent combustion (Peters-Borghi) diagram for hydrogen under engine conditions. Fuel-air equivalence ratio variation from 0.25 to 0.55, intake pressure of 0.7 and 0.9 bar, and engine speed of 900, 1200 and 1500 rpm. Laminar flame properties calculated with the Burke kinetic mechanism [29] and turbulent characteristics taken from [49].

Variations in the equivalence ratio within the ultra-lean mixture range have a significant impact on the combustion diagram. The highest tested equivalence ratios ($\phi = 0.45$ to 0.55) fall

within the "Wrinkled Flamelets" combustion regime. With a slight reduction in the equivalence ratio ($\phi = 0.35$ to 0.45), the experimental conditions shift into the "Corrugated Flamelets" region. At $\phi = 0.30$, the conditions enter the "Thin Reaction Zone" region, and at the leanest tested equivalence ratio ($\phi = 0.25$), they approach the "Broken Reaction Zone". The same behavior is also observed in turbulent NH_3/air flames [94, 154], primarily due to their very low flame speeds and large flame thickness, similar to both ammonia/air and ultra-lean hydrogen/air flames.

Engine speed variation, while less impactful compared to the equivalence ratio, still causes the conditions to move higher on the diagram, indicating greater interaction between turbulence and the combustion chemical reaction. This shift is expected due to the increase in turbulent intensity while other parameters remain constant. Finally, the increase in intake pressure shifts the data points toward less turbulent flame regimes, characterized by a decrease in u'/s_L , indicating an increase in s_L , and an increase in L_T/δ_L , reflecting a decrease in δ_L .

These results highlight the importance of conducting a detailed analysis of both the in-cylinder flow characteristics specific to this spark-ignition engine architecture and the flame development measurements to gain a more comprehensive understanding of hydrogen combustion in ultra-lean mixtures within internal combustion engines. Therefore, the following chapters will focus on characterizing the in-cylinder flow and hydrogen combustion development, with a sensitivity analysis of multiple parameters, including intake pressure, engine speed, equivalence ratio, and spark discharge.

Conclusion

This chapter examined the performance of hydrogen and its fundamental flame characteristics under ultra-lean mixtures. First, the engine geometry was defined, alongside an analysis of the hydrogen injection position and spark plug type. The methodology was then developed, tested, and validated. Hydrogen was tested as fuel in an all-metal spark-ignition engine during a load analysis, showing stable operation with a fuel-air equivalence ratio as lean as 0.2, from 1 to 4 bar of IMEP. The combustion phase most affected was the flame initiation phase (from spark timing to 10% of MFB), which was studied in greater detail under constant intake pressure and spark timing conditions, comparing combustion duration across seven equivalence ratios (from 0.25 to 0.55) and three engine speeds (from 900 to 1500 rpm). From the characteristic timescales analysis, the flame was found to depend on both turbulence and thermodiffusive instabilities, likely interacting in a synergistic manner. It is important to note that the relationship between hydrodynamic and thermodiffusive instabilities are not further explored. The experimental results were plotted on the Peters-Borghi diagram, showing that small variations in the hydrogen/air mixture significantly impact the turbulent combustion regime experienced by the hydrogen/air premixed flame. Further analysis is proposed to better understand in-cylinder turbulent flames through flow and combustion measurements in the next chapters.

The methodology developed in this chapter was applied to two different engines and led to the publication of two conference papers.

- C. Ramalho Leite, R. Oung, P. Brequigny, J. Borée, F. Foucher, "Combustion Cycle-To-Cycle Variation Analysis in Diesel Baseline Hydrogen-Fueled Spark-Ignition Engines", SAE Technical Paper 2023-01-0290, 2023.

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- C. Ramalho Leite, M. Laignel, P. Brequigny, J. Borée, F. Foucher, "Experimental Combustion Analysis in a Gasoline Baseline Hydrogen-Fueled Internal Combustion Engine at Ultra-Lean Conditions", SAE Technical Paper 2023-24-0073, 2023.

Chapter 4

Internal aerodynamics

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Introduction

This chapter explores the flow field within the optical spark-ignition engine using high-speed PIV and EMD techniques, focusing primarily on cycle analysis during the intake and compression strokes, as well as on the assessment of kinetic energy and turbulence. The effects of intake pressure, engine speed, and combustion on both the mean and fluctuating flow are examined. Finally, the EMD method is employed to define the turbulence parameters that will be used in the turbulent combustion research discussed in the following chapters.

4.1 Engine cycle characterization

To characterize the flow field within the engine, the three non-simultaneous PIV velocity fields are analyzed to understand the intake and compression strokes, as well as the mean kinetic energy in the cylinder throughout the cycle. This analysis focuses primarily on a single operating condition: 0.7 bar intake pressure and 1200 rpm.

4.1.1 Intake Stroke

Figure 4.1 shows the ensemble-averaged velocity components in the x and z directions ($\langle U \rangle$ and $\langle W \rangle$, respectively) of the in-cylinder flow over 150 cycles for nine crank angles, from 300° to 180° bTDC, in 15° increments. This figure illustrates the intake stroke from valve opening to BDC. From 300° to 270° bTDC, air enters the cylinder at velocities exceeding 20 m/s. With the mean piston speed at approximately 3.4 m/s (about 7 times slower than the intake flow velocity), the intake jet first impinges the cylinder wall and then the piston. Due to the direction of the intake jet and the combined motion of the jet and piston, this process eventually generates a general rotating flow perpendicular to the cylinder axis, known as tumble, which is desired for faster flame development in spark ignition engines [155].

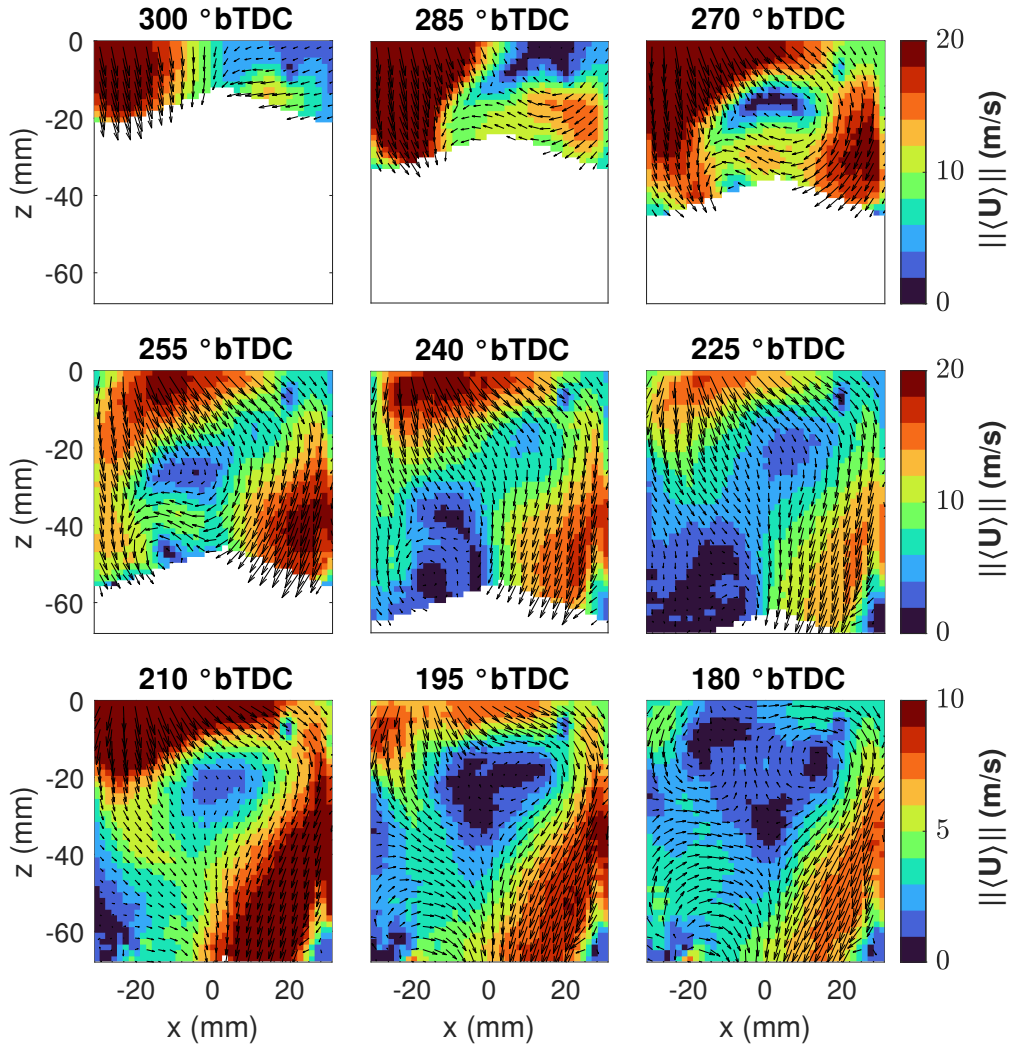


Figure 4.1: Ensemble-averaged velocity components in the x and z directions (U and W , respectively) of the in-cylinder flow during the intake stroke over 150 cycles, measured using high-speed PIV in the VC configuration. Measurements are shown at intervals of 15° , ranging from 300 (upper-left) to 180° bTDC (bottom-right).

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As the jet travels inside the cylinder and impinges on the piston, it flows back upward, interacting with the incoming intake jet. This creates a region of near-zero mean velocity, visible at 270 and 255 °bTDC. Later in the cycle (between 240 and 210 °bTDC), the downward piston movement and intake jets from both sides of the piston create another interaction zone. From this point onward, the jet on the right side of the cylinder becomes stronger than the one from the left, generating a rotating motion in the bottom left-hand corner of the cylinder, rotating in the positive y -axis direction as the piston approaches BDC (from 195 to 180 °bTDC). At this stage, a distinct tumble center is already visible. Additionally, at BDC, the first interaction zone shows two counter-rotating mean motions around $z = -20$ mm, caused by the ongoing intake jet and the already forming tumble motion.

For a more quantitative analysis of the flow, the z -component velocity is plotted at a specific height of $z = -20$ mm. Figure 4.2 presents this component as a function of the x position across the same nine crank angles. At the early crank angles, as the piston descends, the intake jet reaches its maximum value, with a peak velocity of -28 m/s at 285 °bTDC. At this point, a positive velocity is observed at $x = 0$ mm, due to the interaction between the jet that has already impinged on the piston and the jet still entering from the intake valves, as shown in Figure 4.1. As the crank angle progresses, the velocity magnitude in the z direction decreases and becomes positive on the intake side of the cylinder near BDC, where the rotating motion becomes more dominant. At this stage, the flow at this location shows two counter-rotating mean velocity fields, indicated by the positive W velocity (around 2 m/s) in the center of the cylinder at 180 °bTDC, along with a negative velocity (nearly -5 m/s) at the two x -axis extremes ($x = \pm 25$ mm).

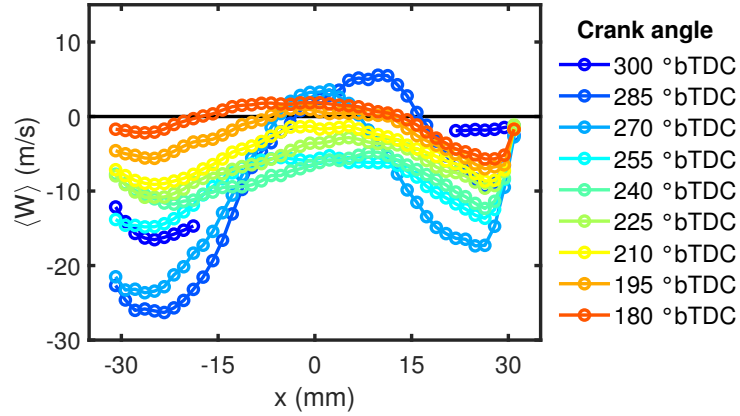


Figure 4.2: Ensemble-averaged W velocity component over 150 cycles as a function of the x position at $z = -20$ mm, measured from 300° to 180 °bTDC in the VC configuration.

Figure 4.3 shows the magnitude of the ensemble-averaged velocity in the x - y directions at the $z = -7.5$ mm plane for four crank angles (ranging from 195 to 180 °bTDC). In the measured velocity fields, the piston is near BDC, and the intake valves are still open. The intake jets from both valves converge along the symmetry plane at $y = 0$, resulting in a velocity magnitude exceeding 9 m/s at 195 °bTDC. As the crank angle increases, this high velocity magnitude decreases in this plane, dropping from over 9 m/s to around 4 m/s in just 15°. At BDC, the flow also begins to deviate from symmetry, with an overall positive value appearing in $\langle V \rangle$.

The ensemble-averaged x -component velocity is evaluated at $x = 0$ mm. Figure 4.4 illustrates the evolution of the ensemble-averaged x component of the velocity field as a function of

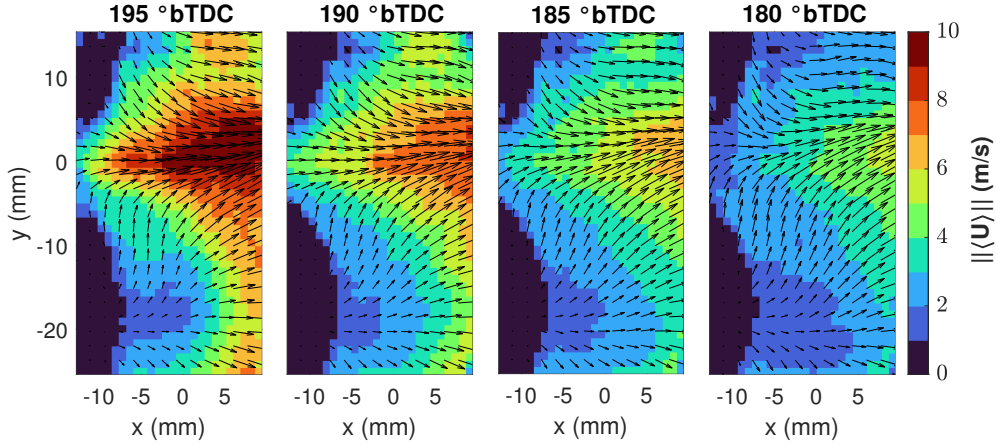


Figure 4.3: Ensemble-averaged velocity components in the x and y directions (U and V , respectively) of the in-cylinder flow over 150 cycles, measured using high-speed PIV in the HCC configuration. Measurements are for four crank angles: 195, 190, 185, and 180 °bTDC.

crank angle at the end of the intake stroke. At 195 °bTDC, the U velocity is nearly symmetric at $y = 0$ mm, with a maximum of 8 m/s and a minimum of 2 m/s at both x extrema, 10 mm away from the center. This graph also highlights the significant decrease in air velocity entering the cylinder as the piston approaches BDC, with a reduction of about 60% of the maximum, or approximately 2 m/s for every 5° of crank angle. This explains the difference in intensity between the early and late intake jets and their interaction throughout the engine cycle, as well as how this difference affects tumble formation, which finally occurs only when the piston reaches the bottom of the stroke. The minimum value of 2 m/s at $y < -10$ mm is maintained constant during these four crank angles.

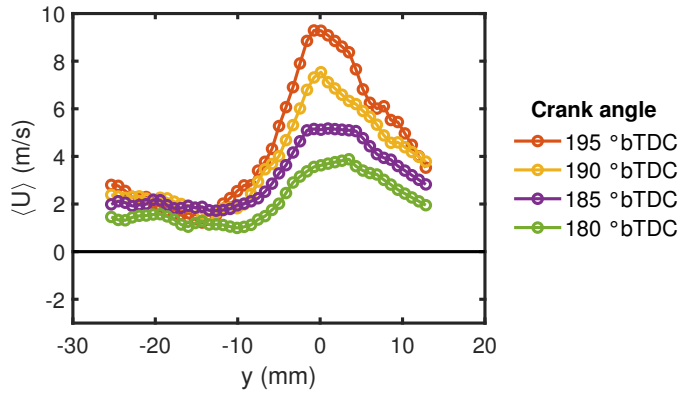


Figure 4.4: Ensemble-averaged U velocity component over 150 cycles as a function of the y position at $x = 0$ mm, measured from 195° to 180 °bTDC in the HCC configuration.

To understand the variability of the flow across the entire measured domain and at multiple crank angles using the Reynolds Decomposition method, Figure 4.5 is presented. It illustrates the ensemble-averaged velocity magnitude (and its directions), the magnitude of the turbulence intensity (i.e., the standard deviation of each velocity component), and the ratio between these two magnitudes for four crank angles: 270, 240, 210, and 180 °bTDC. These crank angles are selected to highlight different stages of the intake stroke. The first shows the early intake jet

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entering the cylinder, the second illustrates the jet impinging on the wall and piston, forming two interaction zones, the third demonstrates the point where the later intake jet becomes less dominant than the earlier impinged jet, and the fourth shows the beginning of tumble motion at the end of the intake stroke, with a mean rotation center at the bottom left of the cylinder. As previously discussed, the ensemble-averaged velocity captures the distinct phases of the engine cycle, emphasizing the large-scale motion. During the intake stroke, velocity magnitudes vary significantly, with values two to three times greater in the early intake stroke compared to the rest of the cycle.

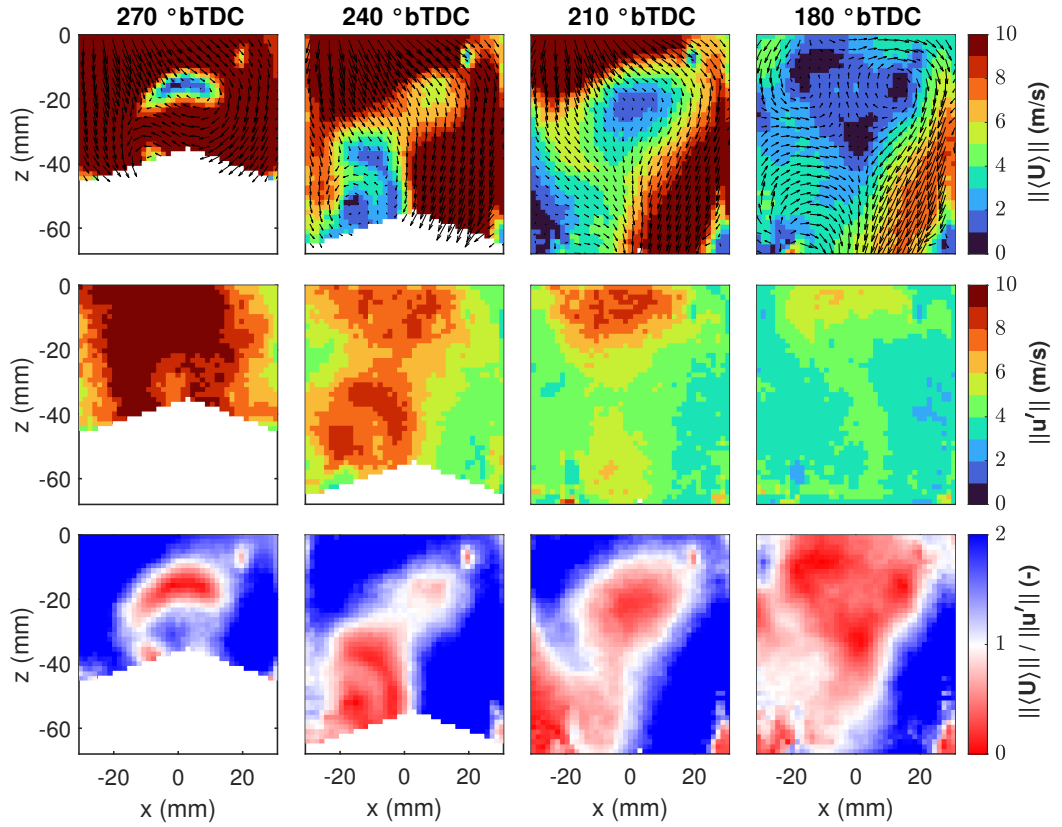


Figure 4.5: Ensemble-averaged velocity in the x and w directions (first row), turbulent intensity magnitude, $\sqrt{u'^2 + w'^2}$ (second row), and mean-to-turbulence ratio (third row) at four crank angles during the intake stroke: 270, 240, 210, and 180 °bTDC, in the VC configuration.

Analyzing flow variability in the second row of the figure, one can observe how this evolves as the cycle progresses. At 270 °bTDC, the flow shows considerable variation, particularly in the center of the cylinder, with turbulence intensities exceeding 10 m/s, primarily due to the intake jet's high variability upon entering the cylinder, as documented in the literature [118, 19, 136]. By 210 °bTDC, turbulence intensity near the intake is around 9–10 m/s, while in the cylinder center, it ranges from 4–5 m/s as the intake velocities weaken. This decreases further at 180 °bTDC, with values generally between 3–4 m/s across the cylinder.

The ratio between the ensemble-averaged velocity and turbulence intensity provides insight into where flow variations are strongest relative to the mean flow. A ratio of 1 indicates that variability is on the same order as the mean flow, while a ratio of 2 or higher (blue) suggests that

the mean flow dominates over fluctuations, indicating a more organized flow. In contrast, a ratio near 0 (red) implies that fluctuations outweigh the mean flow, signifying a turbulence-dominated region. During the early intake stroke, the intake jet velocity dominates the turbulence on the right, left, and bottom parts of the cylinder, showing consistent impingement on the walls and piston. However, where the piston-impinged jet interacts with the intake jet from the valves, a highly turbulent zone appears, characterized by significant cycle-to-cycle flow variation. At 240 °bTDC, this counter-flow zone decreases in intensity and size, and a new interaction zone emerges in the bottom-left corner, where the later intake jet interacts with the earlier jet that impacted the walls and piston. As the piston continues to descend, both counter-flow regions increase in size and in the mean-to-turbulence ratio. Finally, at BDC, a large variable flow zone develops across most of the cylinder, resulting from these interaction zones. This expanded red zone extends diagonally, forming a broad turbulent region, largely due to the low mean velocity magnitude and variation in position of these zones between cycles, as will be further explained.

4.1.2 Compression Stroke

The same analysis is performed for the compression stroke. First, Figure 4.6 shows the mean flow dynamics from 180 to 60 °bTDC in the VC configuration, with measurements taken every 15°. At the beginning of the compression stroke, it is clear that the tumble center is formed in the bottom-left part of the cylinder. From this point onward, the early intake jet follows a more structured path, moving from the right side of the cylinder, traversing the piston, and returning upward on the left side. This jet becomes much more dominant than the intake jet still entering through the intake valves (as the IVC occurs around 120 °bTDC), making the top-left region of the cylinder less turbulent and generally following this large-scale motion, as seen at 165 and 150 °bTDC.

By 135 °bTDC, the two distinct zones - the tumble center at the bottom left and the counter-flow region at the top right - merge into a single tumble center region. As the piston approaches the end of the compression stroke, the tumble center moves upward ($dz/dt > 0$) and rightward ($dx/dt > 0$), while also shrinking in size. Due to limitations in optical access for this configuration, the in-flow measurements are taken only up to 50 °bTDC.

Figure 4.7 displays the z -component of the ensemble-averaged velocity at $z = -20$ mm. At the beginning of the compression stroke, the influence of the intake jet on the overall velocity is visible, along with the two counter-rotating motions, as previously described. As the piston rises, the jet on the negative side of the x -axis intensifies, reaching a peak velocity of about 9 m/s at 90° and 60 °bTDC. On the positive side, the z -component of the ensemble-averaged velocity remains mostly negative, directed toward the piston. This component weakens as compression progresses, and by 60 °bTDC, it turns positive, signaling the onset of tumble motion breakdown.

The flow field during the compression stroke was also measured in the combustion chamber in the x - y plane, as shown in Figure 4.8. As the tumble motion begins to develop and the piston moves upward, the inflow deviates from symmetry, exhibiting a generally stronger positive V component. Thirty degrees later, a flow pattern emerges along the y -axis with a velocity magnitude of around 2 m/s, likely due to counter-flow interactions near this plane during the later phase of intake. From this point through mid-compression, the motion becomes more symmetric, with the velocity magnitude increasing to 5 m/s at $x = -10$ mm, indicating that the tumble front (extending from the intake to the exhaust valves) is reaching the measured plane. At 75° and 60 °bTDC, U continues to increase in magnitude, and a small mean rotating motion

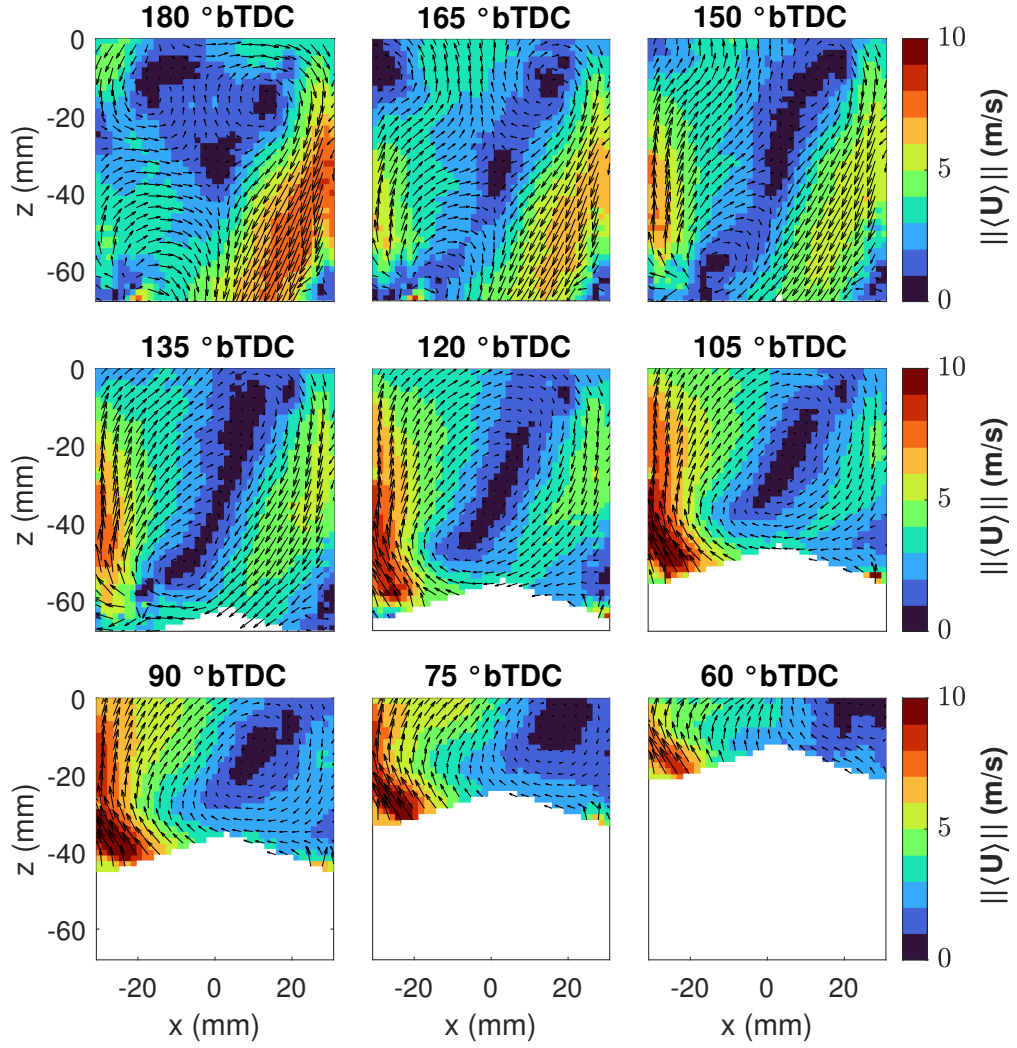


Figure 4.6: Ensemble-averaged velocity components in the x and z directions (U and W , respectively) of the in-cylinder flow during the compression stroke over 150 cycles, measured using high-speed PIV in the VC configuration. Measurements are shown at intervals of 15° , ranging from 180° (upper-left) to 60° bTDC (bottom-right).

with negative z vorticity appears in the lower-right part of the measurement window. Finally, by 30° bTDC, two counter-rotating mean motions form in the lower and upper-right sections of the velocity field (near the exhaust valves), with the large-scale flow slightly shifting away from symmetry towards the positive y direction.

As with the intake stroke, Figure 4.9 shows the ensemble-averaged U velocity component over 150 cycles as a function of the y position at $x = 0$ mm. At 175° bTDC, the velocity reaches a maximum of 1.5 m/s at $y = -20$ mm. From this point, the magnitude begins to increase as the tumble front enters the domain. The U velocity progressively increases and shifts to the positive side of the y -axis between 120° and 60° bTDC, rising from 1.5 m/s at $y = -20$ mm to approximately 4 m/s at $y = 5$ mm. At 60° bTDC, a change of sign is identified on the negative side of the y -axis, where the U component reaches 0 m/s. By 45° bTDC, the velocity

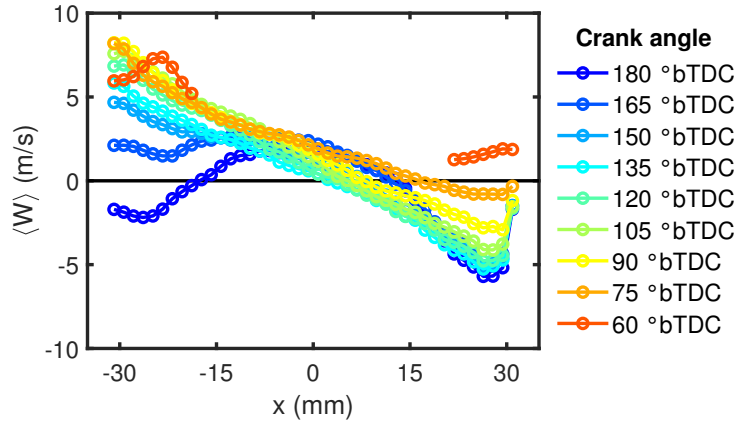


Figure 4.7: Ensemble-averaged W velocity component in the VC configuration over 150 cycles as a function of the x position at $z = -20$ mm, measured from 180 to 60 °bTDC.

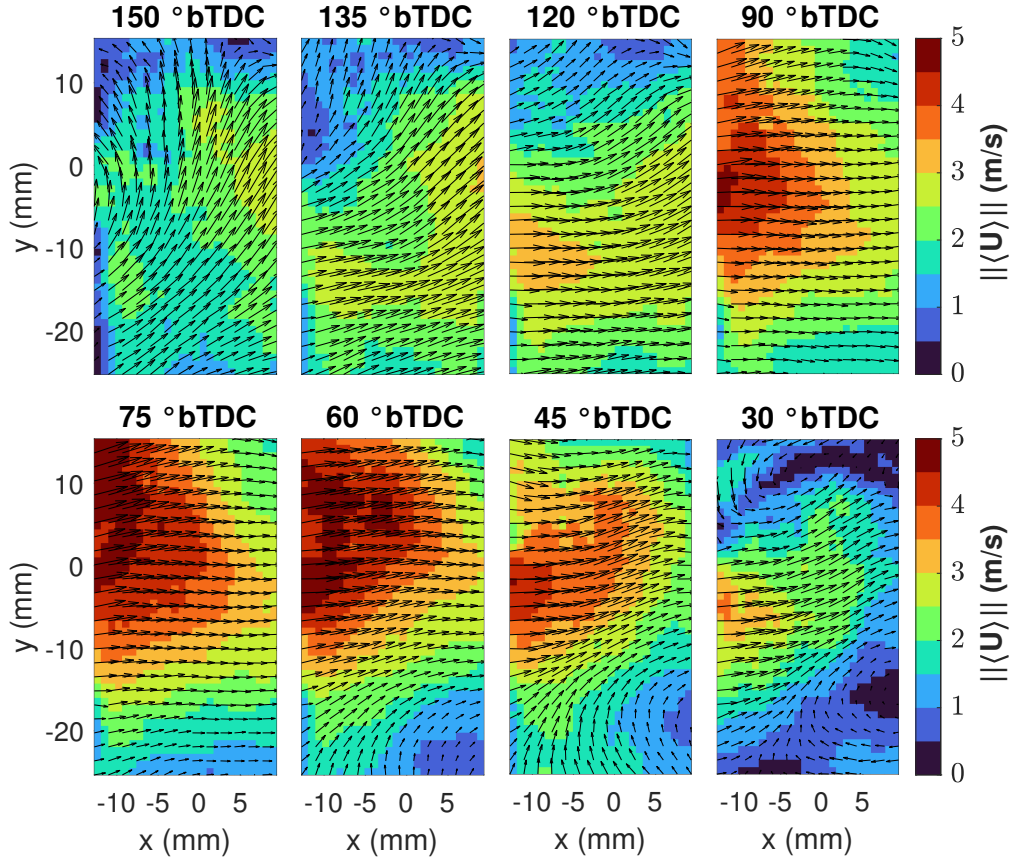


Figure 4.8: Ensemble-averaged velocity components in the x and y directions (U and V , respectively) of the in-cylinder flow over 150 cycles during the compression stroke, measured using high-speed PIV in the HCC configuration. Measurements are shown from 150 (upper-left) to 30 °bTDC (bottom-right).

magnitude decreases slightly, followed by a sharper drop to 2 m/s at $y = 0$ mm at 30 °bTDC. At this stage, the signature of the mean counter-rotating motions are visible on the graph, indicated by negative values of the U component for $y < -15$ mm and $y > 10$ mm.

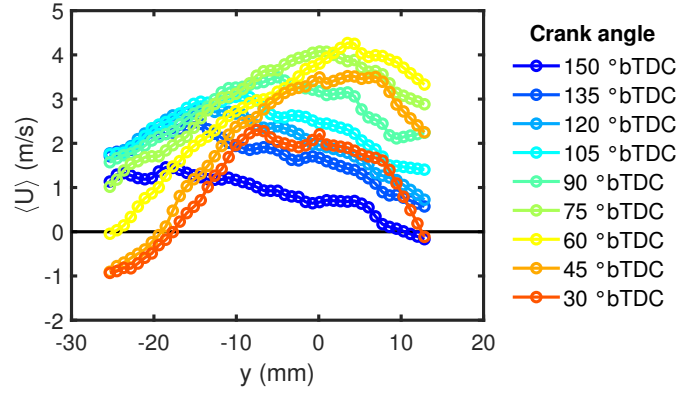


Figure 4.9: Ensemble-averaged U velocity component over 150 cycles as a function of the y position at $x = 0$ mm, measured from 150° to 30° bTDC in the HCC configuration.

Finally, the flow is analyzed in the VCC configuration during the compression stroke, from 146° bTDC to TDC. Figure 4.10 displays the magnitude of the ensemble-averaged velocity in the x and z directions for nine crank angles. In the early compression stroke, the flow is directed toward the intake valves, likely highlighting the backflow of air due to the extended intake valve opening (from 360° to 120° bTDC). At 120° bTDC, the tumble motion begins to form in the combustion chamber, with its velocity increasing and reaching a peak near 46° or 30° bTDC. At this point, the tumble center is located in the bottom-right region of the vertical combustion chamber plane. As the piston moves into the domain, the tumble front passes through the field of view. The mean velocity decreases at the subsequent crank angles (16° and 0° bTDC).

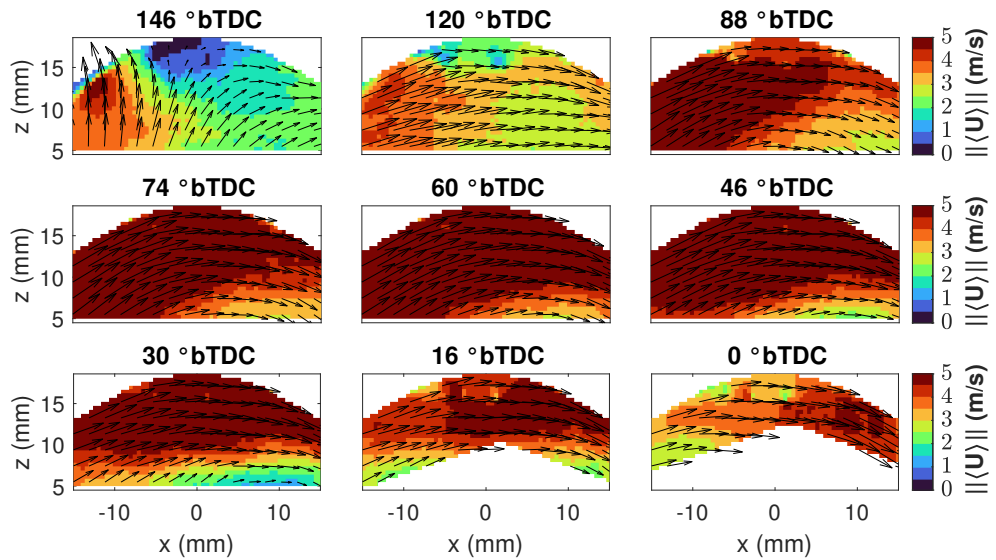


Figure 4.10: Ensemble-averaged velocity components in the x and z directions (U and W , respectively) of the in-cylinder flow during the compression stroke over 150 cycles in the VCC configuration, measured using high-speed PIV in the VC configuration. Measurements are illustrated from 146° (upper-left) to 0° bTDC (bottom-right).

These conditions are also quantitatively assessed at $x = 0$ mm for the $\langle U \rangle$ component in Figure 4.11. As previously discussed, the flow strength increases as the crank angle progresses

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from 146° to 30° bTDC, with the maximum velocity rising from less than 2 m/s to over 6 m/s. Furthermore, the peak velocity is consistently observed at $y = 13$ mm, the location of the spark plug's center electrode. From 30° bTDC to TDC, the ensemble-averaged velocity decreases to 4 m/s, which is desired for the power stroke with the tumble breakdown, converting the ensemble-averaged kinetic energy into turbulent energy to enhance flame speed [155].

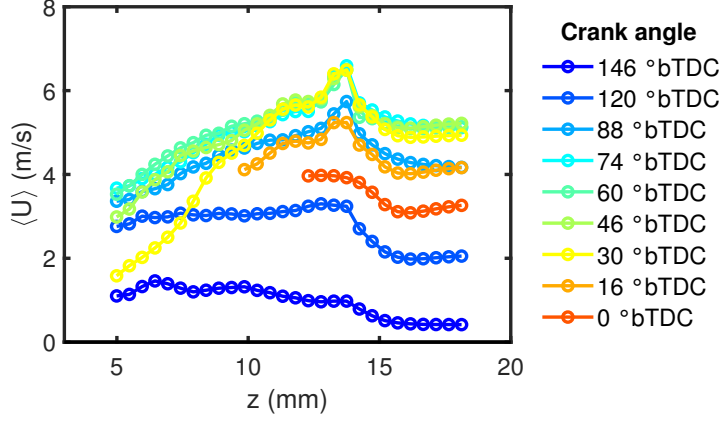


Figure 4.11: Ensemble-averaged U velocity component over 150 cycles as a function of the z position at $x = 0$ mm in the VCC configuration, measured from 146° to 0° bTDC.

The Reynolds Decomposition method is also applied during the compression stroke to analyze flow variability during this phase. Figures 4.12, 4.13, and 4.14 present the ensemble-averaged velocity components (first row), the turbulence intensity magnitude (second row), and the mean-to-turbulence ratio, which indicates whether the flow in a given location is dominated by mean flow or turbulence.

In the VC configuration (Figure 4.12), the tumble structure is clearly formed by 150° bTDC, resulting in a reduction in turbulence intensity to around 2 to 3 m/s compared to 3 to 4 m/s at BDC, with the flow becoming more uniform within the cylinder. As the piston moves upward, the fluctuating velocity magnitudes decrease further, generally converging around 2 m/s, except for a 3 m/s zone near the upper right part of the cylinder at 60° bTDC, where the tumble center is located. Examining the relationship between turbulent intensity, mean flow, and the structured tumble motion, the central part of the cylinder ($z = -30$ mm) displays an organized up-and-down motion, with a mean-to-turbulence ratio of around 2 on both sides of the cylinder. By 120° bTDC, the two interaction zones merge into the tumble center, an area of high variability relative to the mean flow due to low-magnitude velocities, which shifts upward and to the right. In the left region of the cylinder, motion in the positive z -direction, driven by the piston, shows minimal fluctuations. At 90° and 60° bTDC, the region of higher variability shifts and is predominantly found in the upper-right part of the cylinder, where high turbulent velocities and low mean flow are present. In contrast, the left side of the cylinder exhibits a consistently high mean velocity, around 7 m/s, directed upward, following the piston's motion.

The horizontal plane in the combustion chamber (Figure 4.13) also illustrates the variability in the flow field within the field of view (FoV) and how it relates to the mean flow at the four depicted crank angles. From 120° to 60° bTDC, the arrival of the tumble front in the measured plane is visible, accompanied by an increase in the overall U component's magnitude. During this period, the magnitude of u' remains approximately constant across the entire domain, around 2 m/s. At 30° bTDC, as the piston approaches TDC, the emergence of counter-rotating

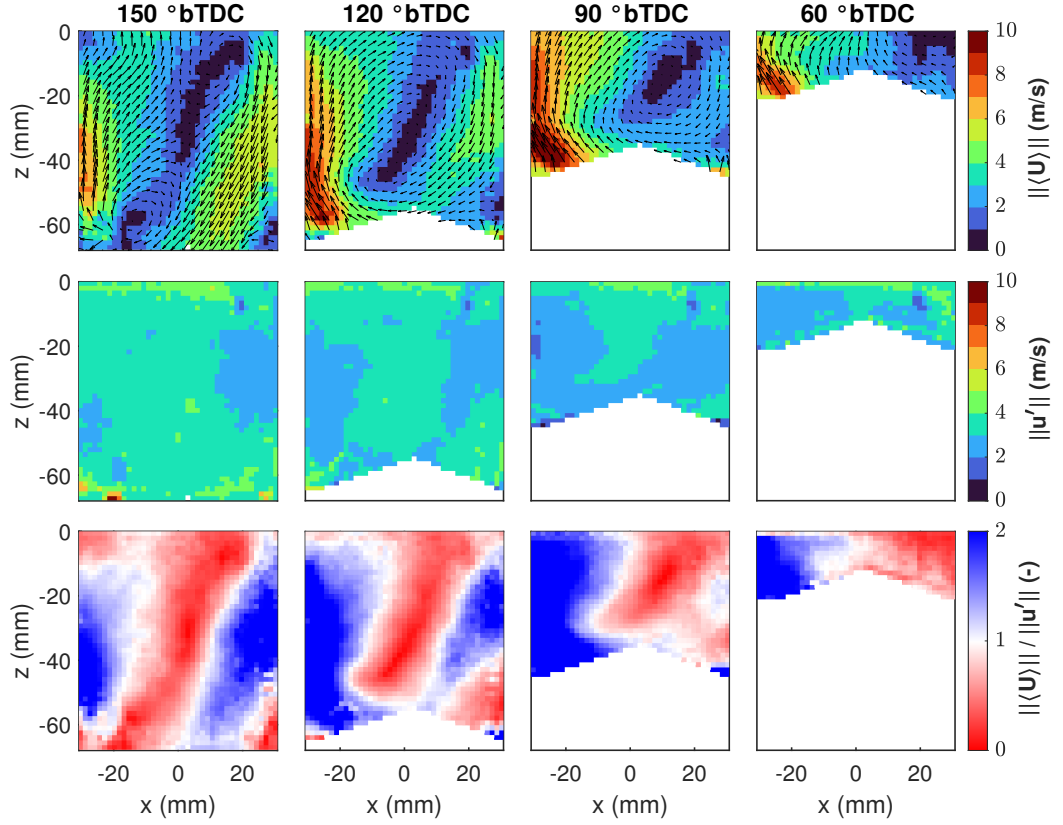


Figure 4.12: Ensemble-averaged velocity in the x and w directions (first row), turbulent intensity magnitude, $\sqrt{u'^2 + w'^2}$ (second row), and mean-to-turbulence ratio (third row) at four crank angles during the compression stroke in the VC configuration: 150, 120, 90, and 60 °bTDC.

motions in the mean flow is noticeable, along with a reduction in mean flow velocity. Simultaneously, the turbulent intensity increases to about 2.5 m/s throughout the domain, indicating the onset of the tumble breakdown phase.

Analyzing the mean-to-turbulence ratio reveals that, at 120 °bTDC, before the tumble flow had fully developed, turbulent zones were present on both sides of the combustion chamber ($y < -20$ mm and $y > 0$ mm). As the tumble front progresses, the flow becomes more symmetric around $y = 0$ mm, with the turbulent zones aligning more closely to this axis. By 30 °bTDC, this turbulent zone consolidates in the center of the chamber, becoming more intense in the core of the counter-rotating vortices. This qualitatively highlights the progression of tumble breakdown occurring within the engine.

The VCC configuration (Figure 4.14) also shows the evolution of variability at four crank angles (138, 88, 30, and 16 °bTDC). Velocity fluctuations range between 3 and 4 m/s across the FoV throughout the cycle, increasing towards the end of the cycle, near TDC. The most variable regions are located near the intake valve at 138 °bTDC and around $z = 6$ mm in the final stage of the compression stroke, with higher variability near the piston bowl when the piston reaches TDC. Furthermore, the fluctuations are more pronounced on the positive side of the x -axis, which aligns with the measurements in the horizontal plane.

Figure 4.15 presents the ensemble-averaged velocity field obtained from three non-simultaneous

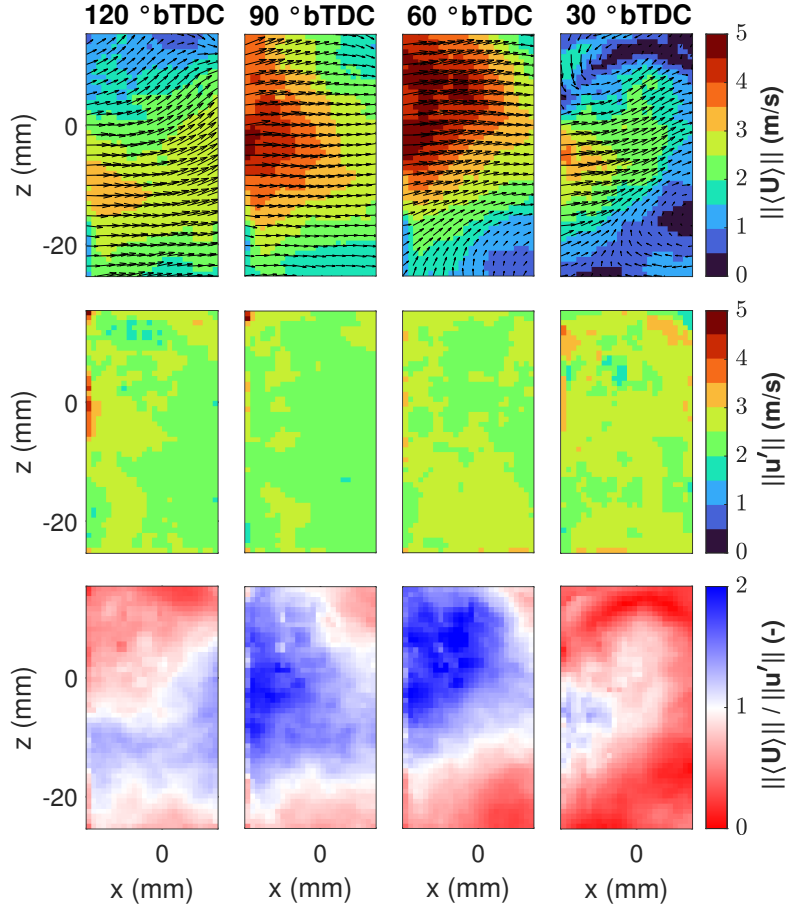


Figure 4.13: Ensemble-averaged velocity in the x and y directions (first row), turbulent intensity magnitude, $\sqrt{u'^2 + v'^2}$ (second row), and mean-to-turbulence ratio (third row) at four crank angles during the compression stroke in the HCC configuration: 120, 90, 60, and 30 °bTDC.

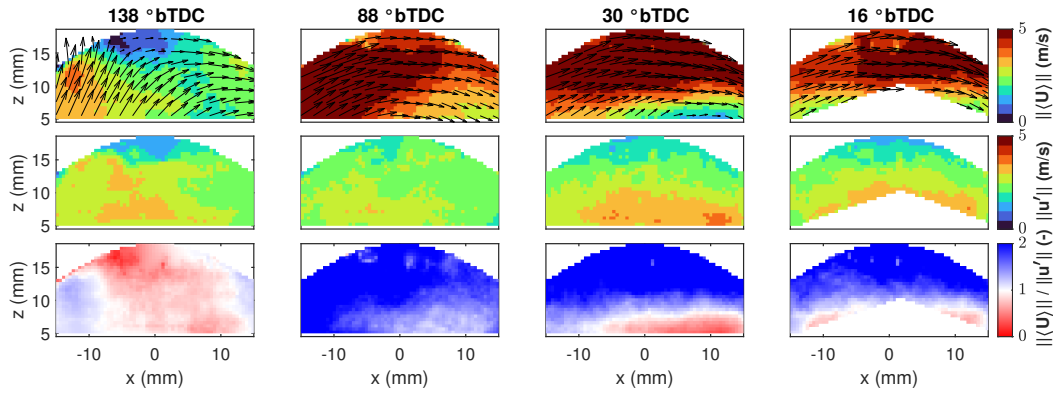


Figure 4.14: Ensemble-averaged velocity in the x and w directions (first row), turbulent intensity magnitude, $\sqrt{u'^2 + w'^2}$ (second row), and mean-to-turbulence ratio (third row) at four crank angles during the compression stroke in the VCC configuration: 138, 88, 30, and 16 °bTDC.

PIV planes during the compression stroke across 10 crank angles. This combination provides an overall view of the large-scale motion and its evolution toward the end of the compression stroke. Additionally, the measured velocity values from the different planes, captured at separate times, demonstrate the consistency and repeatability of the measurements. This is evident in the flow correlation between the VC and VCC configurations (in terms of both direction and magnitude) and in the comparison of the x -direction component between the HCC and VCC configurations, as illustrated at 30 °bTDC. More PIV measurements results are displayed in Appendix C.

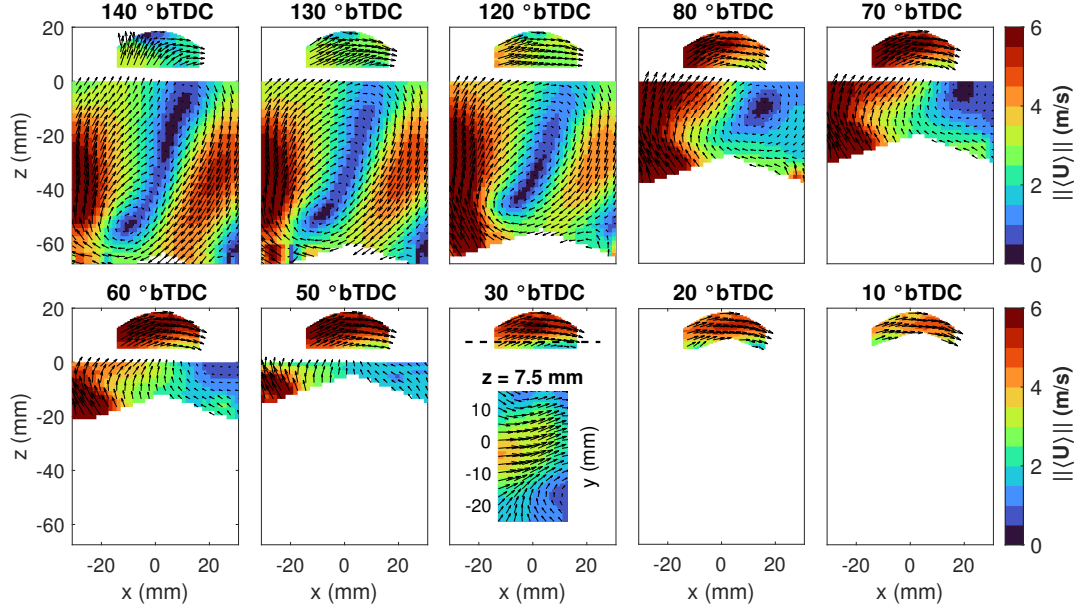


Figure 4.15: Ensemble-averaged velocity magnitude for the VC, VCC and HCC configurations at 0.7 bar intake pressure and 1200 rpm across 10 crank angles.

4.1.3 Kinetic energy analysis

The spatial averaged kinetic energy and the contribution of each component as a function of crank angle in the VC configuration using the Reynolds Decomposition are analyzed in Figure 4.16. Figure 4.16a shows the total kinetic energy (K_{tot}), divided into the sum of the kinetic energy of the ensemble averaged flow (K_{EA}) and the fluctuating, or turbulent, kinetic energy (K_F), as they are orthogonal throughout the cycle. All components exhibit an overall decrease of approximately 10 times, starting from the intake stroke (around $100 \text{ m}^2/\text{s}^2$) to the beginning of the compression stroke (around $10 \text{ m}^2/\text{s}^2$). From the start of the compression stroke to mid-compression, the tumble motion stabilizes, and the total kinetic energy in this plane remains conserved. After 90 °bTDC, the total kinetic energy starts to decrease again, with the ensemble-averaged kinetic energy declining more rapidly, while the fluctuating kinetic energy increases. During the measured crank angles, the energy of the mean flow remains higher than the energy of the fluctuating flow in this plane.

In Figure 4.16b, which compares the contribution of fluctuating kinetic energy to the total kinetic energy as a function of crank angle, it can be seen that at the beginning of the intake

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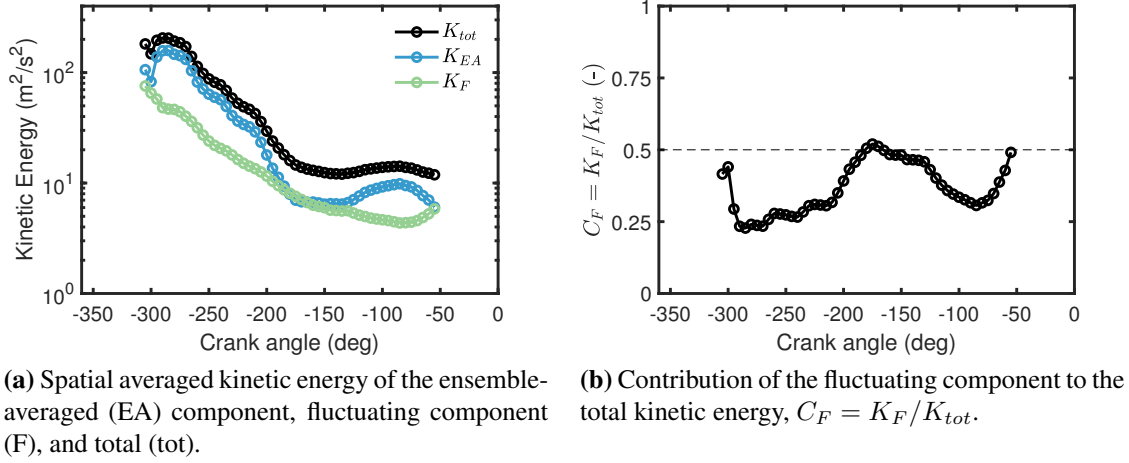


Figure 4.16: Insights into the kinetic energy contributions as a function of crank angle based on the Reynolds Decomposition in the VC configuration.

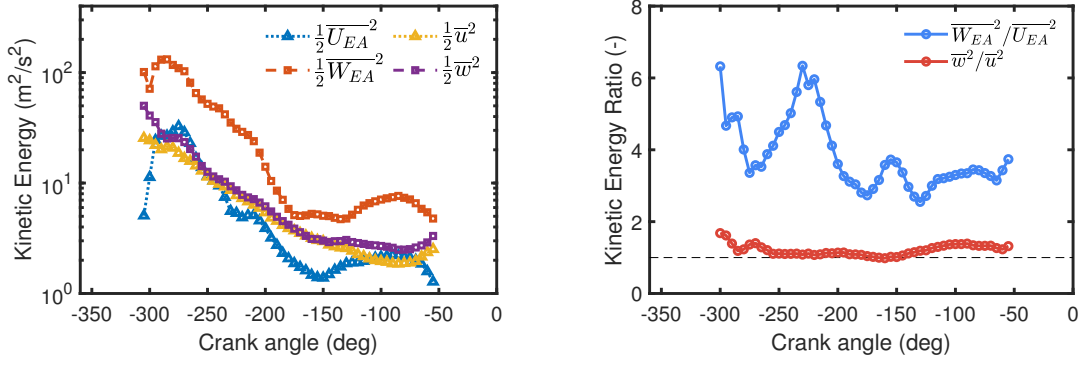
stroke, the ensemble-averaged component has a higher kinetic energy than the fluctuating component. However, both total and ensemble-averaged energy decrease more quickly than the fluctuating energy, leading to the fluctuating contribution reaching 50% at 180 °bTDC. From this point until mid-compression, fluctuations decrease and the large-scale movement becomes more organized, with the fluctuating energy contribution reaching a minimum of 0.3 at -90 °bTDC. Beyond this point, the onset of tumble breakdown becomes apparent, with a rapid decline in ensemble-averaged energy and a corresponding increase in turbulent energy. This shift is reflected in the contribution curve, C_F , which shows a sharp rise and eventually surpasses the ensemble-averaged kinetic energy by the end of the measured crank angles (around 50 °bTDC).

The kinetic energy of each component in the x - z cylinder plane is evaluated in Figure 4.17. Figure 4.17a shows that the kinetic energy of both components follow the same overall trend of the magnitude. For the ensemble-averaged components, the W component energy is consistently 4 to 8 times greater than the U component energy across all crank angles. However, the fluctuating components exhibit similar levels of energy in both directions, suggesting that the turbulence is nearly isotropic, meaning it behaves similarly in all directions from a statistical perspective.

Figure 4.17b provides a quantitative comparison of the difference between the components by showing the ratio between the z and x directions. As estimated previously, $K_{W_{EA}}$ mean over the cycle is approximately 4 times greater than $K_{U_{EA}}$. This ratio changes as a function of crank angle, increasing from 3 to 6 during the early intake stroke due to the downward intake jet, decreasing from 220 °bTDC to BDC to a minimum of 2.5, and then oscillating around 3 from BDC to 120 °bTDC. It slightly increases again until mid-compression before decreasing due to rising fluctuations. Additionally, the ratio of K_w to K_u remains close to unity during all crank angles, with a maximum difference of 38% occurring at 90 °bTDC.

The energy of each velocity component in the HCC plane is displayed in Figure 4.18. In the first measured crank angles, when the intake valves are wide open, the kinetic energy of all components are of the same order of magnitude between 1 and 5 m^2/s^2 . As the crank angle advances, first there is a large-scale flow that starts to take place between 180 and 150 °bTDC with a velocity in the y -axis direction, making the kinetic energy of the $\overline{U_{EA}}$ component decrease

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(a) Spatial averaged kinetic energy of the ensemble-averaged and fluctuating components in the x and z directions. (b) Ratio of the z -direction to x -direction components for both EA and F components.

Figure 4.17: Insight into the kinetic energy contributions of each velocity component as a function of crank angle in the VC configuration.

and from $\overline{V_{EA}}$ increase. Then, around 120 °bTDC, the tumble motion is taken to the combustion chamber, marking the large-scale flow being predominantly in the x -direction. At this point, the KE of ensemble-averaged U component increases to a maximum of $5 \text{ m}^2/\text{s}^2$ at 70 °bTDC while the V component KE decreases to a minimum of $0.07 \text{ m}^2/\text{s}^2$ at 90 °bTDC. From this point on, the flow slightly shifts to the y -direction, making the energy of the y component rise again to a maximum at 50 °bTDC. After this maximum for both EA components, the KE in this plan drops until the last measurable crank angle as it is seen in the VC plane due to the tumble breakdown.

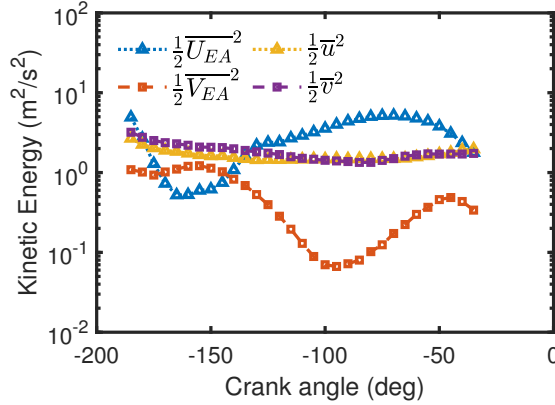


Figure 4.18: Spatial averaged kinetic energy of the ensemble-averaged and fluctuating components in the x and y directions as a function of crank angle in the HCC configuration.

Figure 4.19 shows the kinetic energy for each velocity component using the Reynolds Decomposition method in the VCC configuration, in the x - z plane. During the early compression phase, the development of the tumble motion is indicated by an increase in the kinetic energy of the U_{EA} component, reaching a peak of $100 \text{ m}^2/\text{s}^2$ at 90 °bTDC. After this point, the spatial averaged $K_{U_{EA}}$ decreases slightly. The V_{EA} component shows a KE approximately 10 times lower than the x -axis component, indicating that the flow in the measured plane is primarily along the x -axis. The kinetic energies associated with the fluctuating velocities are similar to

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those in other planes, around $1 \text{ m}^2/\text{s}^2$ during the compression stroke. These values increase slightly from 50 to 25 °bTDC before decreasing again.

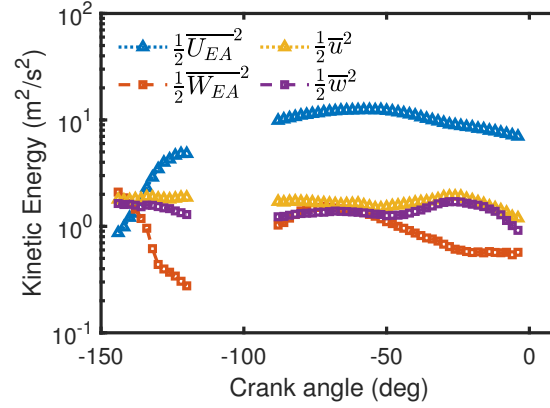


Figure 4.19: Spatial averaged kinetic energy of the ensemble-averaged and fluctuating components in the x and z directions as a function of crank angle in the VCC configuration.

4.1.4 Turbulence characterization

The main turbulence characteristics calculated in this subsection are the turbulence intensity and the integral length scale. The turbulence intensity is calculated in the three directions with two non simultaneous PIV at the same line, which is defined by: $y = -7.5 \text{ mm}$ and $z = 7.5 \text{ mm}$. Furthermore, the mean value in the x line between -10 and 10 mm is proposed in Figure 4.20. The turbulent intensities are proposed as a function of the crank angle at the end of the compression stroke. The error bars are computed with the uncertainty in the PIV vector calculations from Huang et al. [130].

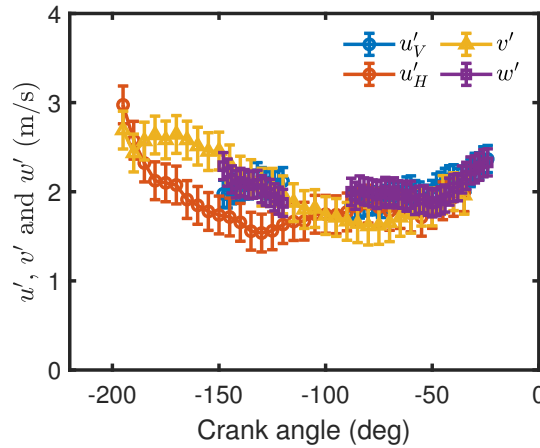


Figure 4.20: Turbulence intensities in the three directions as a function of crank angle calculated with the VCC and HCC configuration over the intersection line. Error-bars characterize measurement uncertainty.

The turbulent intensity in all three directions showed similar values, fluctuating around 3 m/s at BDC (from the HCC configuration). These values decrease during the compression phase, reaching 1.7 m/s at 50°bTDC , before increasing again to 2.0 m/s at 30°bTDC . In the VCC

configuration, the turbulent intensity starts at 2.1 m/s at 148 °bTDC, decreases to a minimum of 1.8 m/s at 50 °bTDC, and then rises to 2.3 m/s at 24 °bTDC.

With the fluctuating field, the integral length scales of the PIV velocity fields can be calculated at each crank angle in the VC configuration, as shown in Figure 4.21. The autocorrelation maps, $R_{u,x}$, are computed for both velocity components in both directions using Equation 4.1, considering distances ranging from 0 to 20 mm. The mean autocorrelation values over 150 cycles as a function of the correlation distance, ξ , are illustrated in Figure 4.21a for 1200 rpm and 0.7 bar of intake pressure at 170 °bTDC. As expected, the autocorrelation decreases with increasing distance. The longitudinal correlations, $R_{u,x}$ and $R_{w,z}$, are similar, while the transverse correlations, $R_{u,z}$ and $R_{w,x}$, are weaker—a well-documented behavior in the literature [118, 156].

$$R_{u,x}(\xi) = \left\langle \frac{u(x, y) \cdot u(x + \xi, y)}{u^2(x, y)} \right\rangle \quad (4.1)$$

The integral length scale is obtained by integrating the autocorrelation function up to its first zero-crossing point (Equation 4.2). Figure 4.21b presents the integral length scales computed for each autocorrelation as a function of the crank angle. Consistent with Figure 4.21a, the longitudinal and transverse length scales are close to each other, indicating a near-isotropic flow behavior. However, the longitudinal length scales remain larger than the transverse ones throughout the cycle. From intake to BDC, all four length scales remain relatively constant before increasing up to approximately 100 °bTDC. At this point, the transverse integral length scales reach a peak of 6 mm, while $L_{w,z}$ reaches 14 mm. In contrast, $L_{u,x}$ reaches its maximum value earlier, around 140 °bTDC, at approximately 12 mm. This earlier peak is likely due to changes in domain size and the influence of the piston's V-shape on the autocorrelation function in the x direction. After these peaks, the integral length scales gradually decrease, with all values dropping below 5 mm by 50 °bTDC.

$$L_{u,x} = \int_0^{\xi^*} R_{u,x}(\xi) d\xi ; R_{u,x}(\xi^*) = 0 \quad (4.2)$$

4.2 Effects of intake pressure and engine speed

Six conditions were compared, involving two intake pressure values and three engine speeds. Figure 4.22 illustrates the in-cylinder airflow at four crank angles, organized by rows. The columns reflect changes in engine speed (from 1200 to 1500 rpm), followed by changes in intake pressure (from 0.7 to 0.9 bar).

With an increase in engine speed, it becomes evident that during the early intake phase, the piston speed influences the intake jet speed near both sides of the cylinder wall, as well as the velocity of the jet that impinges on the piston and moves upward to interact with the remaining intake air. At 210 °bTDC, a much stronger jet with higher velocity is observed on the right side of the cylinder. This jet evolves into a more robust tumble motion, which is visible in the last two crank angles. Additionally, the tumble center is located higher and closer to the cylinder wall near the exhaust valve, creating even stronger flow at TDC inside the combustion chamber. When intake pressure is increased at 1500 rpm during the early intake stroke, it does not significantly alter the behavior of the intake jet along the cylinder walls but does result in

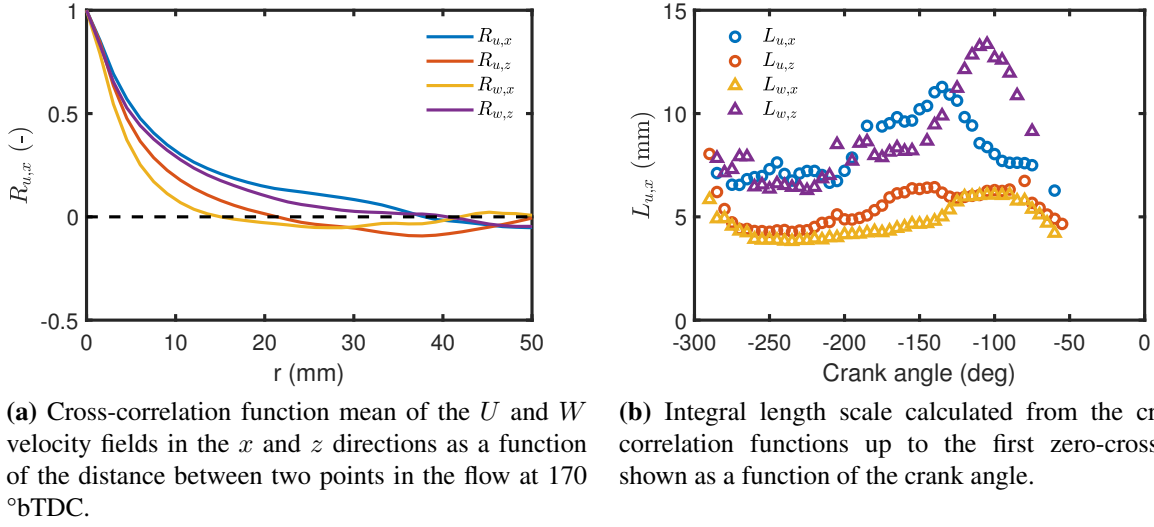


Figure 4.21: Calculation of the integral length scale in the VC configuration.

a stronger impinged jet at $z = -30$ mm. Beyond this point, no clear effect of intake pressure is observed on the ensemble-averaged velocity field.

The z -direction EA velocity is compared at $z = -20$ mm for the same four crank angles across all six cases. Figure 4.23 illustrates the effects of both intake pressure and engine speed. The first notable observation is that engine speed greatly influences the flow within the cylinder, both during the early intake stroke - where a faster downward-moving piston results in higher air velocity near the cylinder walls - and during the mid-compression phase, where the tumble front exhibits higher velocity at increased engine speeds. Additionally, changes in intake pressure did not significantly affect W_{EA} , indicating that engine speed primarily dictates changes in the mean flow.

When normalizing the left-side jet velocity during the intake stroke by the piston speed, all cases show a consistent value of around 7. This indicates that engine speed is directly related to the mean intake jet velocity, with the jet moving seven times faster than the downward piston speed at the start of the intake stroke. A similar analysis was conducted for the mid-compression phase, revealing the same pattern: the tumble front velocity is 2.5 times the mean piston speed. This underscores the direct influence of piston speed on the overall flow field.

Figure 4.24 presents the ensemble-averaged velocity component in the z -direction, normalized by the mean piston speed, for two crank angles under all six conditions as a function of the x position. It also shows the spatial mean velocity fluctuation in the x -direction, also normalized by the mean piston speed, as a function of the crank angle. Both Figures (4.24a and 4.24b) illustrate the influence of engine speed on flow characteristics. Under the tested conditions, the flow in this engine is primarily influenced by engine speed, as both the ensemble-averaged and fluctuating velocities, normalized by piston speed, fall along the same curve. Additionally, the tested intake pressures did not affect either flow parameter. Overall, during the intake phase at 270 °bTDC, the intake jet on the left and right sides of the piston reaches 7 and 5 times the mean piston speed, respectively. At mid-compression, the flow on the left side of the cylinder reaches 2.5 times the mean piston speed, as previously discussed. The fluctuating velocity during the intake stroke shows a root mean square value of 1.5 times the mean piston speed, decreasing

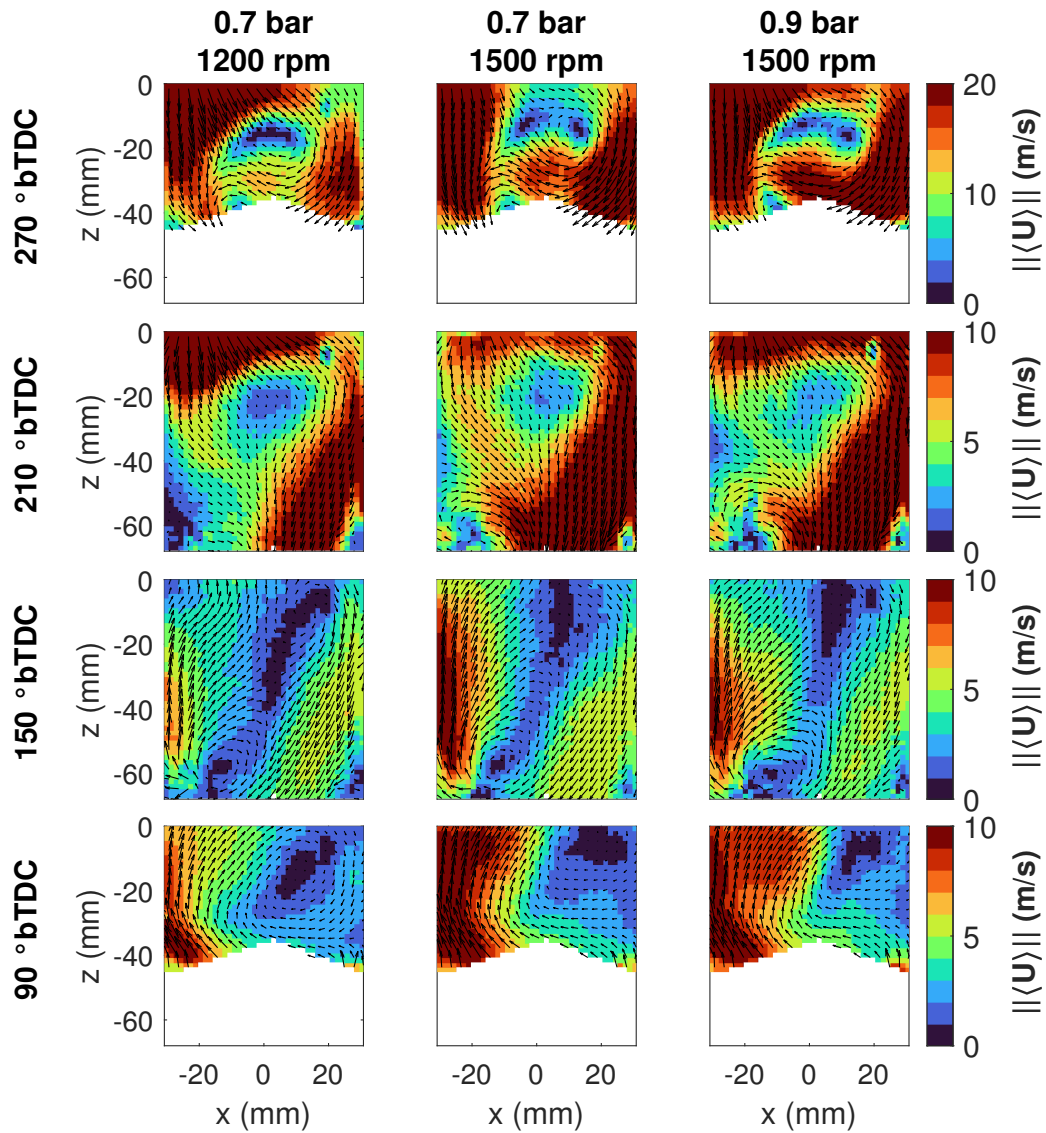


Figure 4.22: Impact of engine speed and intake pressure on the ensemble-averaged velocity field in the VC configuration at four crank angles: 270, 210, 150, and 90 °bTDC.

at the end of the intake and during the compression stroke to 0.5, before increasing again at the final measurement CADs to approximately 0.6. This behavior is consistent across all six conditions.

The same analysis is performed for the VCC configuration in Figure 4.25 with the magnitude of the velocity field normalized by the mean piston speed. The conclusions regarding the effect of intake pressure and engine speed drawn previously also apply here. When the tumble motion forms in the combustion chamber at 60 °bTDC, the flow velocity increases proportionally with the engine speed, from 900 to 1200 rpm, at 0.7 bar intake pressure. This is not the case for earlier crank angles, before mid-compression. The effect of increased intake pressure at 1200 rpm is minimal on the ensemble-averaged velocity at this engine speed. However, an increase in mean velocity in the x direction is observed as engine speed increases from 1200 to 1500

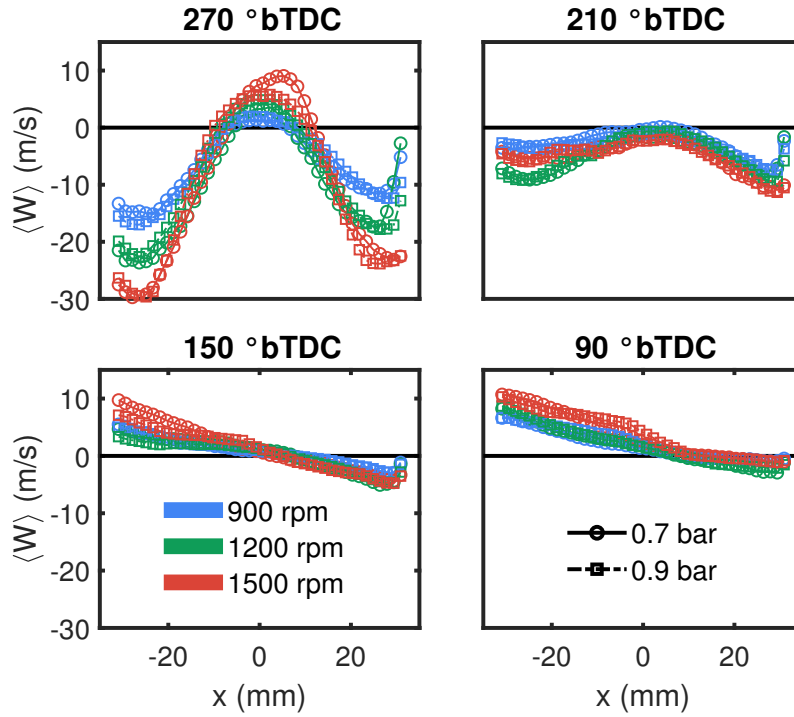
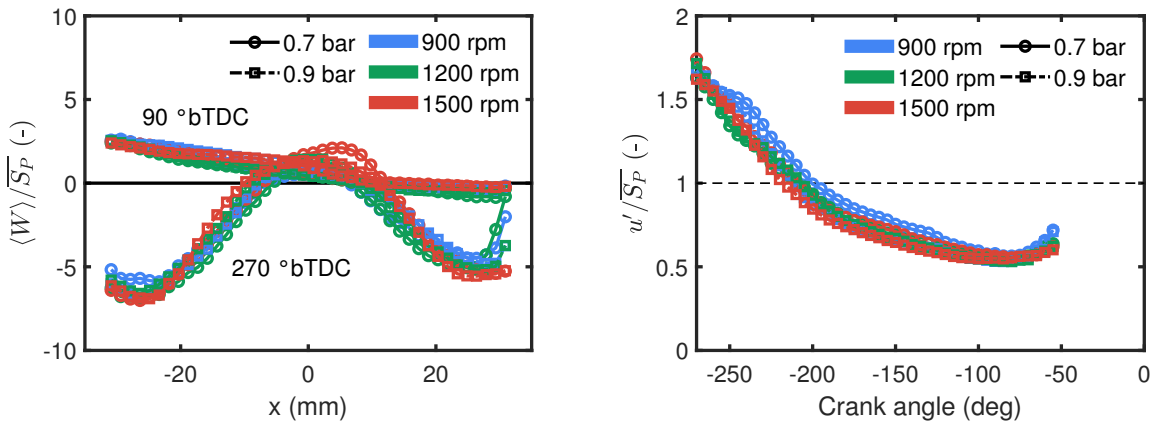


Figure 4.23: W velocity at $x = -20$ mm in the VC configuration for crank angles of 270, 210, 150, and 90 °bTDC, with two intake pressures (0.7 and 0.9 bar) and three engine speeds (900, 1200, and 1500 rpm).



(a) Ensemble-averaged velocity component in the z -direction normalized by the mean piston speed as a function of the x position for all conditions in two crank angles.

(b) Spatial mean velocity fluctuation in the x -direction normalized by the mean piston speed as a function of the crank angle.

Figure 4.24: Ensemble-averaged and fluctuating velocities normalized by the mean piston speed.

rpm at 0.9 bar. Even though small differences can be observed under the different conditions, the impact of the engine speed remain the most important parameter overall.

The quantitative analysis described earlier for the same configuration is repeated here in Figure 4.26. The evaluation of the U_{EA} component of the ensemble-averaged velocity is plotted

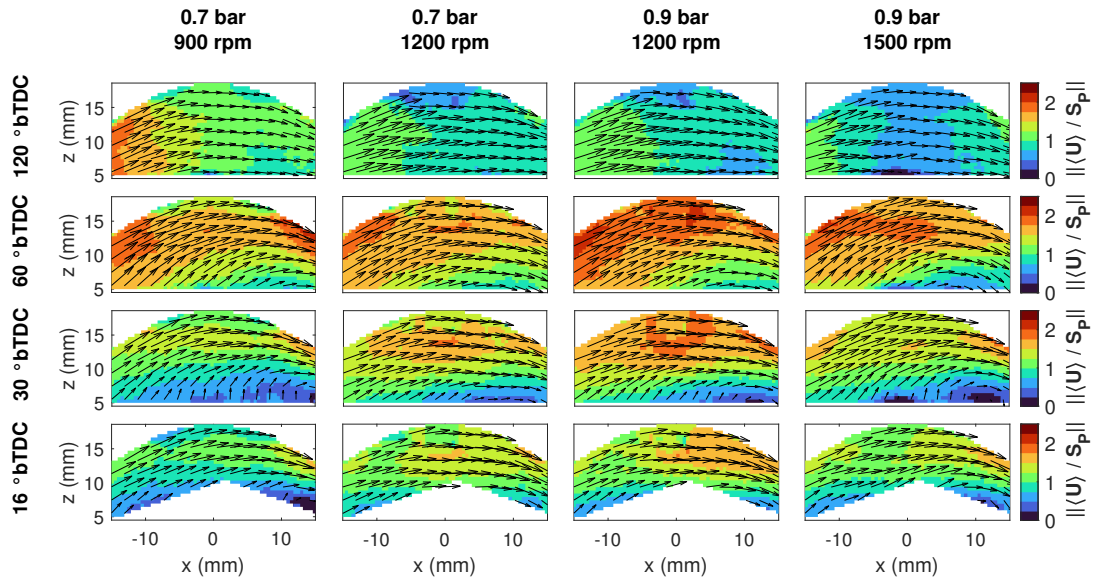


Figure 4.25: Impact of engine speed and intake pressure on the flow field within the combustion chamber in the VCC configuration at four crank angles: 120, 60, 30, and 16 °bTDC.

along the line $x = 0$ mm as a function of y (mm) for the same four crank angles. At 120 °bTDC, the velocity is positive and approximately 3 m/s across all y values for all conditions. By 60 °bTDC, differences between the cases emerge due to the tumble front entering the combustion chamber and the measurement plane. At this point, a clear distinction in mean flow speed is observed based on engine speed, while intake pressure variation has minimal impact. The maximum U_{EA} at 1500 rpm is around 8 m/s, compared to 6 m/s at 1200 rpm and 4 m/s at 900 rpm. After this crank angle, the U_{EA} values for both 1200 and 1500 rpm tend to converge, remaining higher than those at 900 rpm for both 0.7 and 0.9 bar intake pressures.

After analyzing the effects of engine speed and intake pressure on the mean flow, their impact on velocity fluctuations is studied. Figure 4.27 shows the u' and w' values for all cases as a function of the crank angle. All cases exhibit a similar trend in u' , with a maximum at the beginning of the intake stroke, followed by a gradual decrease to about one-third of this value by the mid-compression phase, and then an increase towards the end of the measurements. Additionally, the values of w' closely match those of u' , as indicated by the black points on the line $1 - w'/u'$, which remain near 1 throughout all crank angles. Engine speed also directly affects turbulent intensities, with an increase of approximately 25% from 1200 to 1500 rpm, and a decrease of about 25% when dropping from 1200 to 900 rpm. In contrast, changes in intake pressure did not significantly influence turbulence intensity, similar to what was observed for the mean flow.

The same study is undertaken for the other two configurations in Figure 4.28. Figure 4.28a shows the evolution of u' and v' in the HCC configuration starting at 90 °bTDC. A similar slight increase in turbulence intensity is observed as the piston approaches TDC, as well as the same effects of engine speed and intake pressure. Figure 4.28b, which shows the results for the VCC plane, indicates the same behavior in relation to crank angle and the studied variables. Additionally, in all cases, the turbulence intensity is similar in both directions, a finding that was also confirmed in the single-case analysis with two non-simultaneous PIV measurements taken in the same region. This will be referenced further in this chapter.

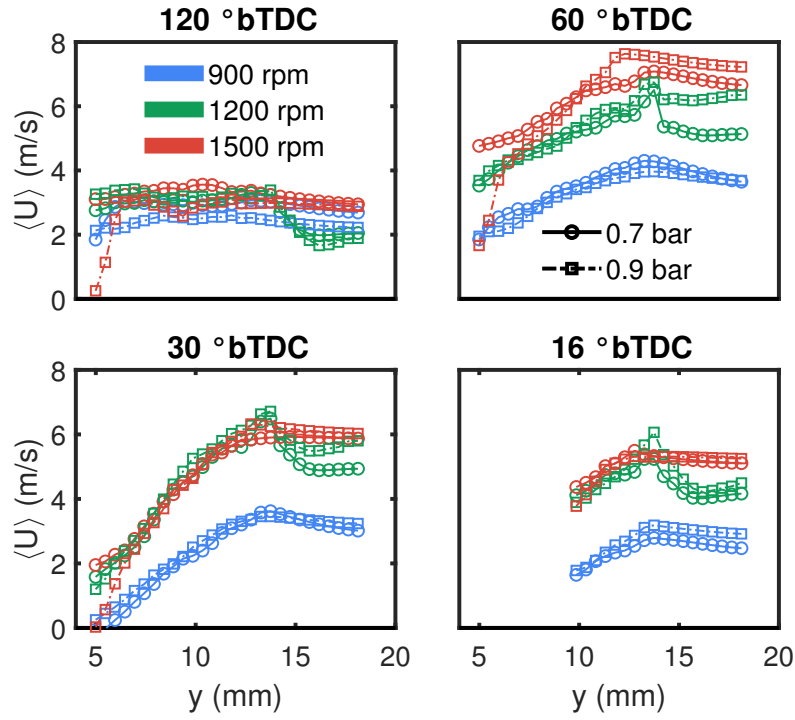


Figure 4.26: U velocity at $x = 0$ mm in the VCC configuration for crank angles of 120, 60, 30, and 16 °bTDC, with two intake pressures (0.7 and 0.9 bar) and three engine speeds (900, 1200, and 1500 rpm).

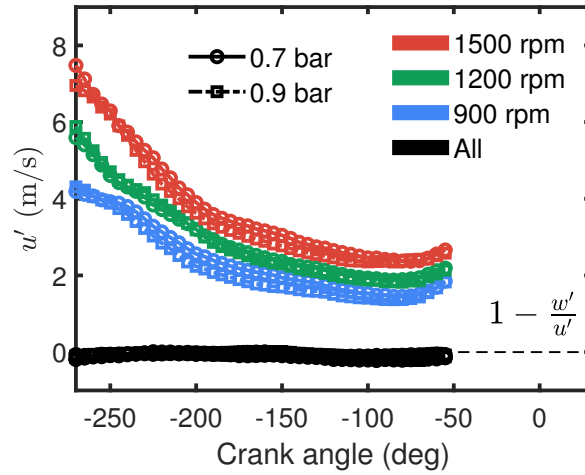


Figure 4.27: Effect of intake pressure and engine speed on u' and w' in the VC configuration.

4.3 Effects of combustion

The effects of combustion were analyzed in the VCC configuration under three operating conditions, both in cold flow (motoring) and hot flow (firing), with a hydrogen/air equivalence ratio of $\phi = 0.40$. The three operating conditions are: 1) $P_{int} = 0.7$ bar and $N = 1200$ rpm; 2) $P_{int} = 0.7$ bar and $N = 1500$ rpm; and 3) $P_{int} = 0.9$ bar and $N = 1500$ rpm. The differences in the flow field due to combustion arise from two main factors. Firstly, when the intake valves

4.3. EFFECTS OF COMBUSTION

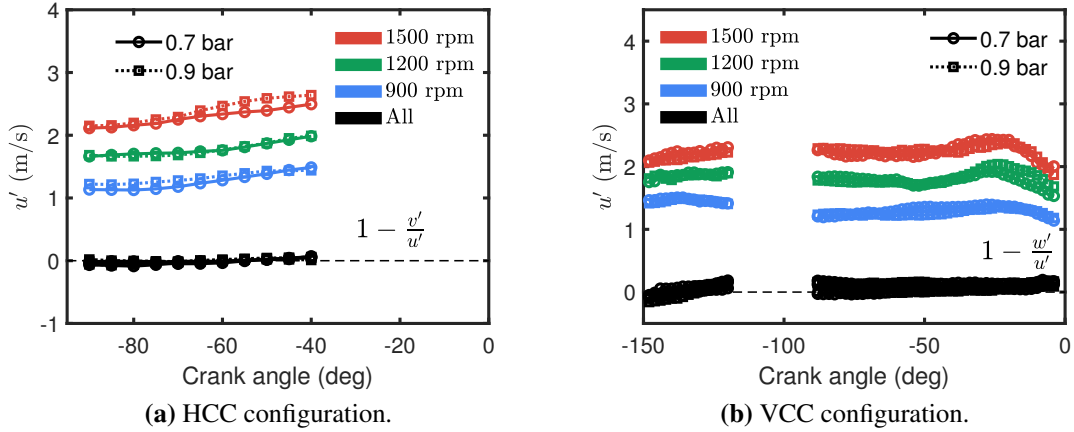


Figure 4.28: Impact of engine speed and intake pressure on turbulent intensities as a function of crank angle.

open, the remaining gases inside the combustion chamber are product gases (and unburned air, given the ultra-lean operating conditions), which have different species and temperatures compared to the motoring condition. Secondly, the mixture entering the cylinder contains about 10% hydrogen by volume, which differs from the full air condition in the motoring reference case. Figure 4.29 shows the effect of combustion on the flow field for the first two operating conditions, also highlighting the effect of engine speed on the velocity results. As previously discussed, the main difference between the two motoring conditions is the strength of the flow field (and tumble front) inside the combustion chamber from mid-compression to TDC. In the fired case, the first condition shows a slightly higher velocity magnitude, especially from 60 °bTDC onwards. However, for the higher engine speed case, the firing cycle has less impact on the flow field, as seen in the ensemble-averaged velocity map.

The U_{EA} magnitude at $x = 0$ mm is plotted at four crank angles for the six operating conditions in Figure 4.30. At 120 °bTDC, all conditions exhibit similar velocity behavior, around 3 m/s across all y positions. At 60 °bTDC, the difference between the motoring and firing cycles is approximately 10%, with the combustion case generally showing a higher velocity magnitude. At 30 and 16 °bTDC, the results are similar, with the main variation due to combustion occurring under the higher intake pressure and engine speed condition, which consistently shows a +2 m/s difference compared to the motoring condition. The first condition performed similarly with and without combustion, as did the second one for $y < 13$ mm.

Finally, the impact of combustion on turbulence intensity for the two extreme conditions (1 and 3) is shown in Figure 4.31, which plots u' as a function of crank angle from 90 °bTDC to 10 °bTDC for both motoring and firing cycles. Throughout the cycle, turbulence intensity under firing conditions shows a slight increase in both cases compared to the motoring condition. This difference becomes more pronounced at the end of the compression stroke, particularly after 40 °bTDC, where the tumble breakdown appears to have a greater effect in the firing case. However, this increase is still within the measurement uncertainty, at least before 20 °bTDC.

4.4. PARAMETERS DEFINITION FOR COMBUSTION ASSESSMENT

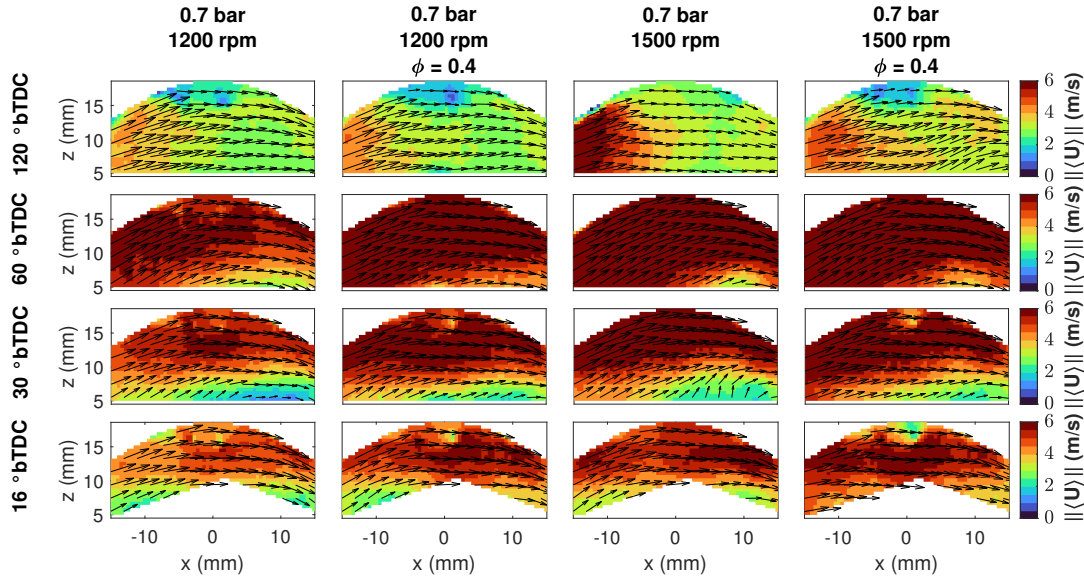


Figure 4.29: Impact of combustion on the flow field within the combustion chamber in the VCC configuration at four crank angles: 120, 60, 30, and 16 °bTDC with an equivalence ratio of 0.4.

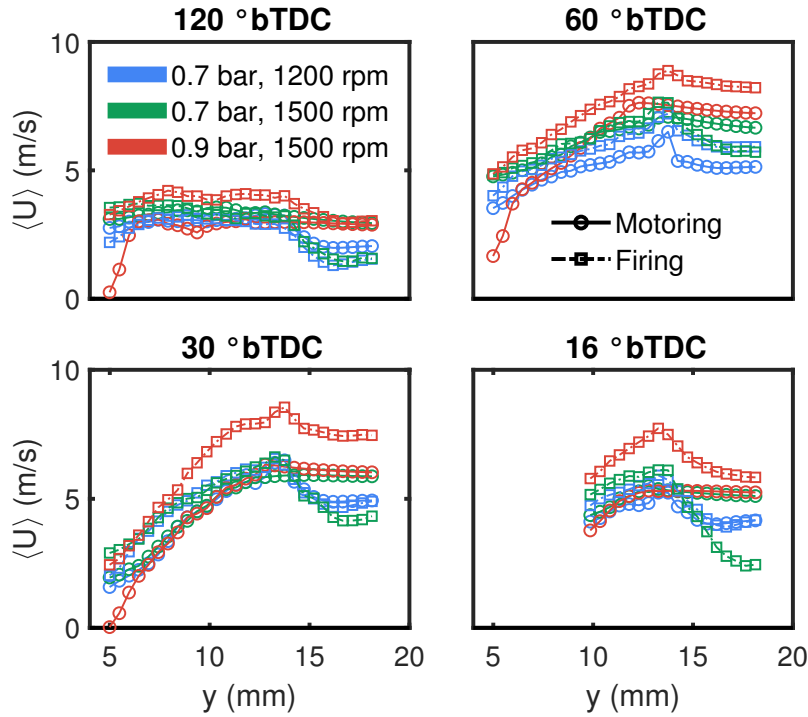


Figure 4.30: Combustion impact on U velocity at $x = 0$ mm in the VCC configuration for crank angles of 120, 60, 30, for three operating conditions.

4.4 Parameters definition for combustion assessment

The last section of this chapter aims to assess turbulence parameters to be used in the turbulent combustion models in the following chapter. The analysis so far has been based on the

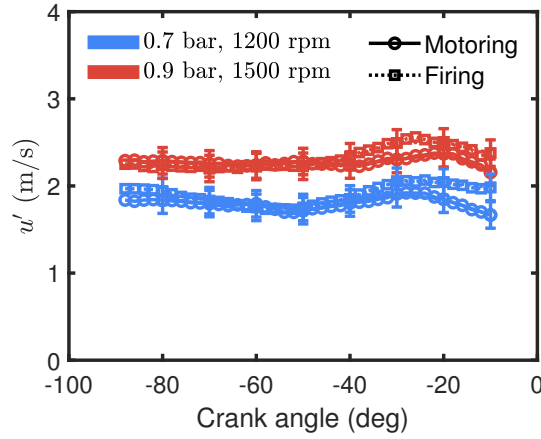


Figure 4.31: Impact of combustion on turbulent intensity as a function of crank angle for two operating conditions in the VCC configuration.

Reynolds Decomposition, which decomposes the flow in an ensemble-averaged velocity and a fluctuating velocity. This fluctuating part takes into account variability in both large-scale and small-scale structures to be part of the turbulence field. Here, Empirical Mode Decomposition is used to differentiate the velocity field fluctuation between a low-frequency fluctuation, which is typically due to large-scale flow changing from one cycle to another, and a high-frequency fluctuation, which is associated to small-scale structures and turbulence behavior [136]. To explore this difference, Figure 4.32 shows the W velocity component at $z = -20$ mm plotted for all measured cycles at a specific crank angle of 120° bTDC at the VC configuration. Three curves are highlighted: the black curve represents the ensemble-averaged velocity and two distinct colored cycles, 45 and 117, are also shown. Additionally, the error bars indicate twice the standard deviation of the velocity at the position.

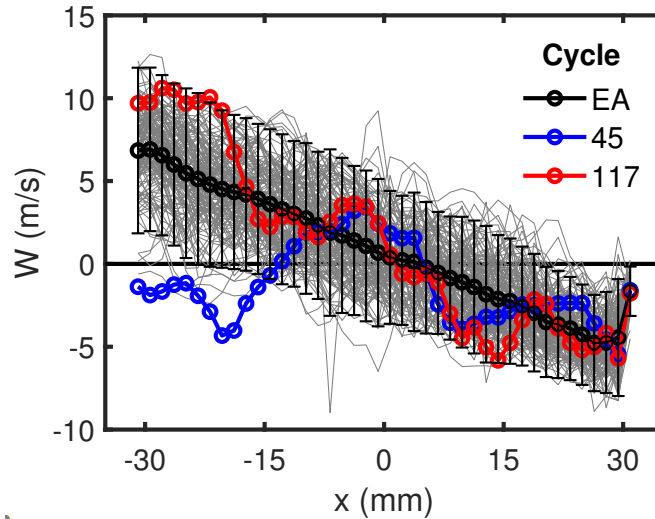


Figure 4.32: W velocity component in the VC configuration for each one of the 150 cycles as a function of the x position at $y = -20$ mm at 120° bTDC. Cycles 45 and 117 are highlighted due to their differing velocities at $x < -20$ mm. The error bars represent twice the standard deviation of the velocity at that position.

4.4. PARAMETERS DEFINITION FOR COMBUSTION ASSESSMENT

The two highlighted cycles exhibit differences from each other and from the ensemble average, particularly on the left side of the cylinder. The ensemble-averaged curve shows a tumble front on the negative side of the x -axis, with velocities around 7 m/s, and -5 m/s on the positive side, indicating a well-defined tumble motion. Cycle 117 shows velocities of about 10 m/s at $x = -25$ to -30 mm and follows a trend similar to the ensemble average from $x = -15$ to $+30$ mm. Cycle 45 also behaves similarly to both the ensemble average and Cycle 117 from $x = -10$ to $+30$ mm. However, on the left side of the cylinder, it exhibits a negative W velocity reaching -5 m/s at $x = -20$ mm, suggesting the absence of a tumble motion in this part of the cycle. Despite these notable differences between the two cycles, overall, the cycles tend to follow the ensemble-averaged trend, and the standard deviation does not seem large enough to significantly alter the large-scale motion between cycles. Further analysis are conducted to confirm this hypothesis.

To further explore cyclic variability, an Empirical Mode Decomposition of the velocity fields was performed, separating the instantaneous velocity into low-frequency and high-frequency components. Figure 4.33 shows the decomposed components for both previously observed extreme cycles (45 and 117) at the same crank angle of 120 °bTDC. From the instantaneous velocity field, it can be seen that the tumble front is stronger and develops more quickly in Cycle 117 compared to Cycle 45. In Cycle 45, the tumble front encounters an opposing flow from the upper-left side of the combustion chamber, a phenomenon already noted in Figure 4.32 with the negative W velocity at $z = -20$ mm. The low-frequency field provides insight into the flow structure. In Cycle 45, the tumble center appears to be established in the lower side of the cylinder, with two zones that seem to be counter-flow regions where the tumble front interacts, and where the high-frequency flow becomes more prominent. In Cycle 117, however, these interaction zones are absent, allowing the tumble to develop more quickly and with greater intensity than in Cycle 45. Additionally, the tumble center in Cycle 117 is located higher in the cylinder and farther to the right, creating a large-scale structure that dominates the entire flow field.

The same analysis for the W velocity component along a line at $z = -20$ mm is shown in Figure 4.34. In Figure 4.34a, the low-frequency components of the velocity for each of the 150 cycles are plotted, highlighting the low-frequency ensemble average (LFEA) along with Cycles 45 and 117. It is evident that the large-scale features of the studied cycles are preserved, enabling an analysis focused on flow structure variability and demonstrating the different development of the tumble within the cycles. At $x = -30$ mm, the probability density function (PDF) of the large-scale velocities in the x and z directions is calculated. The earlier hypothesis, suggesting that the large-scale motion remains consistent between cycles and that variability occurs more in intensity than in flow structure, is validated by Figure 4.34b. A normal PDF is observed in the measured velocities, indicating no bi-modal or other type of distribution in the flow pattern. Thus, the large-scale flow closely follows the ensemble-averaged flow, with a standard deviation that is 30% of the mean tumble front velocity value at this specific crank angle.

Figure 4.35 presents the spatial averaged kinetic energy as a function of crank angle using the EMD method. In this case, since the two velocity components are not uncorrelated, the total kinetic energy is expressed as the sum of the kinetic energy of the low-frequency velocity component (K_{LF}), the high-frequency component (K_{HF}), and the inner product between the low-frequency and high-frequency components (K_{LF-HF}). The K_{LF} closely matches the total kinetic energy at every crank angle, indicating that this component accounts for the majority of

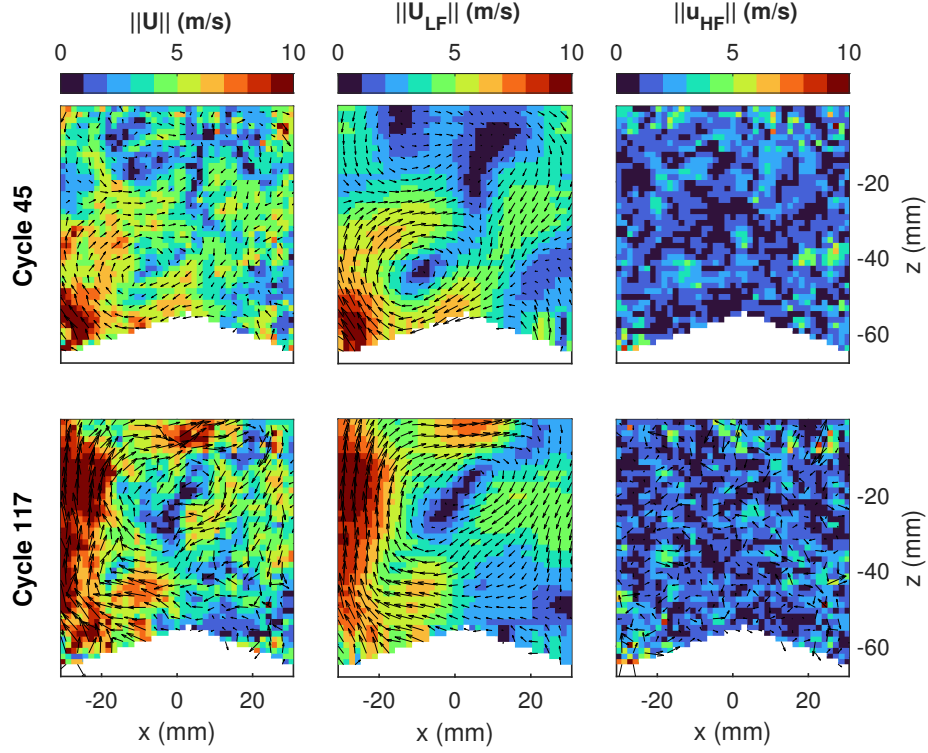


Figure 4.33: Empirical Mode Decomposition analysis of the two extreme cycles (45 and 117) at 120 °bTDC in the VC configuration.

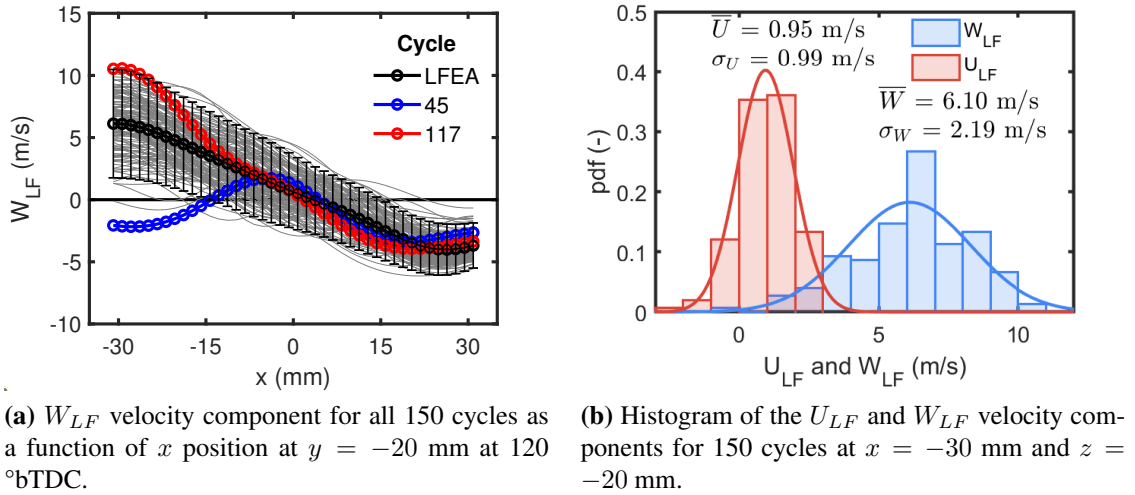


Figure 4.34: Analysis of cyclic variability in the low-frequency velocity field at 120 °bTDC in the VC configuration.

the energy, approximately 90%. The kinetic energy of the high-frequency component is about 10 times lower than that of the low-frequency component. Lastly, the energy representing the correlation between the LF and HF components is 100 times lower than the total kinetic energy. Notably, starting from 90 °bTDC, as also observed in the Reynolds Decomposition graph, the

energy of the high-frequency part of the flow increases while the low-frequency (and total) energy decreases, as it is illustrated in the linear y -axis in Figure 4.35b. This shift results in a greater proportion of the flow's kinetic energy being driven by the high-frequency and turbulent components, as it would be expected in the tumble break down phase [118, 19].

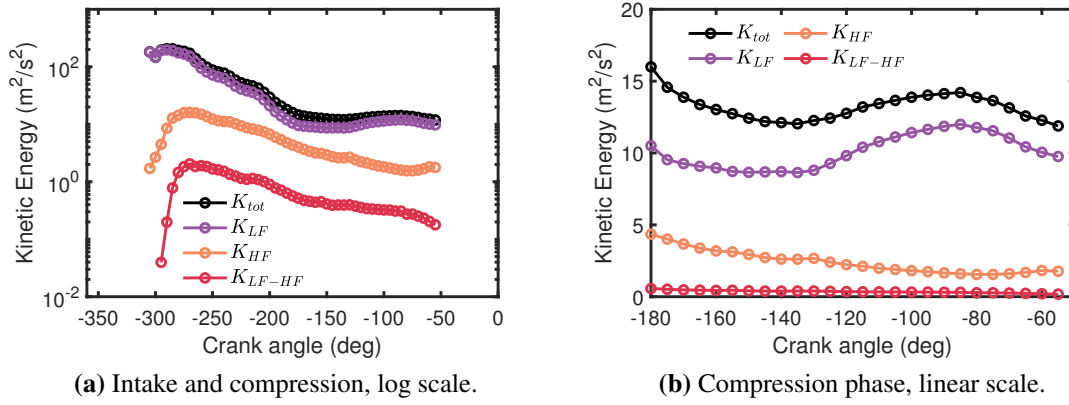


Figure 4.35: Kinetic energy of each component of the EMD in the VC configuration.

The Triple Decomposition method is now applied, breaking down the low-frequency (LF) component into an ensemble average (LFEA) and its fluctuation (CCV). Figure 4.36 presents the velocity magnitude of the Triple Decomposition components (LFEA, CCV, and HF) for each point in the domain across four crank angles. The low-frequency ensemble-average component closely resembles the EA, but it filters out noise caused by reflections and other measurement noises. Consequently, the fluctuating part is split into low-frequency fluctuations and high-frequency fluctuations.

The high-frequency (HF) fluctuations are primarily observed in the intake jet during the intake stroke, and they diminish during the compression stroke, becoming nearly homogeneous with values around 1 m/s throughout the cylinder. In contrast, CCV fluctuations are significant in the counter-flow zone during the early intake phase and remain more prominent in the center of the cylinder than at the sides, where the flow pattern is better defined. By mid-compression, the magnitude of CCV fluctuations becomes more uniform, with values around 2 m/s.

The final row of the figure shows the ratio between LFEA and CCV, highlighting where low-frequency variations dominate over LFEA. This analysis makes it clearer where fluctuations are most significant. Key areas include the interaction zone at the start of the intake stroke and the two counter-flow zones at 210 °bTDC. Additionally, the line formed by the merging of these interaction zones, leading to the creation of the tumble vortex at 150 °bTDC, is clearly visible. Lastly, the location of the tumble center and its upward-right displacement into the right side of the combustion chamber is depicted. The regions of the measured domain where the mean flow is much greater than the variations are also emphasized, providing a clear view of the overall flow pattern inside the cylinder.

The behavior of the kinetic energy of each velocity component as a function of the crank angle and their contribution to the total kinetic energy is examined in Figure 4.37. The kinetic energy calculated from the velocity components shown in the figures are the following: LF (Low-frequency velocity field), LFEA (from the low-frequency ensemble-average), F (fluctuating field in the ReD), CCV (from the low-frequency fluctuating field), HF (high-frequency

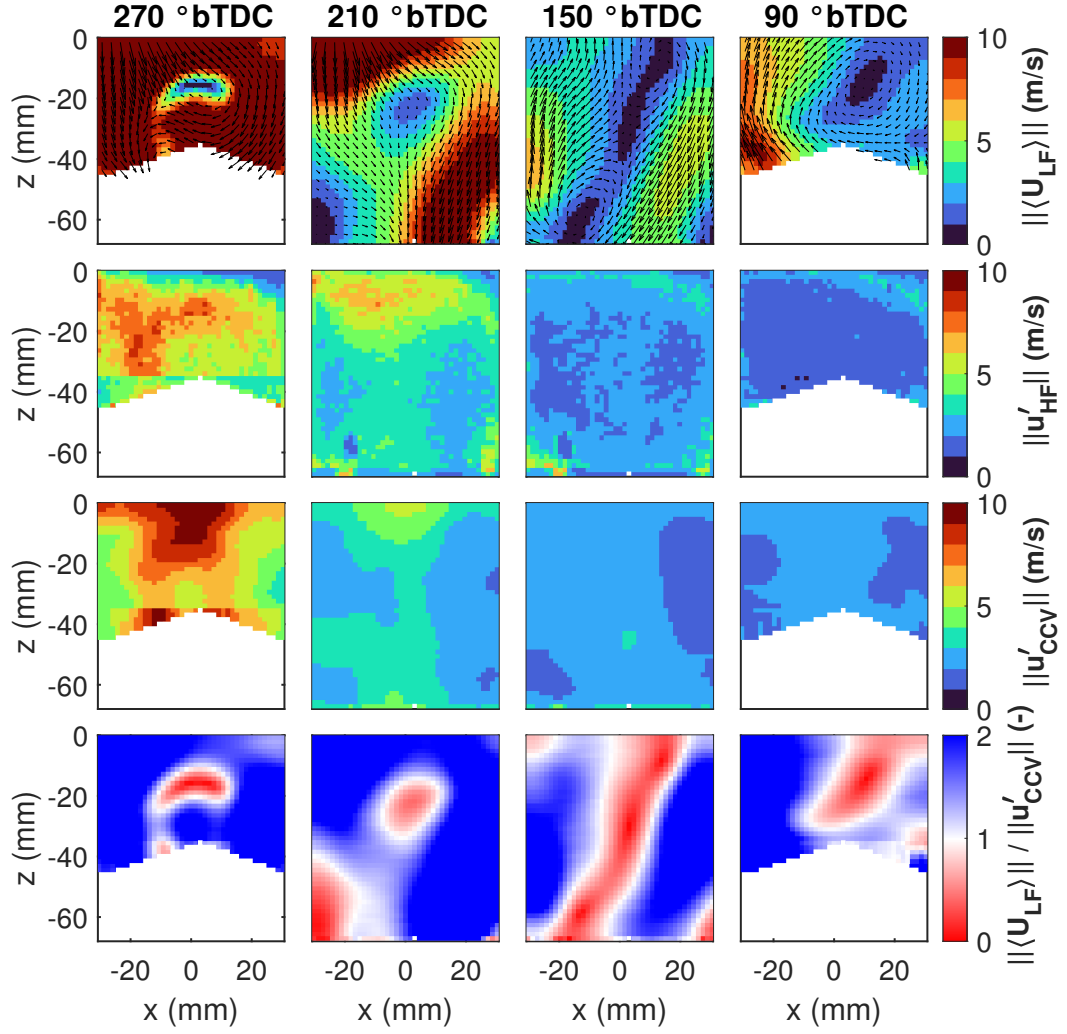
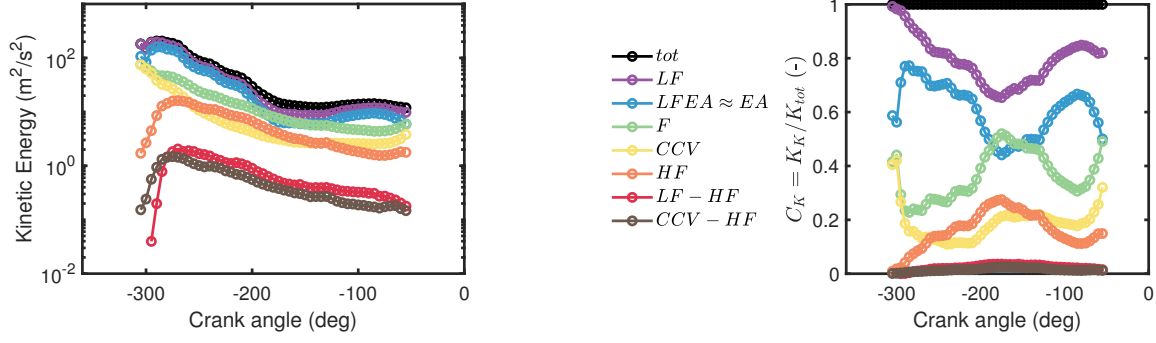


Figure 4.36: Triple Decomposition analysis in the VC configuration: Ensemble-averaged low-frequency (LFEA) velocity magnitude (first row), high-frequency fluctuating velocity turbulence intensity in the x and w directions, $\sqrt{u'^2_{HF} + w'^2_{HF}}$ (second row), low-frequency fluctuating (CCV) velocity turbulence intensity (third row), and the ratio between LFEA and CCV magnitudes (forth row) at four crank angles (270, 210, 150, and 90 °bTDC).

velocity field), LF-HF and CCV-HF (correlations between the LF and HF, and CCV and HF velocity fields, respectively). As mentioned earlier, the kinetic energy of the ensemble-averaged velocity (EA) is similar to the kinetic energy of the low-frequency ensemble-averaged velocity (LFEA), since statistically the mean of the high-frequency field is zero and in practice their difference is much smaller than the correlation values (LF-HF and CCV-HF). The CCV value is higher than that of the HF component, particularly during the early stages of intake and the end of compression, meaning that at the compression phase, variations in the low-frequency motion is greater than that of high-frequency. The kinetic energy from the correlation between the CCV and HF components is even smaller than that of LF and HF.

Analyzing the contribution of each component to the total kinetic energy in Figure 4.37b,



(a) Spatial averaged kinetic energy for each component across all decomposition methods. (b) Contribution of each component, K_K , to the total kinetic energy, K_{tot} .

Figure 4.37: Analysis of kinetic energy contributions from each velocity component for all decomposition methods as a function of crank angle in the VC configuration.

it is clear that the two least significant components are the correlations LF-HF and CCV-HF. These components reach a maximum contribution of 3% and 2% of the total kinetic energy, respectively, at BDC. The largest contributor is the LF component, with an average of 80% of the total kinetic energy. The second-largest contributor is the LFEA, with an average of 60%. Both of these components decrease in kinetic energy as the piston moves down (from 360° to 180 °bTDC) and then increase until 90 °bTDC, after which they both decline.

The fluctuating component, F , behaves inversely to LFEA, as their sum equals the total kinetic energy. This fluctuating velocity is primarily divided between a low-frequency (CCV) and a high-frequency (HF) fluctuation. The HF follows a similar trend to F , but contributes 20% of the total energy compared to 40% for F . The CCV starts the cycle as the more significant component compared to HF, but decreases during the intake stroke, becoming less important than HF at 260 °bTDC. It then remains roughly constant during the compression stroke, but becomes more significant than HF again at 140 °bTDC. From this point, its energy slightly fluctuates, increasing more than HF as the tumble breaks down, and by the end of the measurement, CCV is twice as large as HF (32% and 15%, respectively).

The space averaged longitudinal fluctuation, u' , for both the horizontal and vertical combustion chamber configurations, along with the intersection region (at $y = -7.5$ mm, $z = 7.5$ mm, and $-10 < x < 10$ mm), is divided into a cycle-to-cycle variation component, u'_{CCV} , and a high-frequency component, u'_{HF} . These are plotted as a function of the crank angle. In both configurations, the overall velocity fluctuation of about 2.0 - 2.3 m/s is split into a CCV fluctuation of 1.5 - 2.0 m/s and a HF fluctuation of approximately 1.0 m/s. The HF fluctuation is the component that impacts turbulent flames, as modeled in the LES approach [157].

The influence of engine speed and intake pressure on this fluctuating component is shown in Figure 4.39. The u'_{HF} , normalized by the mean piston speed $\bar{S}_p$, is plotted against the crank angle and reveals that the high-frequency velocity is about 22% of the mean piston speed across all cases. This suggests that intake pressure, within the tested range, does not significantly impact the turbulent velocity, while engine speed has a direct influence. The graph indicates that, for turbulent combustion analysis, the u'_{HF} used in modeling could be $0.20 \cdot \bar{S}_p$, while the fluctuating component (accounting for HF and CCV) is around $0.56 \cdot \bar{S}_p$.

The integral length scale is calculated using the two-point correlation with the high-frequency

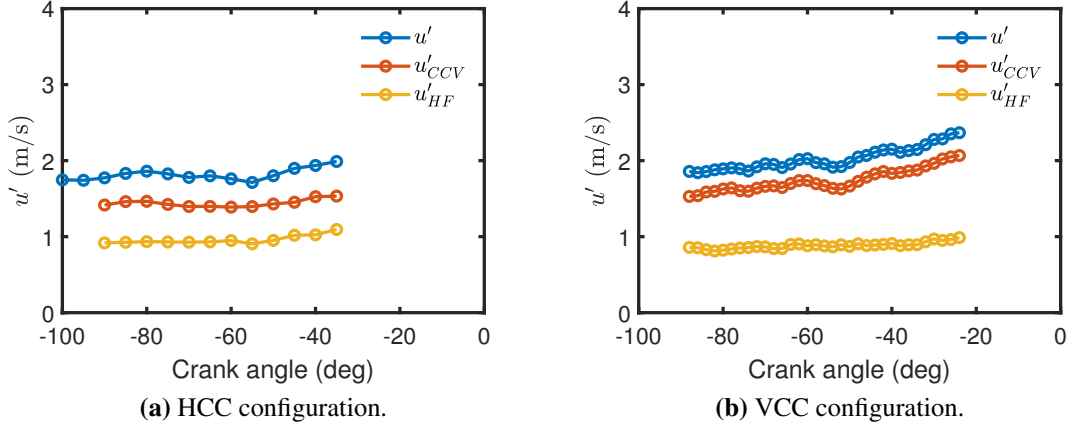


Figure 4.38: Turbulent intensity in the x -direction decomposition into a low frequency (CCV) and a high-frequency (HF) component as a function of the crank angle.

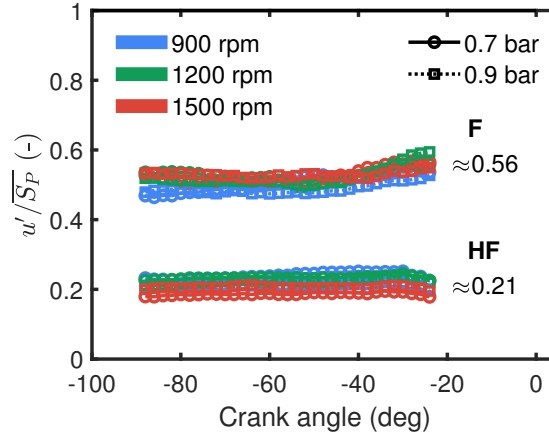


Figure 4.39: High-frequency turbulent intensity normalized by the mean piston speed as a function of the crank angle for three engine speeds and two intake pressures in the VCC configuration.

velocity from the EMD method, u_{HF} . The PIV velocity fields from the VCC and HCC configurations along the intersection line are used to obtain the three components of the integral length scale ($L_{u,x}$, $L_{v,y}$, and $L_{w,z}$). These results are presented in Figure 4.40 as a function of the crank angle. The turbulent scale shows little variation with piston motion during the compression stroke and is similar across all three directions. The mean value across all crank angles and components indicates an integral length scale of approximately 1.5 mm. Since the vectors resolution is 0.49 mm, this value indicates a three vector distance length scale.

Additionally, a study was conducted to evaluate how this value responds to both intake pressure and engine speed, as shown in Figure 4.41. No significant effect was found. Therefore, a constant value of 1.5 mm is selected for all operating conditions.

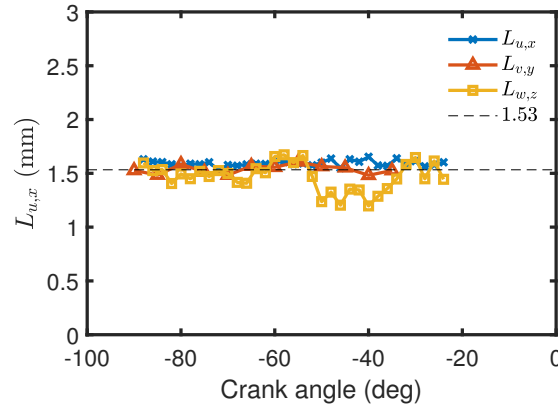


Figure 4.40: The three directions integral length scales calculated in the VCC ($L_{u,x}$ and $L_{w,z}$) and HCC ($L_{v,y}$) configurations over the intersection line as a function of the crank angle.

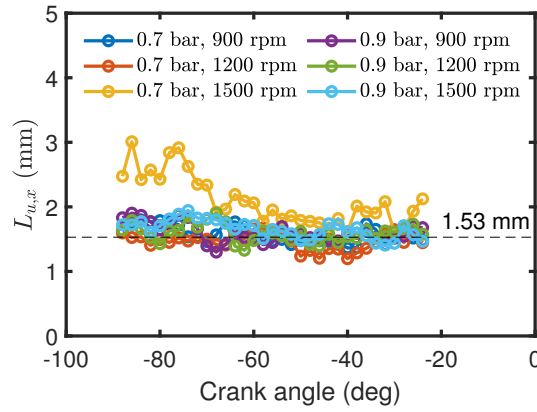


Figure 4.41: Effect of engine speed and intake pressure on the integral length scale of the high-frequency velocity component in the VCC configuration as a function of the crank angle.

Conclusion

The main characteristics of the intake and compression strokes, in terms of both mean flow and variability, were analyzed, revealing the generation and evolution of the tumble motion during the engine cycle until its breakdown phase, which increases turbulence and enhances combustion speed. The kinetic energy from Reynolds Decomposition, Empirical Mode Decomposition, and Triple Decomposition was used to investigate the evolution of each velocity component and the kinetic energy within the combustion chamber. The effects of both engine speed and intake pressure on the flow field were also discussed. Finally, the high-frequency velocity components, which are linked to the turbulence that influences the flame, were studied for use in the following chapters. The high-frequency turbulent velocity was found to be 22% of the mean piston speed in all operating conditions, and the length scale of the high-frequency components was determined to be approximately 1.5 mm, regardless of the conditions. These values will be used for further development.

Chapter 5

In-cylinder flame development

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Introduction

This chapter aims to investigate the development of ultra-lean hydrogen/air flames within the engine during the early flame phase, evaluate their impact on overall performance, and compare them to conventional hydrocarbon fuels. The study begins with a comprehensive analysis of key factors influencing hydrogen combustion, including equivalence ratio, engine speed, intake pressure, and ignition dwell time. Propane/air mixtures are used for comparison due to their well-established combustion characteristics and gaseous phase at normal pressure and temperature conditions. As discussed in Chapter 1, hydrogen/air flames exhibit significantly different behavior based on the equivalence ratio, particularly under ultra-lean conditions, which differ fundamentally from hydrocarbon flames. The laminar flame speed under engine-like conditions is considerably lower than that of stoichiometric propane/air mixtures, while flame thickness is greater, distinguishing the flame’s speed and length scales and potentially affecting the overall combustion behavior. Additionally, covering a wide range of propane/air equivalence ratios help to understand the effect of the Lewis number on the combustion behavior (as it changes from greater than 1 under lean conditions to less than 1 under rich conditions), and the potential impact of thermodiffusive instabilities. By analyzing how these variables impact flame propagation, the goal is to understand their role in enhancing combustion and stability under

ultra-lean conditions. Subsequently, a detailed correlation is established between in-cylinder flame imaging and the heat release analysis from Chapter 3 to assess whether the characteristics observed during the early flame phase can predict the overall combustion heat release. Finally, a turbulent flame correlation is developed based on all tested operating conditions. This correlation is integrated with the heat release analysis and the combustion diagram to provide a comprehensive perspective on hydrogen's potential as a fuel in internal combustion engines.

5.1 Flame Development Comparison: Effects of parameters

In this section, the development of the hydrogen flame within the engine is studied in comparison to propane flames, with variations in several parameters, including equivalence ratio, engine speed, intake pressure, and ignition dwell time.

5.1.1 Equivalence Ratio

The effect of the equivalence ratio on in-cylinder flames is examined for both hydrogen and propane flames under similar thermodynamic conditions at spark timing: an in-cylinder pressure of 10.5 bar and unburned gas temperature of 680 K. Several factors are analyzed and compared between these fuels and their respective equivalence ratios: flame centroid trajectory, equivalent flame radius, equivalent flame speed, flame stretch, and flame circularity.

Figure 5.1 shows the flame centroid path for each equivalence ratio for both propane and hydrogen/air mixtures. The flame generally moves in the positive x -axis direction, indicating it follows the tumble motion, illustrated on the horizontal plane in Figure 4.8. The initial flame center velocity in this direction, for the first measurable crank angle, is 3.1 ± 1.5 m/s for all conditions, which aligns with the 4.0 m/s mean velocity observed at the spark timing in the VCC configuration measurements from the previous chapter, in Figure 4.26.

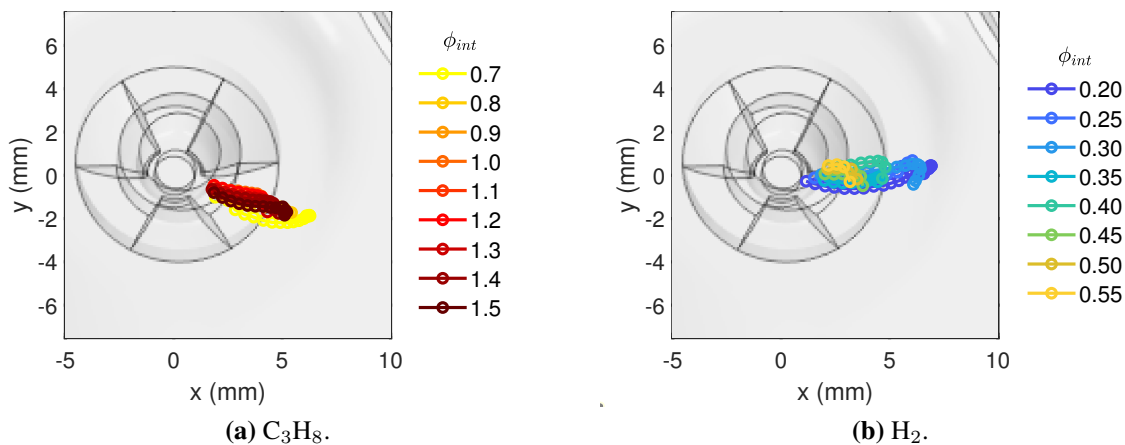


Figure 5.1: Effect of the equivalence ratio on the flame centroid trajectory through the optical piston's view. Each marker represent a crank angle degree.

Additionally, hydrogen flames tend to maintain their position along the y -axis, while propane flames follow a trajectory that moves toward the cylinder's symmetry plane, progressing in the

negative y direction. For both fuels, mixtures closer to stoichiometry show the centroid moving closer to the $y = 0$ position, i.e., the same y -position as the center electrode, compared to richer or leaner mixtures. This suggests that faster flames follow a path with less y displacement. Finally, at the last measurable crank angles, particularly for hydrogen flames, the centroid path curves toward the center of the combustion chamber, likely following the movement of the tumble front as it passes the spark plug, reaches the wall, and moves back down toward the piston.

The equivalent flame surface radius, r_S , calculated from the projected surface as a function of crank angle, is shown in Figure 5.2. For all conditions, the flame growth can be observed as the cycle progresses, with the growth rate varying depending on the equivalence ratio of the mixture. For propane mixtures (Figure 5.2a), as the in-cylinder mixture approaches stoichiometry or becomes slightly richer, the propane/air flame develops more quickly compared to both richer and leaner mixtures, which is in agreement with the laminar burning velocity trend. For instance, a flame radius of 10 mm is reached 8.5 CAD after ignition timing with an intake equivalence ratio of 1.1, compared to 16 CAD and 12.5 CAD for $\phi_{int} = 0.70$ and 1.50, respectively. Furthermore, the faster the flame, the less variability is observed at the same equivalent radius, with standard deviations of 1.31, 1.06, and 1.43 for equivalence ratios of 0.7, 1.1, and 1.5, respectively. The flame variability aspects will be studied in the next Chapter: "Cycle-to-cycle variations".

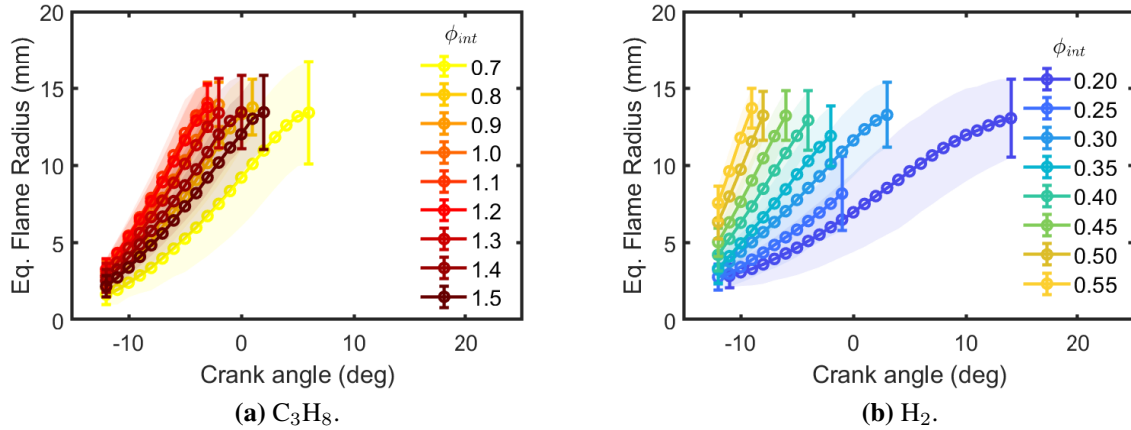


Figure 5.2: Effect of the equivalence ratio on the equivalent flame radius development. The error bars indicate $\pm$ two standard deviations.

For hydrogen (Figure 5.2b), a similar trend is observed. For example, with an equivalence ratio of 0.55, the flame reaches a radius of 10 mm at 11 °bTDC, which is 4 CAD after ignition timing (which is must faster than the stoichiometric C_3H_8 flame), while with an equivalence ratio of 0.20, the flame reaches the same radius only after 20.5 CAD. Additionally, the standard deviation of the radius at a given crank angle increases as the mixture becomes leaner. For these two conditions, the richer mixture shows a standard deviation of 1.17 mm, while the leaner mixture has a value of 1.44 mm, which will be discussed further in the next chapter.

Figure 5.3 presents the laminar flame speed (s_L^0), laminar flame propagation speed (v_L), and expansion ratio (σ) for the studied hydrogen/air and propane/air mixtures at spark timing conditions of pressure and temperature (10.5 bar and 680 K). As previously discussed, as the hydrogen content in the mixture increases on the lean side, both the laminar flame speed and

the propagation speed rise, a behavior observed in engine conditions as well. For propane/air flames, the maximum laminar flame/propagation speed occurs around $\phi = 1.0$ and 1.1, meaning that this flame property highly influences the flame development, as shown in Figure 5.2.

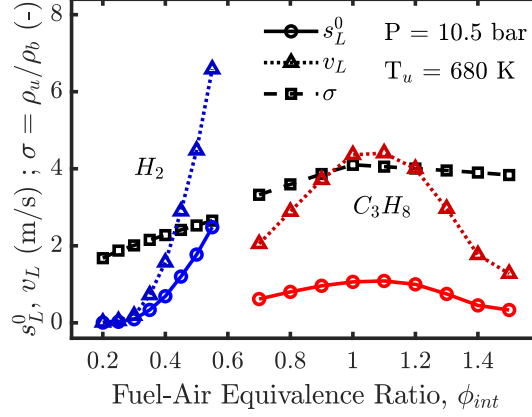


Figure 5.3: Laminar flame speed (s_L^0), laminar flame propagation speed (v_L), and expansion ratio (σ) as a function of the intake equivalence ratio for the studied hydrogen/air and propane/air mixtures at spark timing conditions.

The equivalent flame speed calculated from the derivative of the equivalent flame radius, $v_T = dr_S/dt$, is plotted as a function of the equivalent flame radius for all conditions in Figure 5.4. Figure 5.4a shows the equivalent flame speed of propane flames, which increases similarly across all equivalence ratios during the early flame development phase. The flame speed rises as the equivalence ratio approaches stoichiometry and becomes slightly richer, consistent with the flame radius growth and the laminar flame speed behavior. Specifically, the flame speed varies from 6.60 m/s (at $\phi_{int} = 0.70$) to 10.61 m/s (at $\phi_{int} = 1.10$), representing a 61% increase. This aligns well with the increase in laminar flame speed times the expansion ratio between these two conditions, which rises from 2.12 to 4.50 m/s - a 112% increase. The flame speed variability follows a similar pattern as the radius, with standard deviations between 1.3 and 1.4 m/s for most cases, except for $\phi_{int} = 1.5$, where it reaches 1.58 m/s.

Figure 5.4b illustrates the effect of equivalence ratio changes on the flame speed of ultra-lean hydrogen/air flames. The flame speed increases as the mixture becomes richer, rising from about 4 m/s at an equivalence ratio of 0.2 to 15.6 m/s at $\phi = 0.55$, an increase of approximately 300%. As with propane, this increase in flame speed was expected due to the higher laminar flame speed in mixtures closer to stoichiometry. However, the increase in laminar burning velocity is much greater, with a 295-fold rise, which is not fully reflected in the turbulent flames inside the cylinder.

To understand the effects of laminar flame properties and turbulent intensity on both fuels, Figure 5.5 is presented. This figure shows the ratio of the measured turbulent flame speed ($\rho_b/\rho_u \cdot v_T$) relative to the unstretched laminar flame speed (s_T/s_L), the Damköhler expression outlined in Chapter 3 ($1 + u'/s_L$), and the relative percentage error between them, as a function of the fuel-air equivalence ratio for a given flame radius of 7 mm. For propane flames, s_T/s_L ranges from 5 (at richer mixtures) to 2.2 (at stoichiometric conditions), indicating that the turbulent flame can be 2 to 5 times faster than the corresponding laminar flame. For hydrogen flames, similar trends are observed at higher equivalence ratios (0.40 to 0.55), with s_T/s_L varying from 5.5 to 2.3. At leaner mixtures, due to low flame speeds predicted by 0D/1D Cantera simulations

5.1. FLAME DEVELOPMENT COMPARISON: EFFECTS OF PARAMETERS

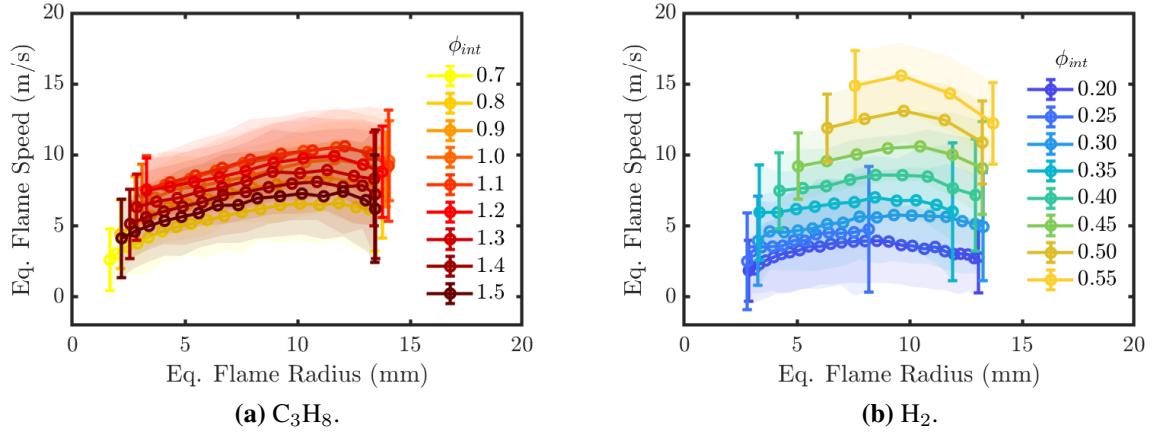


Figure 5.4: Effect of the equivalence ratio on the equivalent flame speed. The error bars indicate $\pm$ two standard deviations.

but significant speeds observed experimentally, the turbulent enhancement can reach as high as 300 at $\phi_{int} = 0.20$, highlighting the impact of turbulence on flame speed.

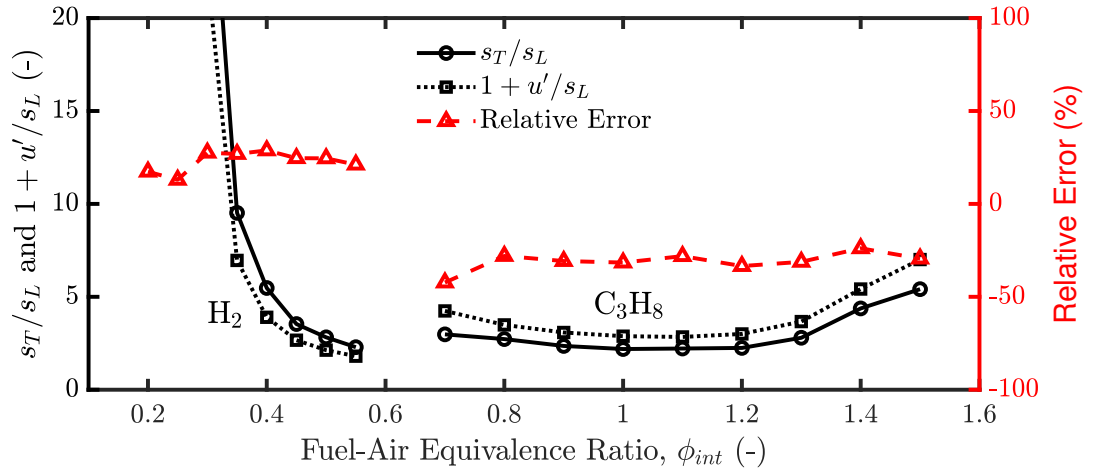


Figure 5.5: The ratio between the measured turbulent flame speed with regards to the unburned gas and the unstretched laminar flame speed (s_T/s_L), the Damköhler like expression relating turbulent fluctuations ($1 + u'/s_L$) and the relative error in percentage between them both, regarding the s_T/s_L , as a function of the fuel-air equivalence ratio for both hydrogen/air and propane/air mixtures at $r_S = 7$ mm.

The Damköhler expression, relating turbulent flame speed to the product of laminar flame speed and the term $1 + u'/s_L$, is also plotted and aligns well with the observed enhancement trends. This suggests that the expression can indicate flame speed trends for both fuels under the tested conditions. The relative error between the measured flame speed and the modeled speed using turbulent intensity and laminar flame speed remains consistent across conditions. For hydrogen/air mixtures, the error is approximately +25%, indicating the Damköhler model underpredicts the flame speed, potentially due to stronger turbulence effects or additional properties such as flame instability. For propane/air mixtures, the error is around -30%, implying that the calculated flame speed exceeds the measured speed, possibly due to a reduced influence

of turbulence or counteracting effects present in propane combustion at these conditions.

Another interesting variable to be studied is the equivalent flame stretch rate, which is defined as the derivative of the flame surface area divided by the surface area, measuring the amount of flame surface stretch due to curvature and the outer velocity strain. This parameter calculation assumes the stretch that would be experienced by a sphere that is developing, $2/R \cdot dr_S/dt$. This variable is shown in Figure 5.6 as a function of the equivalent flame radius for all equivalence ratio mixtures.

Figure 5.6a illustrates that for propane flames, the stretch rate decreases as the flame radius increases, which aligns with the increase in flame surface area, by which the strain is normalized. The initial decrease is non-linear, but beyond a flame radius of about 7 mm, the decrease becomes linear in all cases, with the same slope. For a flame radius of 3 mm, the stretch rate ranges from a minimum of 2500 s^{-1} to a maximum of 4700 s^{-1} for equivalence ratios of 0.7 and 1.1, respectively. At a radius of 10 mm, this difference narrows, with stretch rates ranging from 1500 to 2200 s^{-1} . The 700 s^{-1} difference remains roughly constant between 7 mm and 13 mm, values that align with known results for well-studied fuels in an in-cylinder environment in the literature [158].

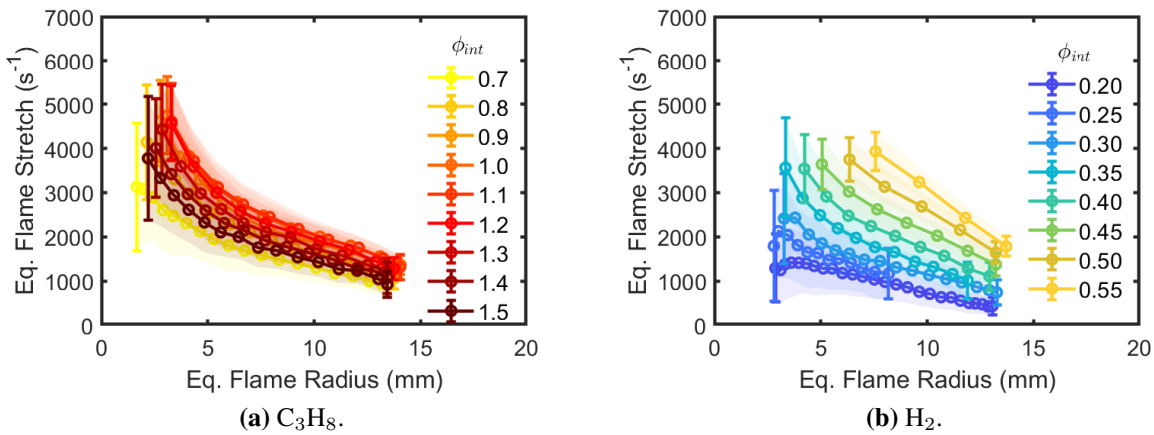


Figure 5.6: Effect of the equivalence ratio on the stretch rate as a function of the flame radius.

For hydrogen flames (Figure 5.6b), a similar trend is observed, with some small differences. As seen with propane, faster hydrogen flames exhibit a higher stretch rate at a given radius, as expected from the calculation. The early flame development, up to a radius of 7 mm, is non-linear, but it becomes linear beyond that point. However, unlike propane, the slope of the linear region varies depending on the equivalence ratio; faster flames exhibit a steeper slope. At a 7 mm radius, the stretch rate ranges from 1000 s^{-1} ($\phi_{int} = 0.20$) to 4000 s^{-1} ($\phi_{int} = 0.55$), and from 300 s^{-1} to 2200 s^{-1} at a radius of 13 mm. This reduces the difference in stretch rate from 3000 s^{-1} to 1900 s^{-1} over a 6 mm radius increase. Additionally, for both fuels, the variability in stretch rate decreases as the flame radius grows. This indicates that higher variability occurs during the initial flame formation phase, and as the flame develops, the stretch rate becomes more self-sustained and predictable.

However, as shown by Brequigny et al. [159], analyzing the stretch as a function of flame radius under engine conditions effectively represents the flame speed. The previous figure indicates that the flame speed (and flame stretch) of hydrogen/air mixtures differ more significantly from one another than those of propane/air flames, a trend already observed in Figure 5.4. To

further investigate the effect of stretch, flame speed as a function of equivalent flame stretch for both hydrogen and propane flames is plotted in Figure 5.7. This figure illustrates differences in stretch rates and flame speeds, as well as the sensitivity of flame propagation speed to stretch, denoted by $-dv_T/dK$ (mm). Propane/air flames under engine-like conditions exhibited an overall consistent behavior in flame speed relative to flame stretch across lean, stoichiometric, and rich mixtures, with sensitivity values ranging from 1.4 mm ($\phi_{int}^{C_3H_8} = 1.50$) to 2.0 mm ($\phi_{int}^{C_3H_8} = 0.70$). These values are similar to those found by Brequigny et al. in multiple flame speed sensitivity analyses conducted in constant volume chambers with laminar and turbulent flames, as well as in optical engines, for lean propane/air flames. For lean hydrogen/air flames, the sensitivity of flame speed to stretch within the combustion chamber was also consistent across all equivalence ratios and less pronounced than for propane, with sensitivity values ranging from 1.0 mm ($\phi_{int}^{H_2} \geq 0.35$) to 1.6 mm ($\phi_{int}^{H_2} \leq 0.25$).

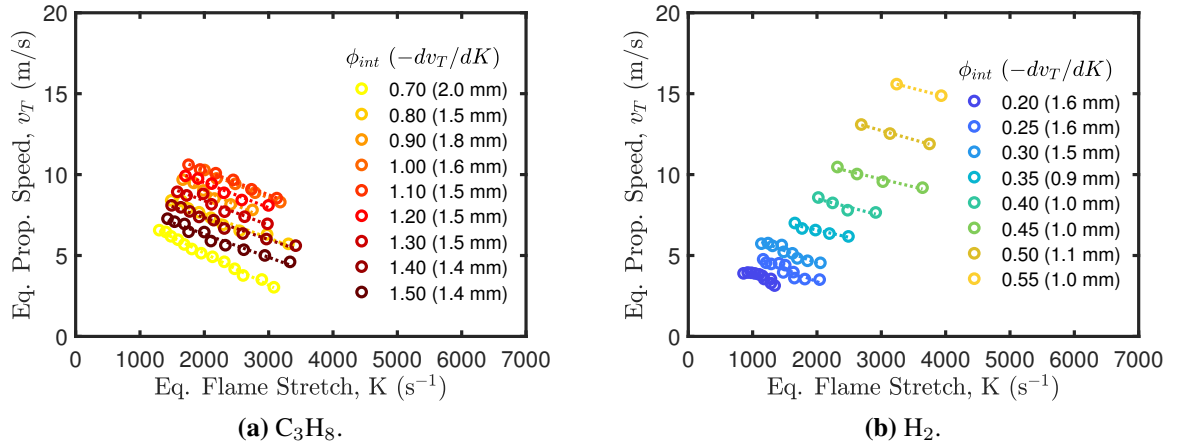


Figure 5.7: Flame propagation speed sensitivity to equivalent flame stretch for both fuels.

Finally, the flame circularity, Ξ , is evaluated. It is calculated as the ratio of the square of the flame radii determined by the contour perimeter to that determined by the surface area, r_P^2/r_S^2 , indicating whether the flame is closer to a circle ($\Xi \approx 1$) or deformed ($\Xi > 1$). For propane flames, shown in Figure 5.8a, Ξ remains close to 1, suggesting that the propane flames maintain a nearly circular shape across all equivalence ratios. However, for richer mixtures ($\phi_{int} = 1.4$ and 1.5), the flame becomes slightly deformed as it develops, with circularity reaching a value of 1.2 at 2 °aTDC and presenting higher variability.

In contrast, Figure 5.8b shows that hydrogen flames exhibit different behavior. At higher equivalence ratios, the flames retain a circular shape with low variability. However, as the mixture becomes leaner, the flame shape becomes increasingly deformed, even at the earliest measurable crank angles (equivalent radius greater than 3 mm). The circularity index increases significantly, reaching a value of 2 at $\phi = 0.30$ and 4 at $\phi = 0.20$, indicating that the flame's perimeter is substantially larger than its surface area, possibly due to the low laminar flame speed, which leads to strong deformation by bigger structures of the turbulent flow field.

To illustrate this parameter, four flame images (two for each fuel) are shown in Figure 5.9. These images capture flames with an equivalent radius of approximately 9.5 mm from cycles that most closely represent the average flame radius growth. The projected flames of both stoichiometric and rich propane/air mixtures display an overall circular shape. The stoichiometric

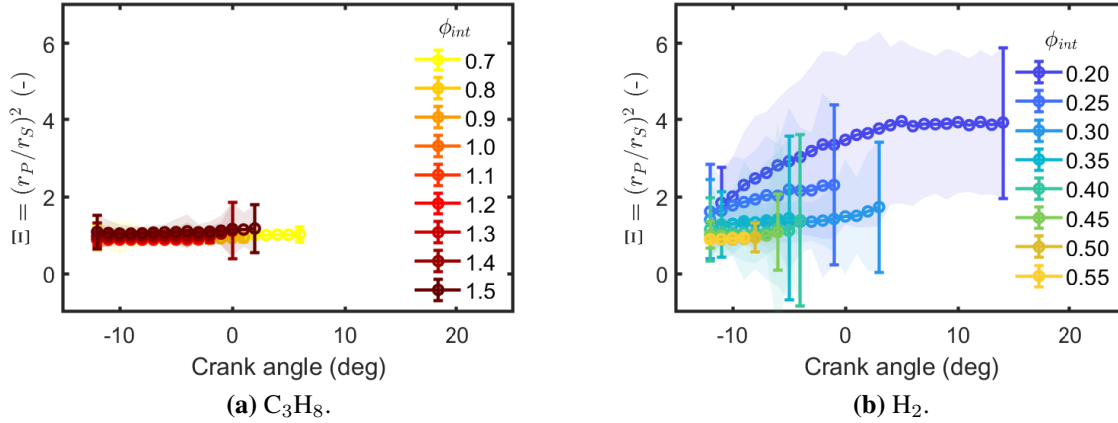


Figure 5.8: Flame circularity indicator, Ξ , as a function of the crank angle for different equivalence ratios.

flame appears more rounded and exhibits higher chemiluminescence intensity compared to the flame at a higher equivalence ratio, which starts to deviate from circularity and shows deformation due to flow motion, illustrating the increased variability in the circularity index for this mixture. In contrast, hydrogen/air flames show significant differences in shape between the two extreme equivalence ratios tested. At $\phi_{int} = 0.55$, the hydrogen flame maintains a more circular shape, similar to the stoichiometric propane mixture (as seen in Figure 5.8). However, under ultra-lean conditions, the chemiluminescence image (captured with higher IRO gain, resulting in more noise) shows a flame that is more deformed, elongating more rapidly along the tumble direction and potentially exhibiting a more wrinkled surface, slightly visible in Figure 5.9c.

5.1.2 Engine Speed

Subsequently, the effects of engine speed on hydrogen combustion are studied and their results are illustrated in Figure 5.10. Figure 5.10a demonstrates that the size of the flame radius at a given crank angle depends on both engine speed and equivalence ratio, consistent with the findings of Meier et al. [84]. The discrepancy in flame development is more pronounced at higher equivalence ratios (e.g., $\phi = 0.55$), where at an engine speed of 900 rpm, the flame develops faster on a crank angle basis compared to 1200 rpm, which in turn is faster than at 1500 rpm. Conversely, at $\phi = 0.35$, the flame development is consistent across all engine speeds, a phenomenon also observed in Chapter 3, using heat release analysis.

Analyzing it at a constant crank angle of -10° aTDC, Figure 5.10b illustrates that the influence of engine speed on the early flame radius is more significant at equivalence ratios higher than 0.35. This could be explained by the fact that the higher the equivalence ratio, the higher the flame speed. When the flame speed is more important than its turbulence enhancement, the flame is primarily driven by laminar flame properties. Consequently, since the time it takes to reach a given crank angle at 900 rpm is greater than at 1200 and 1500 rpm, it will develop more rapidly in a crank angle basis. Moreover, the engine speed does not appear to have a significant impact on flame development variability at a given crank angle, even though the exposure time to the velocity field differs.

The impact of engine speed on flame propagation speed is depicted in Figure 5.11a. Since

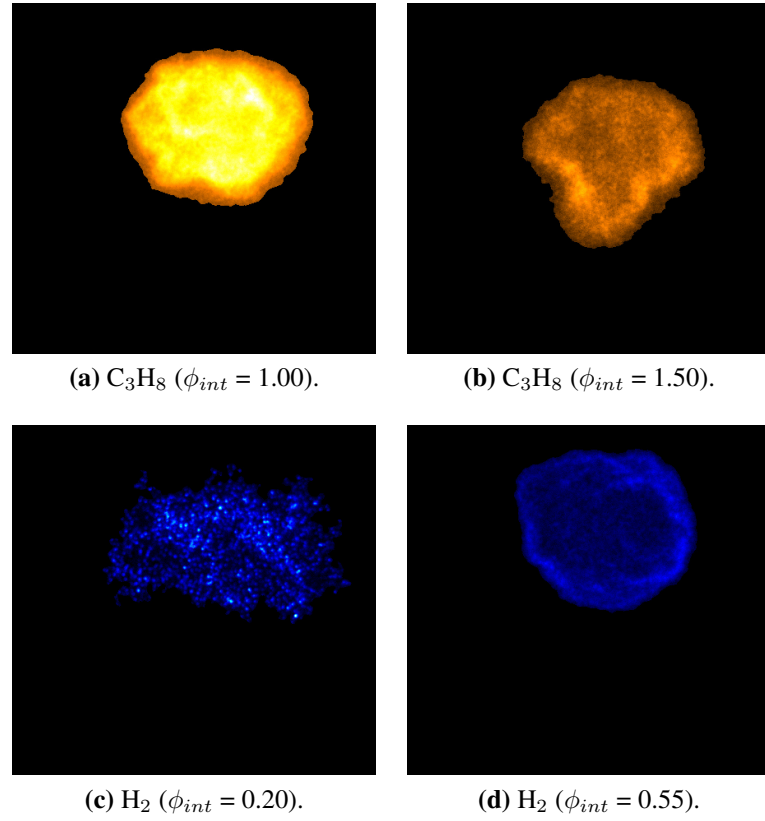


Figure 5.9: Chemiluminescence images of propane/air and hydrogen/air flames at two equivalence ratios, captured at a flame radius of 9.5 mm within cycles exhibiting the most similar flame radius growth.

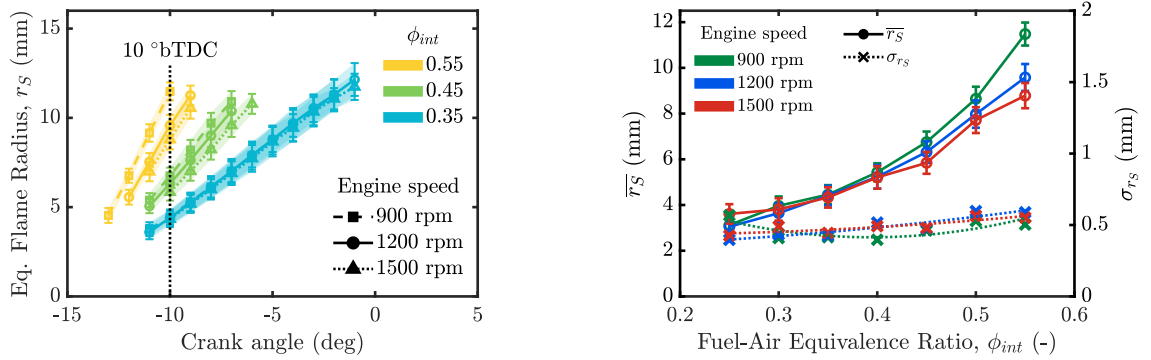
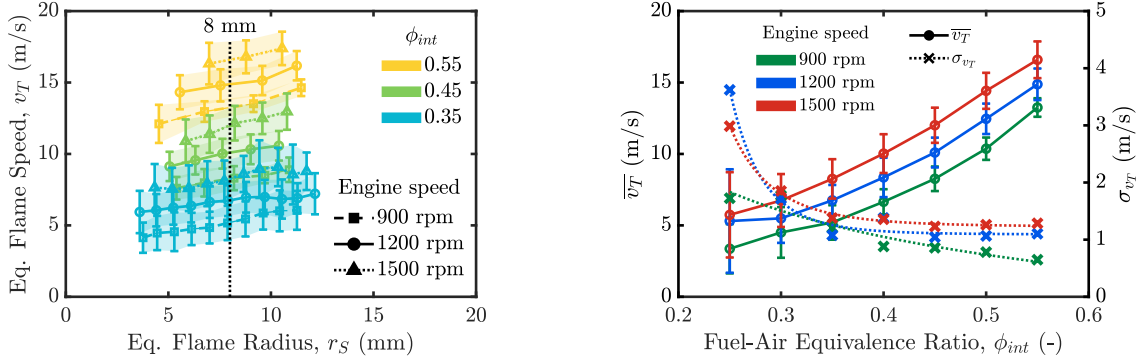


Figure 5.10: Effect of the engine speed on the flame radius development.

velocity is calculated as the derivative of the equivalent flame radius over time and expressed in meters per second, it is a quantity unaffected by the difference in in-cylinder time between engine speeds. The figure illustrates that flame speed is consistently higher with faster engine

speeds, and the increase in propagation speed with engine speed appears to be linear with all tested equivalence ratios.



(a) Equivalent flame speed (m/s) as a function of the equivalent flame radius (mm) for three equivalence ratios and three engine speeds.

(b) Equivalent flame propagation speed (m/s) as a function of the equivalence ratio (-).

Figure 5.11: Effect of the engine speed on the equivalent flame speed.

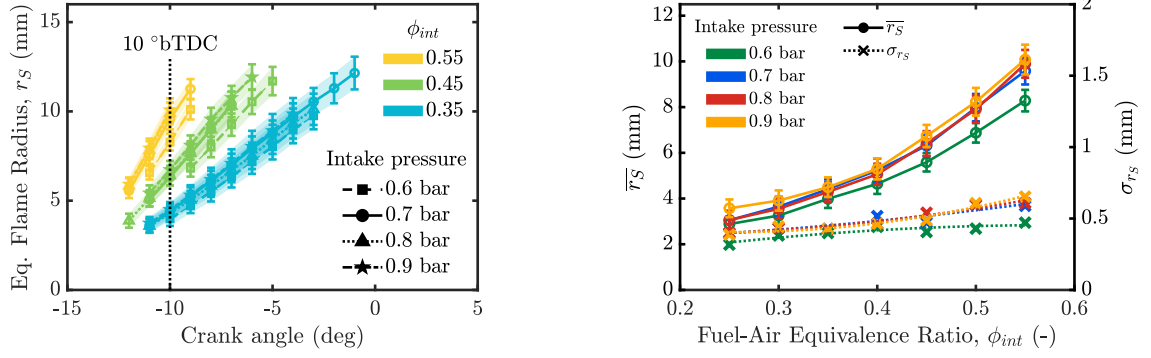
The flame propagation speed at a flame radius of 8 mm, depicted in Figure 5.11b, confirms the apparent linear increase in flame speed with the engine speed due to the increase in turbulence, which increases the surface area of the flame through distortion by wrinkling or entrainment. This phenomenon is well-documented for common fuels, such as iso-octane and methane [160], in spark-ignition engines, and it was also demonstrated for hydrogen/air flames in the study by Meier et al. [84]. Additionally, less combustion variability is observed at lower engine speeds (900 rpm) compared to higher ones (1200 and 1500 rpm), possibly due to lower velocities fluctuation in the former case.

5.1.3 Intake Pressure

The impact of intake pressure on the flame development of in-cylinder ultra-lean/lean hydrogen/air mixtures is depicted in Figure 5.12. Figure 5.12a shows the dependence of flame growth on intake pressure as a function of crank angle. It appears that intake pressure has a limited impact on flame development. For intake pressures of 0.7, 0.8, and 0.9 bar, the flame growth follows a similar trend and exhibits comparable values. However, at 0.6 bar, a slower development is observed for the presented equivalence ratios.

The observation extends to all measured equivalence ratios at 10°bTDC, as shown in Figure 5.12b. It can be seen that flame development at an intake pressure of 0.6 bar is consistently slower across all equivalence ratios, with this effect more pronounced at richer mixtures, characterized by ϕ_{int} greater than 0.35. Conversely, on the ultra-lean side, the 0.9 bar condition yields larger flames at the same crank angle, indicating a positive impact of higher pressures on ultra-lean hydrogen flames. Furthermore, the impact of intake pressure on combustion variability is found to be minor.

The comparison of flame propagation speed as a function of equivalent flame radius is illustrated in Figure 5.13a. Consistent with previous observations, the flame development behavior



(a) Equivalent flame radius (mm) as a function of the crank angle (deg) for three equivalence ratios and four intake pressures.

(b) Equivalent flame radius (mm) as a function of the equivalence ratio at 10 °bTDC.

Figure 5.12: Effect of the intake pressure on the flame radius development.

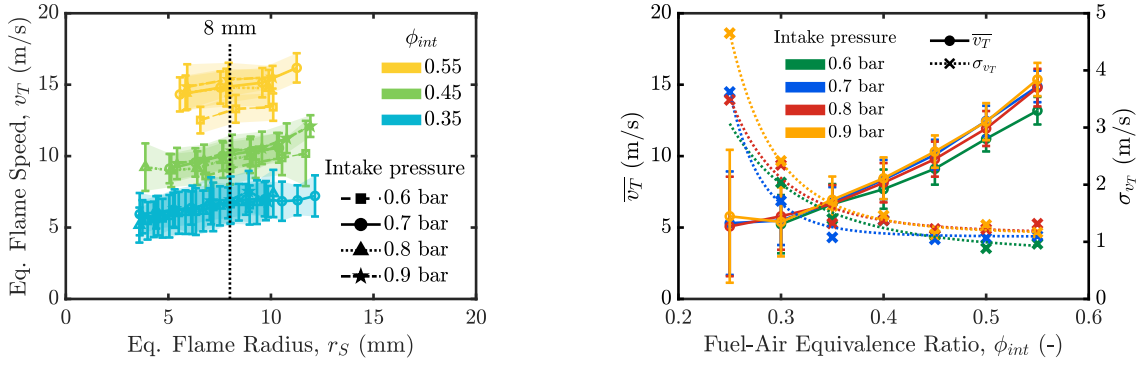
at intake pressures of 0.7, 0.8, and 0.9 bar falls within their respective standard deviations, indicating minimal differences in flame speed. However, at 0.6 bar, significant disparities in flame speed are noticeable, particularly pronounced at higher equivalence ratios.

Figure 5.13b highlights these differences at an equivalent flame radius of 8 mm. Across all tested equivalence ratios, the impact of intake pressure becomes evident when ϕ exceeds 0.35, particularly at an intake pressure of 0.6 bar. One possible explanation for this phenomenon could be the variation in mixture composition at spark timing under lower intake pressure, leading to higher levels of residual gases due to less effective scavenging. Comparing an intake pressure of 0.6 to 0.7 bar, see Table 5.2, the TPA model indicates approximately 20% higher water to hydrogen ratio (WHR) and internal exhaust gas recirculation. This difference in composition may decrease the flame speed and could impact flame development; however, further studies are needed to validate this hypothesis.

5.1.4 Ignition dwell time

Finally, Figures 5.14 and 5.15 illustrates the impact of ignition dwell time on flame development. The growth of radius as a function of crank angle, depicted in Figure 5.14, suggests that dwell time has minimal effect on flame development. Because ignition dwell time affects spark duration, thereby influencing the start of image capturing, direct comparisons at the same crank angle are challenging. This is the reason why the figure relating to the equivalent radius at a given CAD, presented in the previous cases, is not shown here.

Furthermore, Figure 5.15a displays the flame propagation speed as a function of equivalent flame radius for different dwell times and three equivalence ratios. The equivalent flame speed does not appear to be affected by dwell time (and spark duration). An analysis of flame speed at a flame radius of 10 mm is shown in Figure 5.15b. The mean value of flame speed varies within the standard deviation, indicating that ignition duration has little effect on hydrogen/air flame development for the tested equivalence ratios. Moreover, no evident trend is found in terms of combustion variability as a function of dwell time. One possible explanation for this result



(a) Equivalent flame speed (m/s) as a function of the equivalent flame radius (mm) for three equivalence ratios and four intake pressures. (b) Equivalent flame propagation speed (m/s) as a function of the equivalence ratio (-).

Figure 5.13: Effect of the intake pressure on the equivalent flame speed.

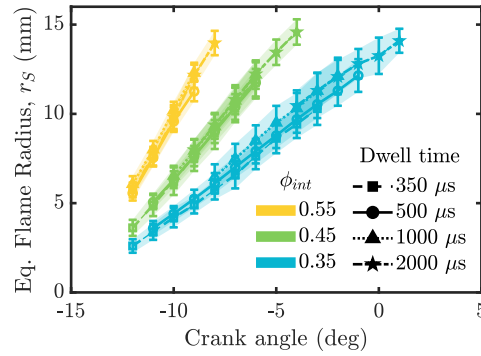
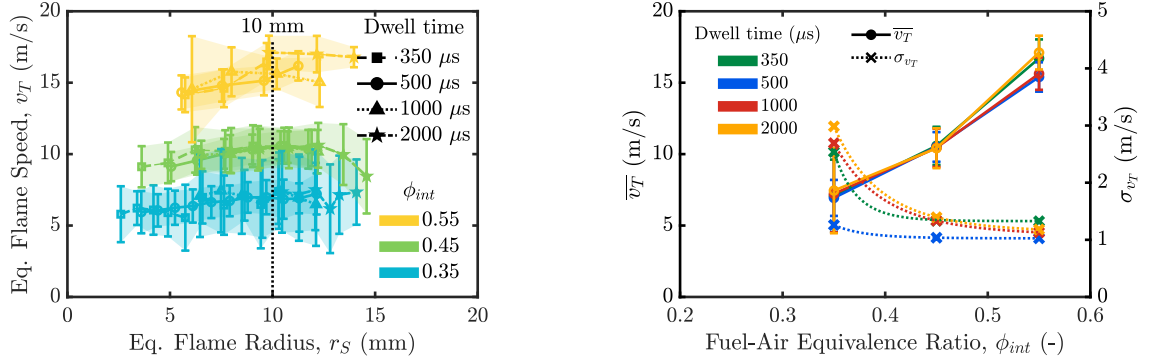


Figure 5.14: Equivalent flame radius (mm) as a function of the crank angle (deg) for three equivalence ratios and four ignition dwell times.

could be the low minimum ignition energy of hydrogen [12], which would facilitate the start of combustion independently of the provided energy. Further investigation with other fuels with different equivalence ratios could help to explore this idea further.

To summarize the effects of equivalence ratio, in-cylinder pressure, and ignition dwell time on the development of ultra-lean hydrogen/air in-cylinder flames, Figure 5.16 is presented. It illustrates the impact of each variable on the ratio between the measured flame propagation speed and the laminar flame speed divided by the expansion ratio, denoted as ρ_u/ρ_b . This figure provides a quantification of the turbulent flame speed enhancement relative to the laminar flame speed under each engine condition. The kinetic mechanism used for calculating the laminar flame speed is derived from the work of Alekseev et al. [143]. In the 0D Cantera simulation, the in-cylinder equivalence ratio, along with pressure and temperature values at which the flame reaches an equivalent radius of 8 mm, obtained from the TPA analysis, are employed.

Figure 5.16a illustrates the behavior of the flame speed ratio, representing the flame speed enhancement, as a function of turbulent intensity for three equivalence ratios. It can be ob-



(a) Equivalent flame speed (m/s) as a function of the equivalent flame radius (mm) for three equivalence ratios and four ignition dwell times.

(b) Equivalent flame propagation speed (m/s) as a function of the equivalence ratio (-).

Figure 5.15: Effect of the ignition dwell time on the equivalent flame speed.

served that for the same u' , the flame speed enhancement relative to the laminar flame speed is two to three times higher with an equivalence ratio of 0.35 compared to 0.55 (e.g., from 1.59 with $\phi_{int} = 0.55$ to 4.68 with $\phi_{int} = 0.35$ at $u' = 0.80$ m/s), indicating a more pronounced enhancement in leaner mixtures. This observation aligns with the findings of Berger et al. [47] in DNS simulations of lean hydrogen/air laminar flames. Similarly, variability is more pronounced with lower equivalence ratios. Furthermore, the increase in turbulent intensity results in higher flame speeds for all equivalence ratios, underscoring the significant impact of turbulence on flame speed. For instance, an increase from 0.55 to 1.05 m/s (+90.9%) in turbulence intensity enhances the flame speed from 1.48 to 1.76 (+19.9%) at $\phi_{int} = 0.55$ and from 3.91 to 5.92 (+51.4%) at $\phi_{int} = 0.35$. This suggests that ultra-lean mixtures are more sensitive to turbulence than richer mixtures, in accordance with the conclusions of heat release analysis.

Figure 5.16b shows the flame speed enhancement response to the increase in in-cylinder pressure. A clear increase in speed enhancement is observed, indicating that the turbulent flame speed tends to exceed the laminar flame speed as the in-cylinder pressure increases in ultra-lean mixtures. Notably, the slope of the curve suggests that this effect is more pronounced in leaner mixtures. This trend also aligns with the findings of Berger et al. [47] with a fuel-air equivalence ratio of 0.5 and an unburned temperature of 700 K. In their study, an increase in pressure from 10 to 20 bar (+100%) resulted in an increase in the ratio of flame consumption speed to the laminar flame speed from 1.7 to 1.9 (+11.8%). In this study, although similar thermodynamic conditions are encountered, turbulence is present. Since, as demonstrated earlier, no significant difference in internal aerodynamics occurs with different intake pressures, it can be assumed that the flame enhancement primarily stems from the in-cylinder pressure. The increase in in-cylinder pressure from 10.2 to 15.6 bar (+52.9%) elevated the flame speed ratio from 1.19 to 2.08 (+74.8%). An even higher increase of +89.9% is observed with an equivalence ratio of 0.35. This proves that ultra-lean flames are also more sensitive to in-cylinder pressure.

Finally, the effect of ignition dwell time is summarized in Figure 5.16c. As observed earlier, the flame speed difference is consistently within the measured standard deviations, thus, no significant effect can be drawn from this study. There is no noticeable change in flame propagation

5.2. HEAT RELEASE VS. FLAME DEVELOPMENT

speed with an increase in ignition dwell time for all equivalence ratios tested.

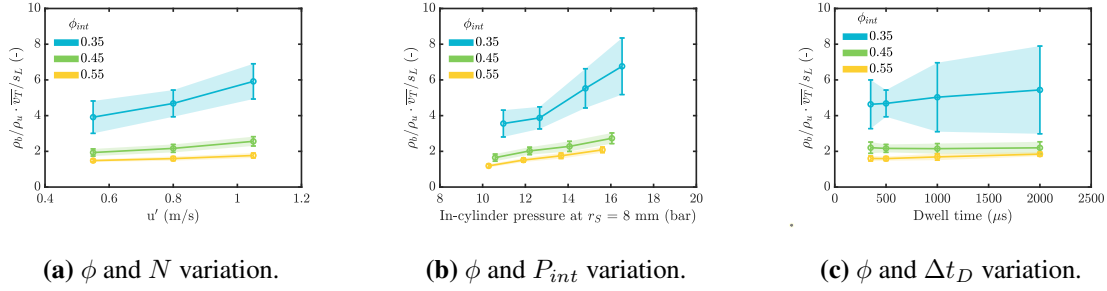


Figure 5.16: Equivalent flame speed enhancement compared to laminar flame speed (-) as a function of (a) Turbulent intensity (m/s); (b) In-cylinder pressure (bar); and (c) Ignition dwell time (μs).

5.2 Heat release vs. Flame development

Once the flame analysis is completed, it is important to verify whether it can be correlated to the in-cylinder pressure analysis. Consequently, two pressure-based variables are compared to the equivalent flame radius and the equivalent flame propagation speed.

Figure 5.17 presents the crank angle at which a radius of 4 mm and 8 mm is achieved as a function of CA2, CA5, CA10, and CA50 for the equivalence ratio variation. A correlation is found for all crank angles and both radii, as it was also observed for conventional fuels [161], indicating that the time it takes for the flame to reach a certain radius (either at the first measurable radius or near the field of view, FOV, limit) is related to the time it takes for the fuel to burn a certain percentage according to the heat release analysis. It is also important to note that when r_s is 8 mm, the CA2 line approaches the equation $CAD_{r_s} = CA$, meaning that these flame images are captured near the 2% of MFB. This highlights that flames as early as CA2 provide insight into the whole combustion duration.

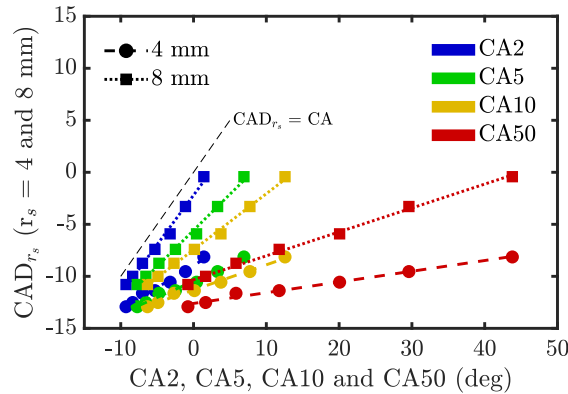


Figure 5.17: Crank angle degrees at which the flame achieves radii of 4 mm or 8 mm, plotted against the crank angles corresponding to 2%, 5%, 10%, and 50% of mass fraction burned.

A strong relation is also found when analyzing the mean equivalent flame propagation speed as a function of the MFB derivative, as depicted in Figure 5.18. The mean in-cylinder flame

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speed in the early flame phase (before CA2) is directly related to the mass fraction burned derivative at a specific CA (and up to CA50), implying again that the knowledge of the early flame phase is crucial for combustion prediction.

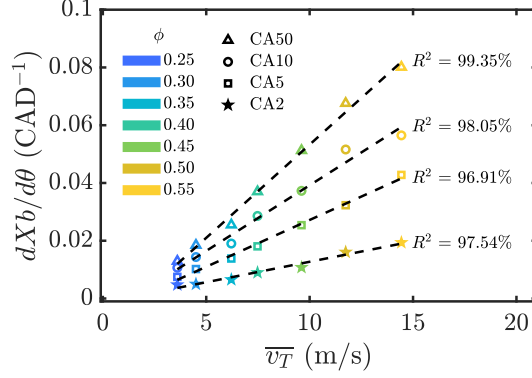


Figure 5.18: Derivative of the mass fraction burned at CA2, CA5, CA10, and CA50 as a function of the mean equivalent flame propagation speed for the equivalence ratio sweep at 1200 rpm.

Figure 5.19 shows the same comparison between the crank angle at which a certain percentage of fuel is burned (2, 10, 50 and 90%) and the crank angle at which the flame reaches an equivalent radius, for operating conditions that vary in equivalence ratio, engine speed, and intake pressure. In all cases, a correlation between heat release and flame size is observed, indicating that observations from both analyses can be related to each other. This justifies the study of in-cylinder hydrogen flames and the specification of a flame correlation for use in subsequent combustion predictive models, which will be addressed in the following section.

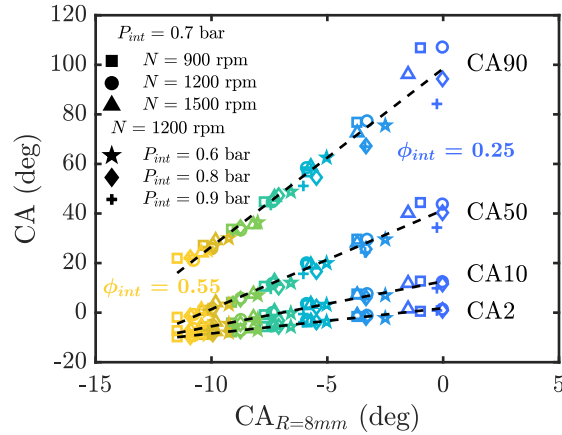


Figure 5.19: Crank angle degrees at which the flame achieves a radius of 8 mm, plotted against the crank angles corresponding to 2, 10, 50, and 90% of mass fraction burned.

5.3 Turbulent flame speed correlation

Having established that a thorough understanding of the early flame development phase contributes to a comprehensive insight into the overall hydrogen combustion process within the

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engine cylinder, it becomes capital to characterize this flame initiation accurately. To achieve this, a description of the measured equivalent flame propagation speed with the fundamental flame properties of the mixture is proposed.

As previously discussed, the flame propagation speed does not directly correlate with the laminar flame speed of the mixture, indicating that the early flame phase is likely influenced by the turbulent environment. To account for this, a correlation for turbulent flame speed is established across all tested conditions. Figure 5.20 depicts the enhancement of turbulent flame speed as a function of the ratio between turbulent intensity and laminar flame speed. Correlations are proposed for both Reynolds Decomposition (Figure 5.20a) and the Empirical Mode Decomposition (Figure 5.20b) turbulent velocity, represented as u' and u'_{HF} , respectively. This distinction is made due to their differing behavior and implications for engine modeling. While u' represents total velocity fluctuations and is inherently linked to the Reynolds Averaged Navier-Stokes (RANS) modeling approach through turbulent kinetic energy, u'_{HF} represents high-frequency velocity fluctuations, aligning with LES modeling. This is because u'_{HF} captures intrinsic high-frequency modes within the velocity field, representing the filtered portion of the flow field excluding large-scale structures. For this analysis, the flame propagation speed, v_T , and the laminar flame speed, s_L , were evaluated when the flame reached an equivalent radius of 8 mm. The graph demonstrates that all experimental conditions (including changes in equivalence ratio, engine speed, and intake pressure) converge onto a single curve. The turbulent flame speed correlation used in this study is based on a Damköhler-type expression proposed by Zimont [37]:

$$\frac{s_T}{s_L} = 1 + A \left(\frac{u'}{s_L} \right)^n \quad (5.1)$$

This expression follows the same trend as the experimental results and can be fitted to them. A good agreement is achieved with R^2 values of 98.90%. This indicates that despite significant differences in the laminar flame speed under various conditions, particularly with changes in equivalence ratio (e.g., at $P_{int} = 0.7$ bar and $N = 1200$ rpm, where $\phi_{int} = 0.25$, $s_L = 3.7$ cm/s, and when $\phi_{int} = 0.55$, $s_L = 3.1$ m/s, resulting in an almost 100-fold increase), the correlation holds a good fit overall. Additionally, since both velocity fluctuations are proportional to the mean piston speed, the exponent, n , of the ratio u'/s_L remained the same (1.02) in both cases, with the final difference reflected in the constant A . These values are close to others in the literature, such as the ones calculated by Giménez et al. [162] in H_2 ICEs from pressured-based measurements with lean mixtures, where both parameters are close to unity at the early flame phase (when the flame and piston radii ratio is less than 0.2).

Considering the strong correlation between the measured flame velocity and the calculated flame speed based on laminar flame properties and in-cylinder turbulent intensity, one can estimate the time it takes for the turbulent flame to traverse the cylinder and compare it with the time it takes for 10% of the fuel to burn in the heat release approach. Therefore, the combustion duration from spark timing to CA10 (in crank angle degrees) for all experiments is converted into physical time by dividing it by $6N$, where N is the engine speed in rpm. Additionally, a characteristic engine length, h , is chosen to be the height between the spark plug and the bottom of the piston bowl at the moment of the spark discharge. Since in all the experiments the spark occurs at a fixed crank angle (-15° aTDC), this height is 17 mm for all conditions. Finally, the burning time is calculated as the characteristic length, h , divided by the turbulent flame speed, s_T , obtained from the correlation introduced in Figure 5.20.

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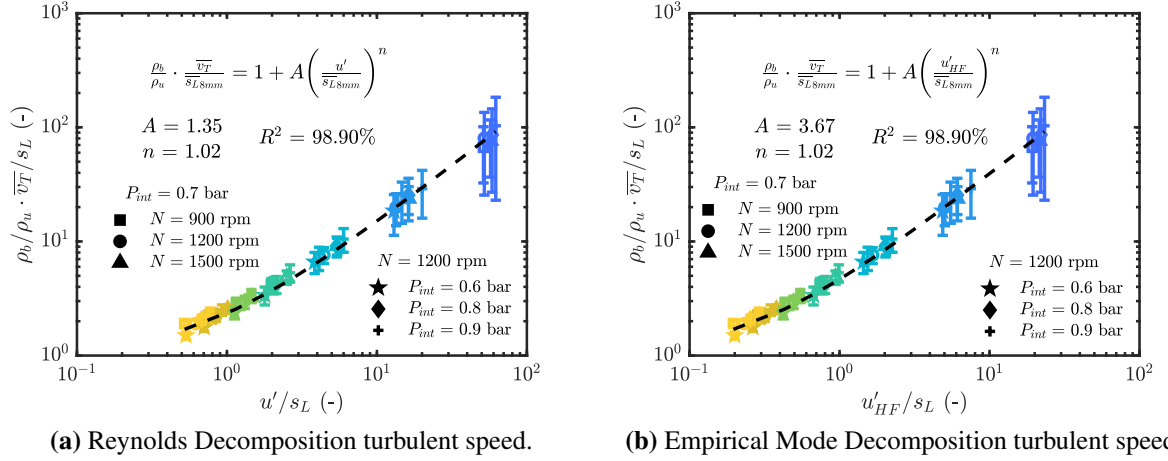


Figure 5.20: Flame speed enhancement as a function of u'/s_L with two turbulence models for all experimental conditions. The Zimont [37] turbulent flame speed correlation fitted with the measurements from this study shows good overall agreement ($R^2 = 98.90\%$).

Figure 5.21 displays the combustion duration from spark timing to CA10, in milliseconds, as a function of the flame time for both the engine speed and equivalence ratio sweeps. A strong and direct relationship is found between these two times ($R^2 = 99.42\%$), indicating that the calculated turbulent flame speed can be employed in predicting the early flame development phase and, consequently, the total combustion duration. This approach is validated in this work for a wide range of equivalence ratios (from 0.2 to 0.55), low engine speeds (900 to 1500 rpm) and low loads (0 to 3 bar of IMEP) in a tumble-motion spark ignition hydrogen-fueled engine. Finally, the flame development combustion duration, in crank angle degrees, can be estimated as a function of the engine speed, N (rpm), a characteristic engine length, h (m), and the turbulent flame speed with known turbulent flow parameters and laminar flame properties. The calculation is done with Equation 5.2.

$$\Delta\theta_{0-10\%} = C(6N)(h/s_T) \quad (5.2)$$

This early flame combustion duration formulation is based on the equation proposed by Heywood [19], where C is a constant that depends on the engine geometry. In this study, the value of the constant, determined from experimental data, was found to be 0.43 with the Reynolds turbulence decomposition with an R^2 of more than 99%.

One interesting observation is that across a wide range of equivalence ratios (from very lean to ultra-lean) and various turbulent intensities, a linear correlation, taking into account only the laminar flame speed and a classical turbulent combustion model, was able to closely match the experimental results in both flame and heat release behavior. Such a variation results in significantly different values for laminar flame speeds and thickness in hydrogen/air kinetic mechanism predictions and, consequently, in u'/s_L . These results are particularly interesting when analyzing the values in both Tables 5.1 and 5.2, which demonstrate that the flame present a big variation in both turbulence and flame scales, representing in the Peters-Borghi diagram a significant displacement from the "Wrinkled flames" zone to the "Well-stirred reactor" zone, as it was predicted in Chapter 3.

To have an idea of the flame morphology in each zone of the graph, the experimental con-

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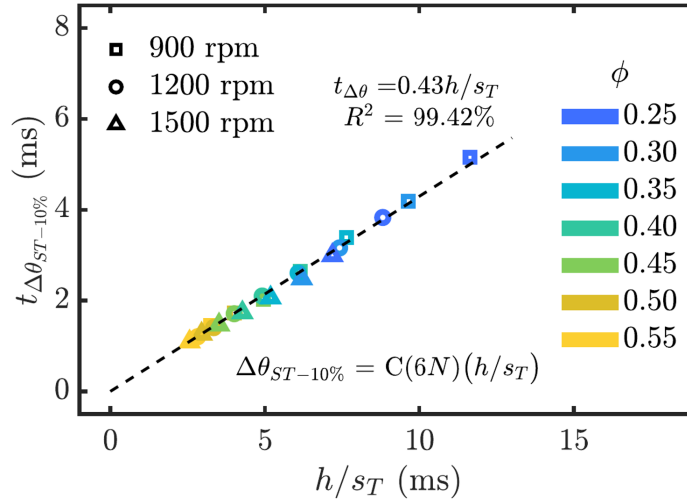


Figure 5.21: Flame development combustion duration, $t_{\Delta\theta_{ST-20\%}}$ (ms), as a function of the characteristic in-cylinder flame time, h/s_T (ms), for variations in equivalence ratio and engine speed.

ditions are placed in the Peters-Borghi diagram and displayed in Figure 5.22. As before, the laminar flame speed and thickness were calculated with the Alekseev et al. kinetic mechanism for each crank angle degree considering the TPA simulated in-cylinder pressure and unburned gas temperature and in this case the turbulence adopted was Reynolds decomposition. An arrow is drawn to describe the flame's path. The hydrogen/air flame image presented in each zone, elucidates its aspects in a given condition. The exhibited images were selected for an equivalent flame radius of 8 mm and for the cycles that approach the most the mean cycle in path and radius evolution.

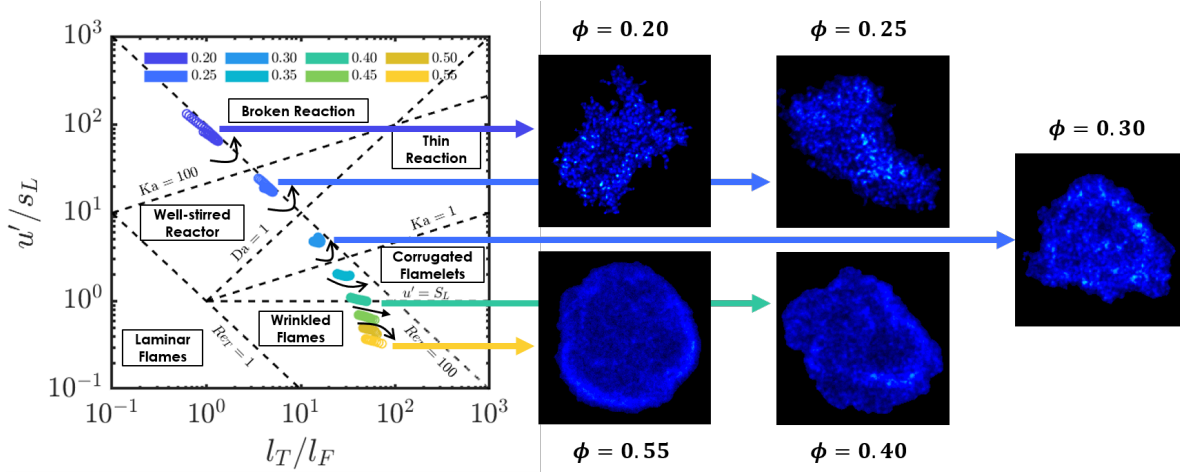


Figure 5.22: Peters-Borghi diagram for all fuel-air equivalence ratios at 1200 rpm. Each mixture is represented by a different color. The combustion development path is displayed for each crank angle from spark timing up to 10% MFB, with the direction indicated by arrows. Chemiluminescent images illustrate flame characteristics in various turbulent combustion zones, all captured at the equivalent flame radius closer to 8 mm.

It is observed that the overall shape of the flame is dependent on the Damköhler number (Da). The flames placed in the wrinkled flames zone ($\phi = 0.45 - 0.55$), where the laminar

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flame speed is higher than the turbulent intensity, presented a spherical form that is gradually advected from the spark plug, following the low-frequency flow created by the tumble motion, but remains minimally wrinkled. In this zone, as the combustion progresses, the Da tends to increase. As the equivalence ratio decreases (as well as the Da), the flame becomes more wrinkled. At equivalence ratios of 0.40 and 0.35, the flame enters the corrugated flamelets zone in the diagram, and since the flame is slower, it is more affected by advection compared to the richer mixtures for the same equivalent flame radius. In the thin reaction zone ($\phi = 0.30$), the flame starts to lose its spherical shape, and the Damköhler number decreases with the flame expansion. Upon reaching the well-stirred reactor zone, the flame is even more wrinkled and flattened, probably due to a longer exposition to the flow field caused by its slower expansion speed and by the turbulent eddies that start to penetrate the flame thickness [51]. This flame wrinkling increase as the equivalence ratio decreases can be observed in Figure 5.23, where the flame contour evolution for 4 hydrogen/air mixtures are illustrated. Finally, at the broken reaction zone ($\phi = 0.20$), the flame is distorted and advected further away towards the cylinder wall and the spherical shape is lost. Despite the low equivalence ratios and flame speeds, the flame maintains a consistent ellipsoidal shape, driven by the flow and developing without extinction – an uncommon characteristic for flames in this region of the turbulent combustion diagram. Figure 5.23 highlights this behavior for an equivalence ratio of 0.25, which also occurs at $\phi_{int} = 0.20$.

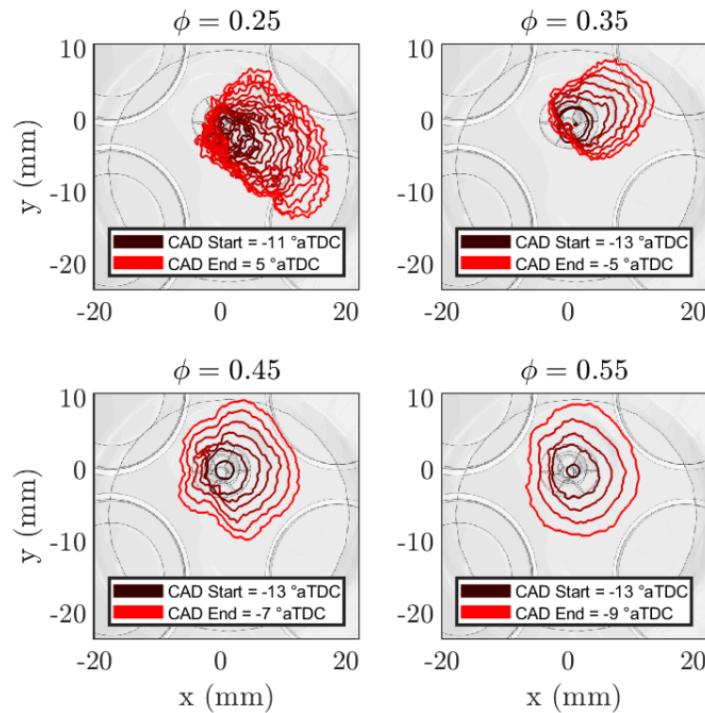


Figure 5.23: Evolution of hydrogen/air projected flame contours within an optical spark-ignition engine for four equivalence ratios (0.25, 0.35, 0.45, and 0.55). Each contour corresponds to a crank angle degree that develops from the black to the red lines.

The Zimont model approach was able to reproduce the flame and turbulence interactions from the wrinkled flames regime ($u'/s_L < 1$) up to the well-stirred reactor. Recently, Xie et al. [45] proposed a correlation for the critical radius at which cellular instabilities begin to

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appear in hydrogen/air flames. Extrapolating this correlation to the experimental conditions, it is observed that, for all cases, the critical radius is reached before the first flame imaging, suggesting that hydrogen flames are unstable inside the cylinder in all instances. Even though it is an extrapolation, this calculation shows a trend and could explain the possibility of having a single v_T/s_L correlation that fits all the data, despite the presence of multiple Damköhler numbers. At the broken reaction zone, however, the prediction was not found. At this condition, the flame properties resulting from the 1D flame calculations present very low laminar flame speeds (≈ 1.6 cm/s) and a large flame thickness (≈ 1.35 mm). These results do not seem to agree with the measurements, as the latter indicate a non-negligible flame speed of 2.5 m/s, and an initial flame kernel with 2 to 3 mm radius, while the theoretical flame thickness would be 1.35 mm. It also suggests that these values, not having been validated at such a low equivalence ratio and high temperature (> 700 K), and not aligning with the in-cylinder flame measurements, may not accurately represent the physical behavior at this configuration.

A final turbulent combustion diagram is presented in Figure 5.24, which includes all tested conditions (with an intake equivalence ratio equal to or greater than 0.25). The diagram highlights the zones explored within the flame imaging experiments conducted inside the engine. Both definitions of turbulence intensity are applied here, and their effect on the graph is indicated by the colors of the markers. When the turbulence intensity is defined as the high-frequency fluctuation of the velocity field, all conditions shift downward on the graph, with values decreasing to less than half of the y -axis, due to a reduction in turbulence from 0.56 to $0.21 \bar{S}_p$. This change can lead to significant variations in the turbulent combustion diagram and may require re-evaluating the combustion regime previously identified.

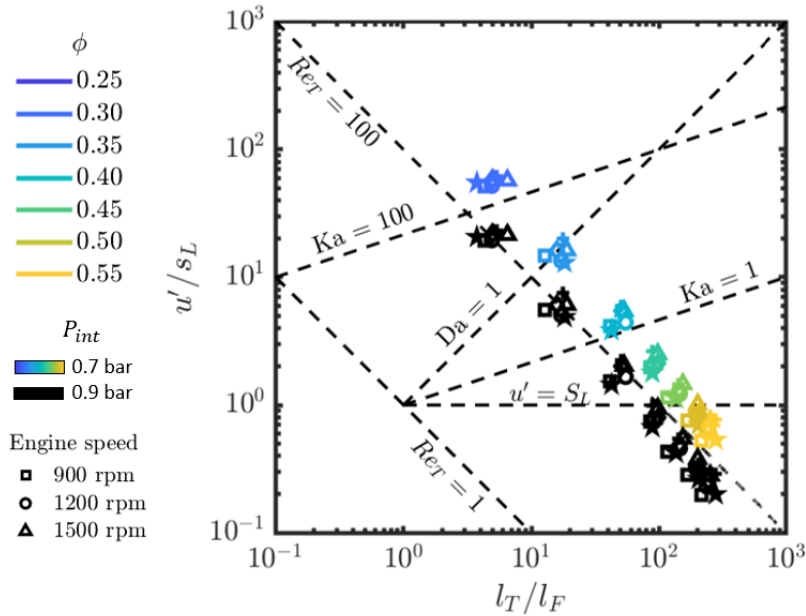


Figure 5.24: Peters-Borghi diagram for all experimental conditions. Each equivalence ratio is represented by a distinct color, while variations in intake pressure and engine speed are indicated by different markers. Turbulence intensity, calculated using EMD, is displayed in black, in contrast to the Reynolds decomposition, which is color-coded.

Conclusion

Experimental investigations were conducted on very lean to ultra-lean hydrogen/air flames ($0.20 < \phi < 0.55$) at various engine speeds ($900 < N < 1500$ rpm), intake pressures ($0.6 < P_{int} < 0.9$ bar), and ignition dwell times ($350 < \Delta t_D < 450$) in an optical spark-ignition engine. The impact of each parameter on hydrogen flames was examined, and comparisons with propane flames were made. The early flame development phase was analyzed using chemiluminescence flame imaging techniques and compared with pressure-based heat release analysis.

It was found that heat release analysis is closely linked to flame development. The time required for the flame to reach a specific radius (either at the initial visualization or at the last measurable radius) correlates directly with the time needed for the fuel to burn a certain percentage, as calculated from the pressure rise. The average equivalent flame propagation speed during the early flame development phase (before CA2) was also found to be directly related to the mass fraction burned rate, up to CA50. This demonstrates that understanding the early flame phase is critical for predicting total combustion duration and the in-cylinder pressure trace.

A model for hydrogen premixed turbulent flames, based on the Zimont equation, was developed using the experimental data to predict the combustion behavior during the initial stages. A framework and equation for 0D/1D combustion duration prediction up to CA10 are proposed. The correlation is valid for the wrinkled flame regime up to the well-stirred reactor regime ($Ka < 100$ and $\phi \geq 0.25$) under the experimental conditions. However, at lower equivalence ratios, where laminar flame properties were not validated, the results suggest non-physical quantities, such as a laminar flame thickness theoretically being half the measured flame radius. Therefore, specific data and refined kinetic mechanisms are required for these conditions.

As a perspective, it would be valuable to position ultra-lean hydrogen/air flames within the turbulent combustion diagram while considering the thermodiffusive instabilities that arise under such conditions, particularly at higher pressures. This could be achieved using the ω_2 model or by incorporating the Lewis number into the axis, allowing for comparisons with flames such as those of methane.

The experiments conducted in this chapter were used in the following publications:

- C. Ramalho Leite, P. Brequigny, J. Borée, F. Foucher, "Early flame development characterization of ultra-lean hydrogen–air flames in an optical spark-ignition engine", *Proceedings of the Combustion Institute*, Volume 40, Issues 1–4, 105260, 2024.
- S. Sfriso, F. Berni, S. Breda, S. Fontanesi et al., "Proposal and Validation of 3D-CFD Framework for Ultra-Lean Hydrogen Combustion in ICEs", *SAE Technical Paper* 2024-01-2685, 2024.

Engine speed variation data

Table 5.1: Summary of the measured and calculated parameters at an equivalent radius of 8 mm for the engine speed variation.

Engine speed	ϕ_{int} (-)	ϕ_{cyl} (-)	WHR (-)	$\Delta\theta_{8mm}$ (deg)	P_{cyl} (bar)	T_u (K)	δ_L^{Ze} (mm)	s_L^0 (m/s)	$\bar{v}_T$ (m/s)	σ_{v_T} (m/s)	$\rho_b/\rho_u \cdot \bar{v}_T$ (m/s)	u'/s_L^0 (-)
900 rpm	0.25	0.22	0.63	14.0	12.9	714.6	0.348	0.028	3.36	1.72	1.87	19.64
	0.30	0.27	0.73	11.3	12.8	718.0	0.117	0.098	4.51	1.77	2.33	5.62
	0.35	0.31	0.83	9.1	12.5	721.4	0.036	0.350	5.20	1.21	2.53	1.57
	0.40	0.36	0.94	7.3	12.1	716.2	0.018	0.727	6.65	0.88	3.04	0.76
	0.45	0.41	1.04	5.9	12.1	717.6	0.013	1.245	8.26	0.86	3.59	0.44
	0.50	0.46	1.13	4.6	11.9	715.8	0.009	1.890	10.37	0.78	4.28	0.29
1200 rpm	0.55	0.51	1.22	3.5	11.6	720.9	0.007	2.752	13.25	0.65	5.26	0.20
	0.25	0.23	0.51	15.0	13.3	731.3	0.306	0.037	5.30	3.62	2.96	21.71
	0.30	0.27	0.59	11.7	13.3	735.9	0.087	0.143	5.49	1.72	2.85	5.60
	0.35	0.32	0.66	9.1	12.9	735.1	0.027	0.433	6.75	1.08	3.29	1.85
	0.40	0.37	0.74	7.6	12.8	740.6	0.016	0.930	8.36	1.38	3.86	0.86
	0.45	0.42	0.81	6.3	12.4	740.0	0.010	1.570	10.10	1.04	4.43	0.51
1500 rpm	0.50	0.47	0.87	5.0	12.3	735.7	0.008	2.254	12.46	1.07	5.19	0.35
	0.55	0.52	0.93	4.2	12.0	735.0	0.006	3.109	14.88	1.10	5.92	0.26
	0.25	0.23	0.42	13.5	14.2	739.2	0.231	0.042	5.74	2.99	3.20	25.09
	0.30	0.28	0.50	11.3	14.1	740.3	0.079	0.147	6.74	1.85	3.50	7.13
	0.35	0.32	0.59	9.3	13.7	740.2	0.028	0.441	8.25	1.38	4.03	2.38
	0.40	0.37	0.68	7.7	13.5	747.3	0.015	0.956	10.02	1.36	4.65	1.10
1500 rpm	0.45	0.42	0.75	6.8	13.3	752.3	0.010	1.640	12.01	1.23	5.31	0.64
	0.50	0.47	0.83	5.2	12.6	745.5	0.007	2.370	14.42	1.26	6.05	0.44
	0.55	0.52	0.88	4.6	12.7	745.3	0.006	3.199	16.59	1.29	6.66	0.33

Intake pressure variation data

Table 5.2: Summary of the measured and calculated parameters at an equivalent radius of 8 mm for the intake pressure variation.

Intake pressure	ϕ_{int} (-)	ϕ_{cyl} (-)	WHR (-)	$\Delta\theta_{8mm}$ (deg)	P (bar)	T_u (K)	δ_L^{Ze} (mm)	s_L^0 (m/s)	$\bar{v}_T$ (m/s)	σ_{v_T} (m/s)	$\rho_b/\rho_u \cdot \bar{v}_T$ (m/s)	u'/s_L^0 (-)
0.6 bar	0.25	0.22	0.66	-	-	-	-	-	-	-	-	-
	0.30	0.27	0.77	12.5	11.2	728.9	0.082	0.148	5.23	2.04	2.73	5.42
	0.35	0.31	0.87	10.0	11.0	741.9	0.035	0.499	6.64	1.40	3.30	1.60
	0.40	0.36	0.99	8.4	10.7	748.6	0.017	1.072	7.69	1.37	3.62	0.75
	0.45	0.41	1.11	7.0	10.6	746.5	0.011	1.707	9.11	1.11	4.07	0.47
	0.50	0.46	1.19	5.7	10.5	758.1	0.007	2.721	11.21	0.89	4.81	0.29
0.7 bar	0.55	0.51	1.29	4.8	10.3	754.3	0.005	3.593	13.18	0.97	5.39	0.22
	0.25	0.22	0.57	15.0	13.1	735.3	0.312	0.037	5.30	3.62	2.98	21.59
	0.30	0.27	0.66	11.7	13.1	741.2	0.087	0.146	5.49	1.72	2.87	5.48
	0.35	0.32	0.74	9.1	12.7	756.9	0.026	0.530	6.75	1.08	3.36	1.51
	0.40	0.37	0.83	7.6	12.6	758.6	0.015	1.062	8.36	1.38	3.93	0.75
	0.45	0.41	0.91	6.3	12.2	749.0	0.010	1.648	10.10	1.04	4.48	0.49
0.8 bar	0.50	0.47	0.98	5.0	12.0	763.7	0.007	2.659	12.46	1.07	5.34	0.30
	0.55	0.52	1.05	4.2	11.9	746.6	0.006	3.271	14.88	1.10	6.00	0.24
	0.25	0.23	0.48	15.0	15.0	726.8	0.303	0.033	5.08	3.48	2.82	24.44
	0.30	0.28	0.56	11.7	15.0	738.0	0.094	0.118	5.79	2.35	3.01	6.78
	0.35	0.32	0.63	9.5	14.8	735.9	0.029	0.355	6.65	1.32	3.24	2.25
	0.40	0.37	0.69	7.9	14.6	751.4	0.015	0.898	8.14	1.38	3.79	0.89
0.9 bar	0.45	0.42	0.76	6.3	14.1	743.4	0.010	1.457	9.79	1.23	4.29	0.55
	0.50	0.47	0.82	5.1	13.9	751.7	0.007	2.273	11.93	1.22	5.04	0.35
	0.55	0.52	0.88	4.1	13.7	732.3	0.006	2.826	14.79	1.32	5.87	0.28
	0.25	0.23	0.43	14.7	17.0	724.7	0.282	0.031	5.79	4.50	3.19	25.88
	0.30	0.28	0.48	11.6	17.0	732.9	0.085	0.096	5.39	2.42	2.77	8.36
	0.35	0.33	0.54	9.0	16.5	734.5	0.030	0.320	6.94	1.63	3.36	2.50
	0.40	0.38	0.59	7.6	16.5	738.1	0.017	0.728	8.45	1.46	3.87	1.10
	0.45	0.43	0.64	5.9	16.0	742.2	0.011	1.317	10.32	1.13	4.50	0.61
	0.50	0.48	0.69	4.9	15.7	747.7	0.007	2.067	12.41	1.30	5.20	0.39
	0.55	0.53	0.73	4.0	15.6	723.0	0.005	2.487	15.36	1.16	6.02	0.32

Chapter 6

Cycle-to-cycle variations

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Introduction

This chapter aims to characterize the variability of hydrogen/air combustion in spark-ignition internal combustion engines. To investigate this performance parameter, three main analyses are conducted. First, an overall analysis is performed using both the heat release analysis method and chemiluminescence imaging to identify key differences in in-cylinder pressure, flame images, and parameters derived from these measurements for both propane and hydrogen flames. Second, the effects of equivalence ratio, engine speed, intake pressure, and dwell time on flame variability are explored. Finally, extreme conditions identified in the overall analysis are examined on a cycle-by-cycle basis, dividing the measured cycles into fast and slow categories. The aerodynamic patterns and flame propagation of fast and slow cycles are compared to understand the impact of the flow field on flame variability.

6.1 Overall variability

The overall variability of parameters is assessed in both the heat release (e.g., maximum in-cylinder pressure, indicated mean effective pressure, combustion duration) and flame imaging approaches (e.g., radius and flame speed at a given crank angle, CA timing or a given radius).

These parameter values and variations are discussed and compared between hydrogen/air and propane/air mixtures at 1200 rpm and 0.7 bar of intake pressure.

6.1.1 Heat release analysis

Figures 6.1 and 6.2 illustrate the in-cylinder pressure traces for the equivalence ratio variation in operating conditions for propane and hydrogen flames over 100 and 500 cycles, respectively. In both figures, the mean value is highlighted with a thick line, and the variation around this mean is represented by two times the standard deviation, shown in the corresponding equivalence ratio color with a degree of transparency.

For the propane case, the pressure traces show higher maximum pressures at equivalence ratios closer to 1.0 and 1.1. As the equivalence ratio deviates from these values, the in-cylinder maximum pressure decreases, and the peak is shifted to a later point in the cycle, which is expected if the flame is propagating more slowly inside the combustion chamber. Furthermore, the pressure trace variability appears slightly higher at both extremes of the equivalence ratio and lower near stoichiometric mixtures. For the hydrogen flames, richer mixtures, with their higher flame speeds, result in greater in-cylinder pressures. The maximum pressure achieved with an equivalence ratio of 0.55 is comparable to the highest pressure found in propane mixtures (close to stoichiometry). As the equivalence ratio of the hydrogen/air mixture decreases, the maximum pressure also decreases, and the crank angle at which this maximum occurs shifts to higher crank angles, indicating slower combustion.

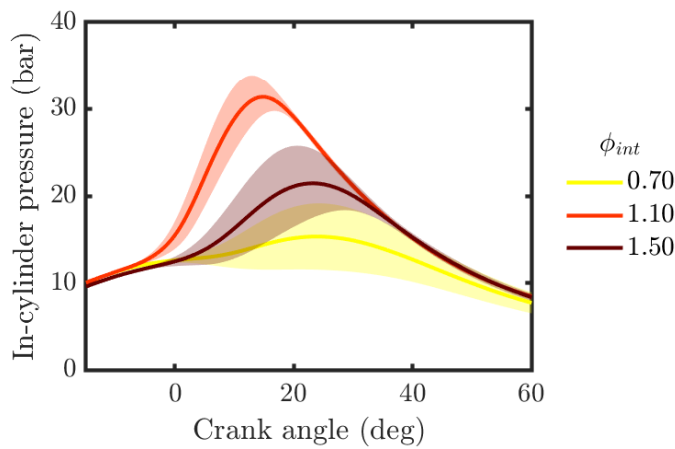


Figure 6.1: In-cylinder pressure as a function of crank angle for propane/air mixtures at three equivalence ratios (0.70, 1.10 and 1.50).

In terms of standard deviation, hydrogen and propane flames behave differently at the same maximum pressure. Hydrogen flames exhibit less variability compared to propane flames. Additionally, even with very slow flames, the pressure trace in hydrogen conditions shows minimal variation between cycles. This suggests that slow hydrogen flames propagate effectively even when the mixture is highly diluted with air, and that this propagation is not significantly impacted by sources of cycle-to-cycle variation (such as, in this case, charge composition and fluid motion), which is in contrast to the behavior of more conventional fuels [98, 71, 163].

The maximum in-cylinder pressure for both fuels is analyzed in Figure 6.3. It shows the maximum pressure for each operating condition, along with two times the standard deviation,

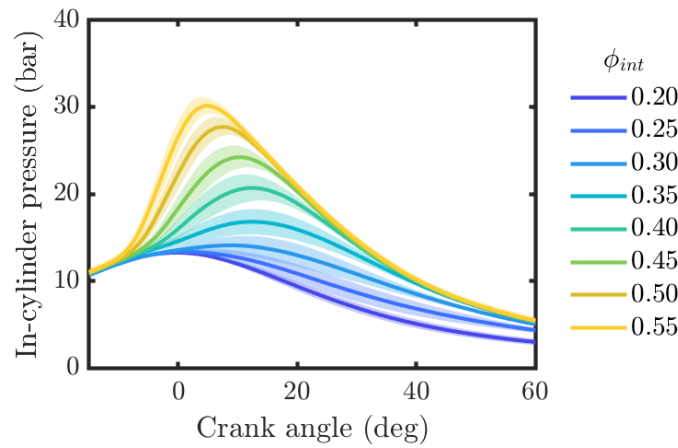


Figure 6.2: In-cylinder pressure as a function of crank angle for hydrogen/air mixtures at eight different equivalence ratios, ranging from 0.20 to 0.55.

as a function of the equivalence ratio. The previously discussed pressure curve behavior is summarized in this graph, demonstrating an increase in maximum pressure with rising equivalence ratios for hydrogen and a peak at an equivalence ratio of 1.1 for propane. The graph also shows that the variability for hydrogen is significantly smaller than for propane across all equivalence ratios.

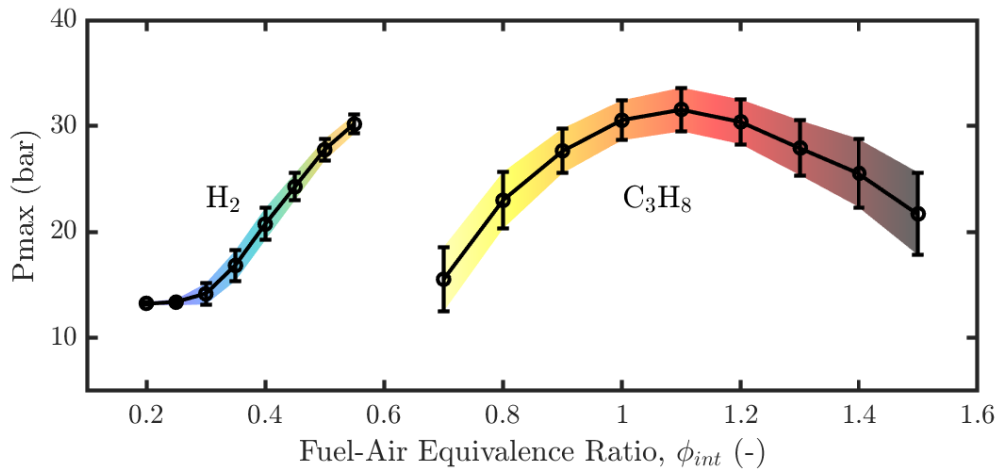


Figure 6.3: Maximum in-cylinder pressure as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent twice the standard deviation.

For propane, the effect of equivalence ratio on maximum pressure variability is clear: it increases as the flame slows and maximum pressure decreases, with minimal variability at equivalence ratios of 1.0 and 1.1. For hydrogen, the relationship is less straightforward, while higher equivalence ratios (i.e., faster flames) exhibit less variability than medium equivalence ratios (e.g., $\phi_{int} = 0.4$), this variation decreases again at leaner equivalence ratios.

This behavior is influenced by the timing of combustion within the engine cycle. If the flame is fast and well-timed, the maximum pressure occurs during the combustion phase, as seen in all propane cases and hydrogen flames with equivalence ratios higher than 0.3. However, when the flame is too slow, poorly timed, and has low energy (as in ultra-lean conditions), combustion

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occurs later in the expansion stroke, well after TDC. In such cases, the pressure increase due to combustion does not contribute to the maximum in-cylinder pressure, which is instead reached near TDC due to compression alone. This explains why the maximum pressure variability at ϕ_{int} values of 0.25 or lower is close to zero. Analyzing the highest variability at a given crank angle for the tested hydrogen/air mixtures, it ranges from 0.5 bar to 1.3 bar ($2 \cdot \sigma$) for $\phi = 0.20$ and 0.55, respectively. This variation depends on the combustion development and timing, which is further examined using the mass fraction burned profile.

Figure 6.4 shows the indicated mean effective pressure and its overall variability (standard deviation, σ_{IMEP}) as a function of the equivalence ratio for both fuels. It is evident that the IMEP for hydrogen varies between 0.2 and 2.6 bar, while for propane, it ranges from 3.7 to 5.4 bar, reflecting the energy released per cycle for each fuel.

Considering a piston at TDC, with a volumetric efficiency of approximately 80% (regardless of the mixture), a displacement volume of 0.4 L, and hydrogen's energy density of 9.6 MJ/m³ (as indicated in Table 1.3), the energy content inside the cylinder at TDC is 298.9 J for a hydrogen/air mixture with an equivalence ratio of 0.25 (where hydrogen occupies 9.5% of the mixture volume). For an equivalence ratio of 0.5 (with hydrogen occupying 17.4% of the mixture volume), the energy content is 545.9 J. For propane, the corresponding analysis for equivalence ratios of 0.7 and 1.0 yields energy contents of 759.1 J and 1071.4 J, respectively. These values align with the increase in IMEP, from 2.6 bar for hydrogen at $\phi_{H_2} = 0.50$ to 5.4 bar for propane at $\phi_{C_3H_8} = 1.00$, reflecting an increase of 108%, compared to a 96% increase in energy content (from 545.9 J to 1071.4 J). The relationship between IMEP and in-cylinder energy content is also evident with increasing equivalence ratios for both fuels. When the hydrogen equivalence ratio increases from 0.25 to 0.50, IMEP rises by 136%, compared to an 83% increase in energy content. For propane, an increase in equivalence ratio from 0.7 to 1.0 leads to a 46% increase in IMEP, compared to a 41% increase in energy. While combustion timing plays a role in converting fuel energy to work, due to combustion and thermal efficiency, the energy content of the unburned mixture remains a key factor in understanding the effect of each mixture on engine performance.

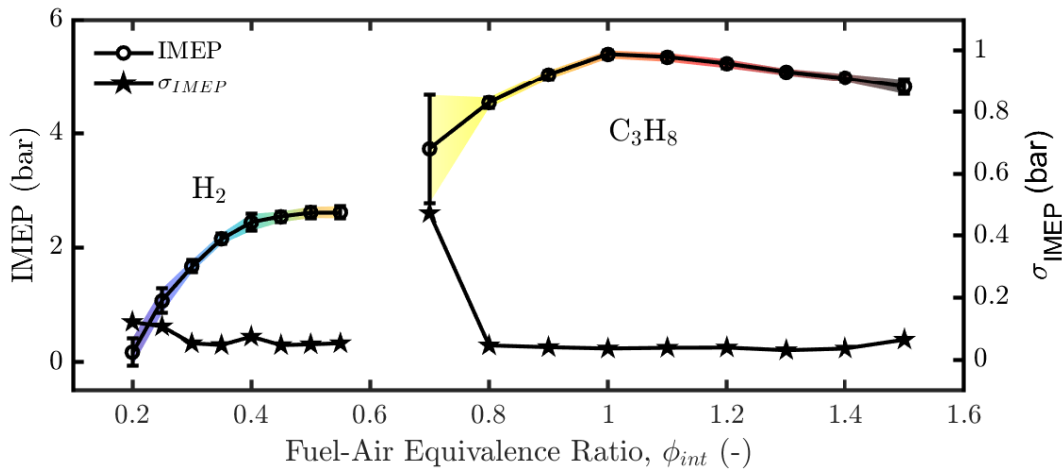


Figure 6.4: Indicated mean effective pressure as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent twice the standard deviation.

Examining the effect of equivalence ratio on IMEP for propane, it is clear that maximum IMEP is achieved at an equivalence ratio of around 1.0, which corroborates the fact that faster

flames lead to better overall engine performance in terms of both load and efficiency, in agreement with the theoretical Otto's cycle. As the equivalence ratio deviates from stoichiometry, IMEP decreases. The standard deviation of IMEP remains below 0.1 bar but increases at the extreme equivalence ratio values. The highest variability occurs at an equivalence ratio of 0.7 (approaching the flammability limit for propane), where the standard deviation exceeds 0.4 bar with an IMEP of 3.7 bar, corresponding to a coefficient of variation of 10.8%, indicating an unstable operating condition.

For hydrogen, despite the large variation in IMEP with changes in equivalence ratio, especially near the lean side of the lower flammability limit (around an equivalence ratio of 0.17), the standard deviation is consistently low (below 0.15 bar). This highlights hydrogen's strong ability to ignite and sustain combustion even at very low equivalence ratios and under low-load conditions, which is in contrast to conventional fuels [71].

Figures 6.5 and 6.6 show the mass fraction burned for multiple equivalence ratios for propane and hydrogen mixtures. Similar to the in-cylinder pressure trace curves, the mean values are represented by thick lines, with the $\pm$ two standard deviations also displayed. The differences in the combustion progress within the cylinder, the variability of each condition, and the effects of the equivalence ratio sweep are qualitatively assessed in both figures. What is expected based on the pressure curves is more clearly illustrated with this variable: faster combustion occurs when ϕ_{int} is closer to 1.0 for propane and 0.55 for hydrogen. Additionally, as the flame speed decreases, the cycle-to-cycle combustion variability increases, as previously discussed by Ozdor et al. [98]. This pattern is observed for both fuels.

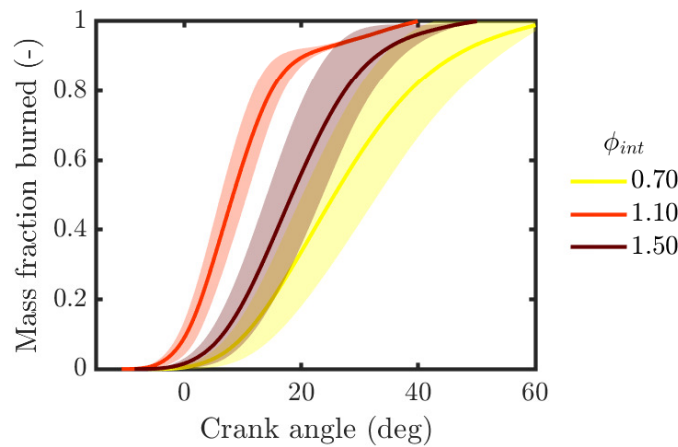


Figure 6.5: Mass fraction burned as a function of crank angle for propane/air mixtures at three equivalence ratios.

To better quantify the combustion characteristics within these curves, Figure 6.7 is introduced. It displays the combustion duration for the 0-10% (initiation) and 10-50% (propagation) phases as a function of the equivalence ratio for both fuels, along with their variability. Under these operating conditions, both the initiation and propagation phases exhibit similar trends in relation to the equivalence ratio. For hydrogen, richer mixtures result in faster combustion and shorter combustion timing. For propane, the minimum combustion timing occurs at an equivalence ratio of 1.1, corresponding to the fastest flame. Furthermore, the graph clearly shows the variation in combustion duration across different equivalence ratios. Faster flames display less variability. The greatest variation in combustion duration during the flame initiation phase

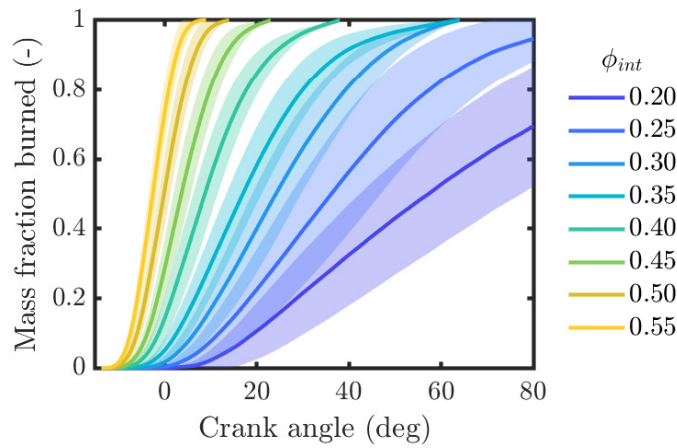


Figure 6.6: Mass fraction burned as a function of crank angle for hydrogen/air mixtures at eight different equivalence ratios.

is observed in hydrogen/air mixtures at an equivalence ratio of 0.20, with a standard deviation of 4.0 CAD. Conversely, the least variation is found in hydrogen/air mixtures at an equivalence ratio of 0.55, with a standard deviation of 0.3 CAD. Notably, these conditions also coincide with the longest combustion duration (35.2 CAD) and the shortest combustion duration (7.7 CAD), respectively.

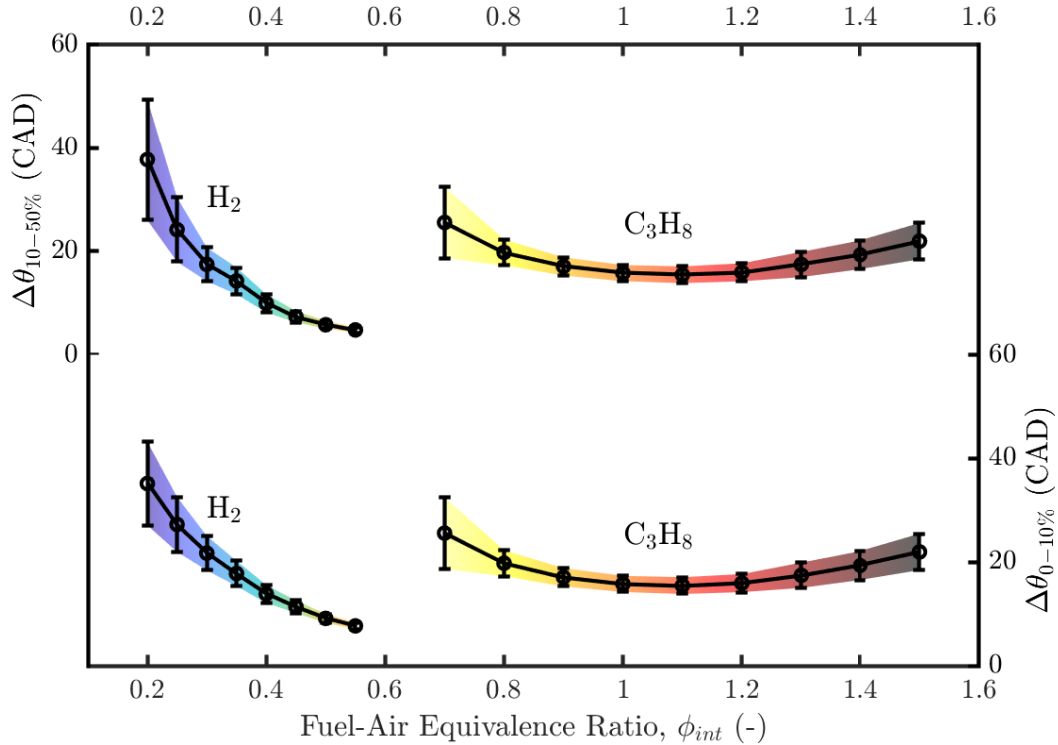


Figure 6.7: Combustion duration for the flame initiation phase (0–10% MFB, bottom) and flame propagation phase (10–50% MFB, top) as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent twice the standard deviation.

The combustion duration and variability for propane flames at $\phi_{int} = 1.1$ (15.5 ± 0.8 CAD) are comparable to those observed for hydrogen flames at equivalence ratios between 0.35 (17.8 ± 1.2 CAD) and 0.40 (13.9 ± 0.7 CAD). In general, the combustion duration during the flame propagation phase is slightly longer than during the flame initiation phase. However, this analysis should be interpreted with caution, as the combustion timing is not optimized, a condition that is typically managed through engine control in real-world applications.

6.1.2 In-cylinder flames

A similar analysis of cyclic variability is conducted using chemiluminescence measurements. Figure 6.8 presents the equivalent flame radius and its standard deviation at 10 °bTDC (i.e., five crank angle degrees after ignition) as a function of the equivalence ratio for each fuel. As expected, for propane, the largest radius at 10 °bTDC is 5.47 mm, achieved with an equivalence ratio of 1.1. At an equivalence ratio of 0.7, the radius is 2.43 mm, and at an equivalence ratio of 1.5, it is 3.40 mm. For hydrogen, the smallest flame is observed at the lowest equivalence ratio, 0.20, with a radius of 3.10 mm. The largest flame at 10 °bTDC has an equivalent flame radius of 11.80 mm, corresponding to the highest tested hydrogen/air equivalence ratio. The standard deviation across all conditions is similar, ranging from 0.5 to 0.6 mm.

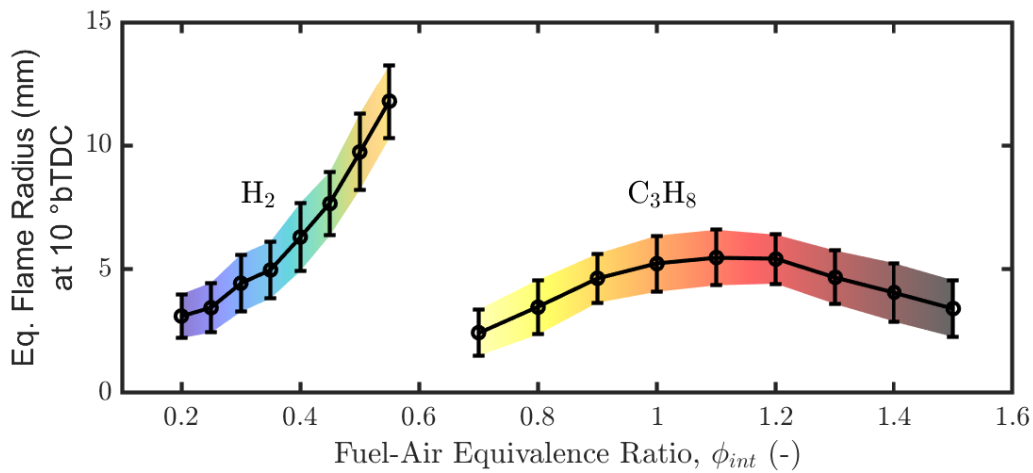


Figure 6.8: Equivalent flame radius at 10 °bTDC as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent twice the standard deviation.

Figure 6.9 displays the equivalent flame speed as a function of the equivalence ratio. The equivalent flame radius and speed (its derivative) follow the same pattern. The highest speed for propane flames is found at $\phi_{int} = 1.1$, with a value of approximately 8.5 m/s, compared to 3.5 m/s at $\phi = 0.7$. For hydrogen, the speeds range from 1.9 m/s to 14.3 m/s at $\phi_{int} = 0.20$ and 0.55, respectively. The highest flame speed for propane is similar to that observed for hydrogen/air flames with equivalence ratios between 0.40 and 0.45. The standard deviation is about 1.2 m/s for propane flames and slightly higher, around 1.3 m/s, for hydrogen flames.

Another way to analyze the flame, rather than comparing certain parameters after a fixed amount of time, is to compare parameters for flames of the same size. Figure 6.10 introduces the idea of comparing the time it takes for the flame to reach an equivalent radius of 8 mm as a function of the equivalence ratio. The results of this approach exhibit similar characteristics

6.1. OVERALL VARIABILITY

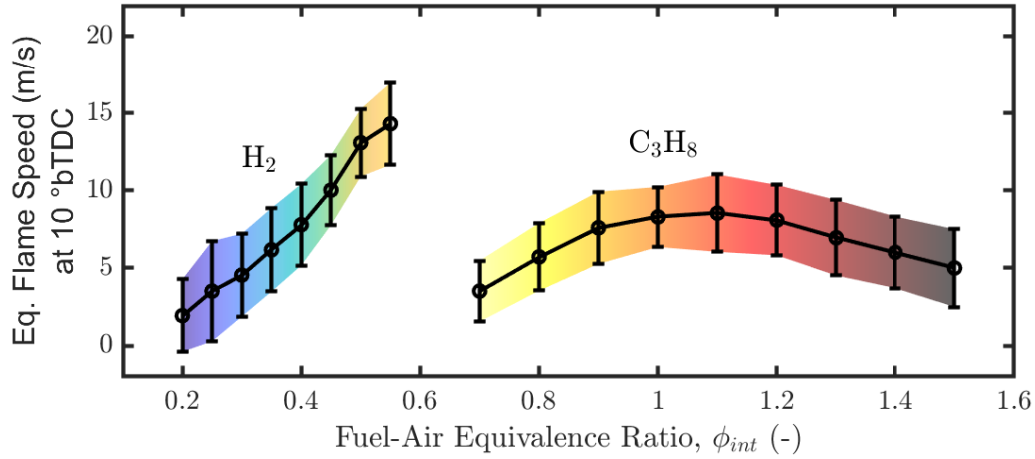


Figure 6.9: Equivalent flame propagation speed at 10 °bTDC as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent twice the standard deviation.

to those observed in the combustion duration, from spark timing to 10% mass fraction burned, as calculated from the in-cylinder pressure. In this case, the time for the flame to reach 8 mm is approximately half the time it takes for 10% of MFB. The highest variability occurs with the slowest flames, as previously discussed. However, when measured by the flame approach, the variability is at least twice as high compared to the flame initiation calculated using the heat release method.

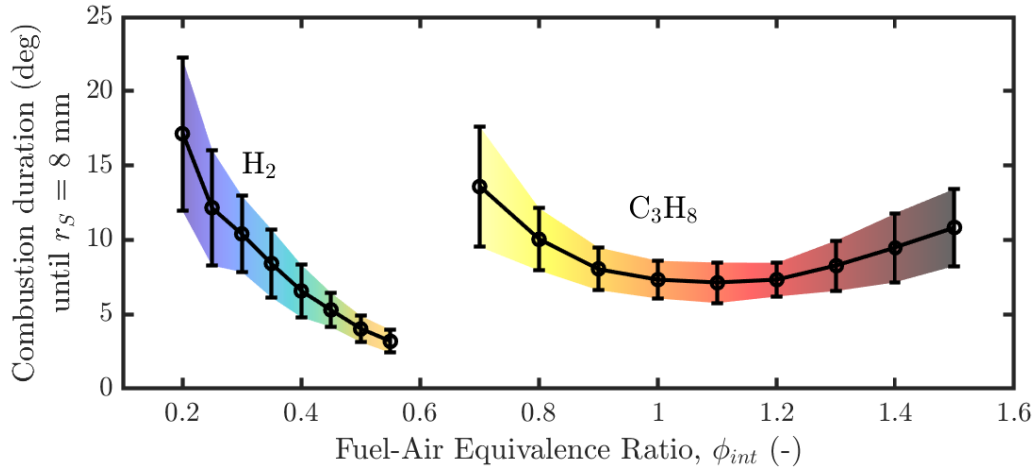


Figure 6.10: Combustion duration from spark timing to an 8 mm equivalent flame radius as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent two times the standard deviation.

Additionally, the equivalent flame speed is assessed in Figure 6.11. The overall flame speed behavior is consistent with the flame speed observed at 10 °bTDC. Higher flame speeds are recorded at higher equivalence ratios for hydrogen (15.1 ± 2.3 m/s) and near stoichiometry for propane flames (9.8 ± 2.4 m/s). However, the variability of this parameter is more sensitive to changes in the equivalence ratio, with higher standard deviations observed in mixtures with lower flame speeds. In comparison to H₂, C₃H₈ flames show a less varying standard deviation

with the equivalence ratio.

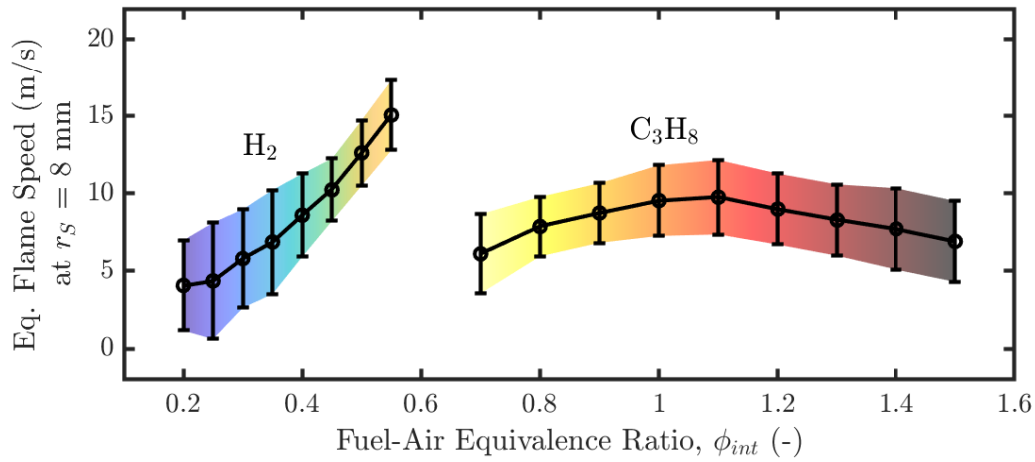


Figure 6.11: Equivalent flame propagation speed at an 8 mm flame radius as a function of the fuel-air equivalence ratio for hydrogen/air and propane/air mixtures. Error bars represent two times the standard deviation.

6.2 Influence of engine parameters on CCVs

In this section, the impact of three variables on cyclic variability is assessed from the chemiluminescence images. Since the effect of equivalence ratio on flame variability has already been analyzed in the previous section, this analysis focuses on understanding the influence of engine speed, intake pressure, and ignition dwell time on flame variability. Specifically, the equivalent flame radius and propagation speed at 10 °bTDC are evaluated for three hydrogen equivalence ratios and propane at stoichiometry.

Figure 6.12 shows the standard deviation of the equivalent flame radius over 100 cycles for each variable sweep. According to Figure 6.12a, flame radius variability does not change significantly with increasing engine speed for both fuels. The only outlier is the hydrogen/air flame at an equivalence ratio of 0.3, which exhibits greater variability at 900 rpm compared to 1200 and 1500 rpm. Figure 6.12b indicates that intake pressure has a greater impact on flame radius variability at higher equivalence ratios for hydrogen flames. At higher equivalence ratios, such as $\phi_{int}^{H_2} = 0.50$, flame radius variability increases with intake pressure, from a minimum of 0.59 mm at 0.6 bar to 0.79 mm at 0.9 bar. For lower equivalence ratios, flame variability remains relatively constant at around 0.62 mm regardless of intake pressure. It is interesting to note that the effect of intake pressure above 0.6 bar is most noticeable at higher equivalence ratios. This could be attributed to the fact that, at lower equivalence ratios, the flame is already highly wrinkled at these conditions and may reach a plateau in flame speed enhancement due to instabilities. In contrast, at higher equivalence ratios, where instabilities are less pronounced, this plateau might be reached at higher intake pressures (between 0.8 and 0.9 bar), as suggested by Figure 6.12b.

The effect of intake pressure on flame radius variability is also observed for propane flames. Although propane flames show lower variability than hydrogen flames, intake pressure still influences them, with a minimum variability of 0.42 mm at 0.5 bar and an increase to 0.55 mm

6.2. INFLUENCE OF ENGINE PARAMETERS ON CCVS

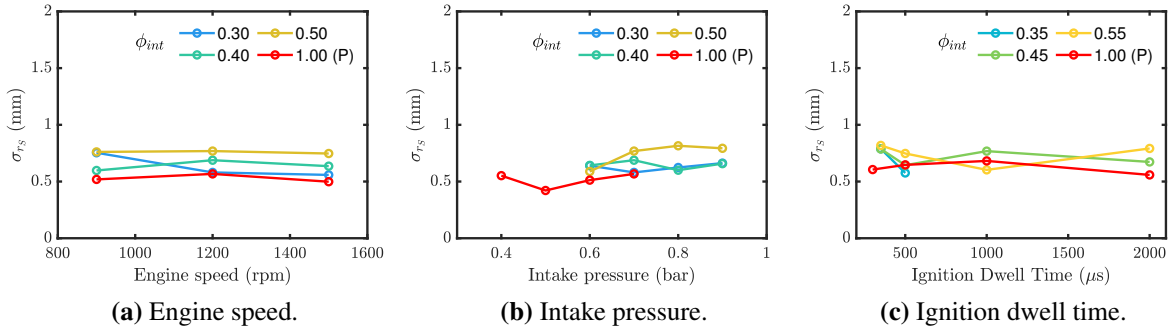


Figure 6.12: Effect of engine speed, intake pressure, and ignition dwell time on the standard deviation of the equivalent flame radius at 10 °bTDC for three hydrogen/air mixtures and a stoichiometric propane/air mixture.

at 0.4 bar and 0.57 mm at 0.9 bar. This is likely due to multiple factors, such as the increase in residual gases at lower intake pressures, changes in laminar flame properties, and greater instabilities at higher pressures. Finally, the effect of ignition dwell time is presented in Figure 6.12c. No clear relationship is observed between ignition dwell time and flame radius variability at a given crank angle.

The effect of these parameters on the standard deviation of equivalent flame propagation speed, under the same experimental conditions and crank angle, is shown in Figure 6.13. The first thing to note is that the variability in flame speed does not mirror the variability in flame radius. Figure 6.13a illustrates that, unlike flame radius, flame speed variability is influenced by engine speed depending on the equivalence ratio. Low equivalence ratio hydrogen/air flames and stoichiometric propane/air flames exhibit greater flame speed variability at higher engine speeds. For example, at an equivalence ratio of 0.40, the standard deviation increases from 0.96 m/s at 900 rpm to 1.69 m/s at 1500 rpm. However, for higher equivalence ratios, hydrogen/air flames are less affected by these changes in the flow field, as already discussed in the heat release analysis, in Chapter 3, and in the flame development characterization in Chapter 5.

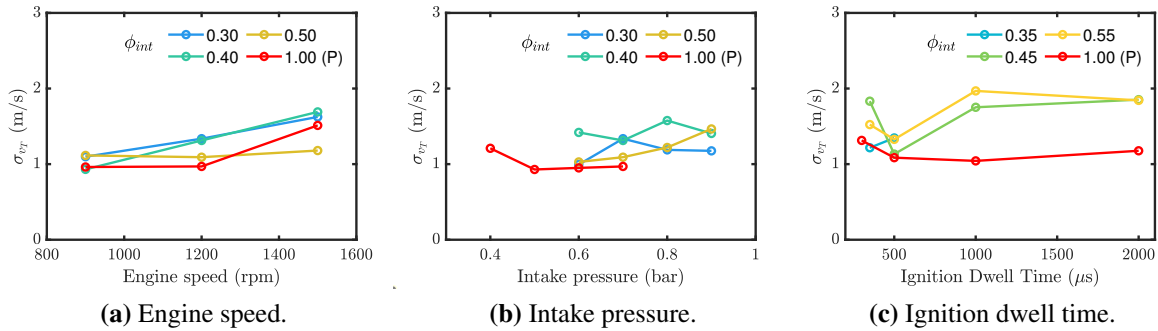


Figure 6.13: Effect of engine speed, intake pressure, and ignition dwell time on the standard deviation of the equivalent flame propagation speed at 10 °bTDC for three hydrogen/air mixtures and a stoichiometric propane/air mixture.

The impact of intake pressure on flame propagation speed variability, shown in Figure 6.13b, also depends on the mixture's equivalence ratio, as observed for flame radius variability.

ity. Changes in intake pressure affect the charge composition, particularly the residual gases at lower intake pressures. For example, stoichiometric propane/air flames are more sensitive to residual gases due to their minimum ignition energy and laminar flame speed characteristics, which leads to higher variability, especially at low loads. At an intake pressure of 0.4 bar, for instance, the standard deviation is 1.21 m/s, compared to 0.93 m/s at other intake pressures. Since hydrogen combustion is more influenced by charge composition at higher equivalence ratios, the impact of intake pressure is more pronounced in mixtures with higher equivalence ratios, such as $\phi_{int} = 0.50$. Conversely, at lower equivalence ratios, the flame development speed is primarily influenced by the flow field, which is less affected by variations in intake pressure, as discussed in Chapter 4. Therefore, flame speed variability for equivalence ratios below 0.40 is not directly impacted by changes in intake pressure.

The effect of ignition dwell time on flame propagation speed variability is examined in Figure 6.13c. For propane/air flames, an increase in variability is observed at the minimum ignition dwell time of $300\mu\text{s}$ compared to longer dwell times. For hydrogen flames, a minimum variability is observed for all three equivalence ratios at a dwell time of $500\mu\text{s}$, though no definitive conclusions can be drawn regarding a clear pattern.

Generally, cyclic variability can be attributed to four main factors: intake charge, mixture heterogeneity, spark discharge, and flow-flame interactions [98, 163]. With this engine, the design of the intake ducts and the positioning of the injector contribute to a generally homogeneous mixture at the time of ignition under all conditions. Moreover, as shown in Figure 6.13c (and further in Figure 6.26), the spark discharge appears consistent in both intensity and location across all cycles, suggesting that the observed variability is mainly due to 1) intake charge variation (the amount of air, hydrogen, and residual gases trapped in the cylinder after the intake valves close) and 2) flow-flame interactions.

The impact of intake charge variation can be assessed through a simple flame development model. A semi-spherical flame development was simulated to estimate the effect of charge composition. The variability measured in both air and fuel mass flow controllers are used to estimate the variability in equivalence ratios inside the cylinder at the end of the intake stroke with a 95% confidence interval. First, a stoichiometric propane flame is studied. With an in-cylinder equivalence ratio for a given cycle as $\phi_{cyl} = 1.00 \pm 0.01$, the resulting flame propagation velocity is $v_L = \rho_u / \rho_b \cdot s_L = 4.46 \pm 0.02$ m/s, which translates to a variability of 0.5%. Thus, the variability of equivalent propagation speed for propane ranges between 12% and 28%, with a flame radius variation of 11% at 10 °bTDC. A study by Hinze and Cheng [99] highlighted the impact of air, propane, and residual gases on early flame development in spark-ignition engines at idle, attributing 10.5% of the cyclic variability in combustion duration (from spark timing to 10% mass fraction burned) to these factors, with the remaining caused by mixture stratification and flow field variations. This trend is also observed in propane flames at higher IMEP (5 bar), where intake charge variations account for 3% of variability, consistent with the Hinze and Cheng study. These results validate the methodology used here, enabling its application to characterize the causes of hydrogen combustion variability.

For hydrogen, two distinct equivalence ratios are compared: $\phi_{int} = 0.25$ and $\phi_{int} = 0.50$. The analysis show that the in-cylinder equivalence ratios are $\phi_{cyl} = 0.226 \pm 0.003$ and $\phi_{cyl} = 0.470 \pm 0.008$, respectively. This leads to flame propagation speeds of 0.056 ± 0.003 m/s and 4.8 ± 0.3 m/s, respectively, indicating that the variation in flame propagation speed due to charge variation is about 5.8% and 6.9%. Thus, the corresponding variability in flame speed at a specific crank angle would be 6-7%. However, analyzing flame speed variability 5 CAD after

ignition, the measurements reveal a variation of about 2.6 m/s for all equivalence ratios, which is distinct from what would be expected from charge variability alone. The coefficient of variation of the flame speeds in both equivalence ratios are 60% and 8%, respectively. Additionally, the measured flame radius variability is around ± 1.2 mm, representing 14% and 8%, respectively of the mean value, for each condition. This analysis shows that intake charge variability is not solely responsible for the combustion variability, and its impact on engine performance depends on the mixture, and that hydrogen flames are overall less sensitive to flow field variations than propane flames under similar intake pressure and spark timing conditions.

Applying this approach to both hydrogen and propane flames, we can estimate the impact of charge composition and flow-flame interactions. Figure 6.14 presents the coefficient of variation (CoV) for flame speed at 10 °bTDC for both fuels. The CoV for equivalent flame propagation speed is highly dependent on equivalence ratio, with higher flame speeds yielding lower CoV values. For example, the CoV is minimal (around 8-9%) for $\phi_{int}^{H_2} = 0.50$ and 0.55 and $\phi_{int}^{C_3H_8} = 1.00$, and maximal (60%) for $\phi_{int}^{H_2} = 0.20$ and 28% for $\phi_{int}^{C_3H_8} = 0.70$. These results suggest that hydrogen combustion is more sensitive to charge composition than propane, especially at equivalence ratios near 0.50.

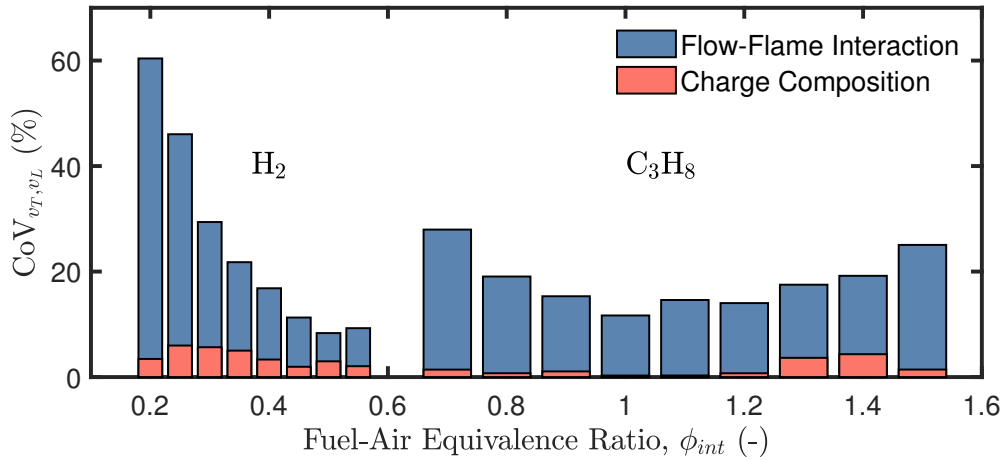


Figure 6.14: Impact of flow-flame interactions and charge composition on the coefficient of variation of the equivalent flame propagation speed at 10 °bTDC (blue) and theoretical charge composition variability effect on laminar flame propagation speed (red) for hydrogen/air and propane/air flames across a wide range of equivalence ratios.

In a homogeneous charge spark-ignition engine, small variations in mixture composition can have a greater impact on combustion than in well-known fuels, such as gasoline, where the mixture is typically heterogeneous due to direct injection. This suggests that in engines operating with direct injection and lean hydrogen/air mixtures, the sensitivity of flame speed to equivalence ratio could significantly increase, making mixture composition a key factor in combustion variability.

6.3 Cycle-by-cycle analyses

After completing the overall variability analysis, a more detailed cycle-by-cycle assessment can be conducted to further investigate differences between cycles under specific experimen-

tal conditions that displayed particular characteristics in the overall study. Two analyses are presented in this section. The first examines the behavior of individual cycles using both heat release and flame imaging techniques, comparing both fuels. The second analysis compares in-cylinder flame behavior with the specific aerodynamics of the given cycle, aiming to understand the influence of turbulence and large-scale flow structures on hydrogen flame development.

6.3.1 Heat release and in-cylinder flames

The cycle-by-cycle comparison of both heat release and flame images is conducted for two distinct cases for each fuel. The analyzed flames are: propane/air mixtures with equivalence ratios of 0.70 and 1.00, and hydrogen/air mixtures with equivalence ratios of 0.25 and 0.50. These operating conditions were selected due to their contrasting performance characteristics in both analyses, representing two different scenarios: one fast and one slow. The slower scenarios are more prone to higher CCVs.

Propane

Starting with the propane/air flames, Figure 6.15 shows the in-cylinder pressure trace (a) and the mass fraction burned (b) as a function of the crank angle for an equivalence ratio of 1.00. All 100 cycles are displayed in gray, with the 10 slowest cycles highlighted in blue and the 10 fastest in red. These cycles are defined as the slowest and fastest based on when they reach 10% of MFB. The pressure traces for these cycles exhibit similar behavior in the initial crank angles after ignition, with a clear distinction between the fastest and slowest cycles. After 20°, the cycles generally diverge, indicating that cycles which start slower do not necessarily result in the lowest maximum pressure, although they tend to remain below the mean pressure trace.

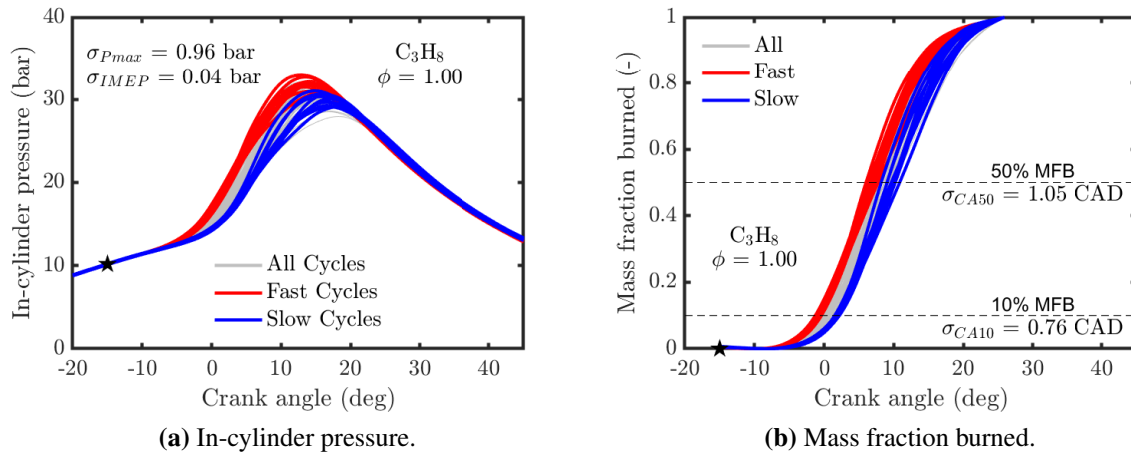


Figure 6.15: Heat release analysis parameters for a propane/air flame with an intake fuel-air equivalence ratio of 1.00. All 100 cycles are plotted in gray, with the 10 fastest cycles in red and the 10 slowest cycles in blue.

Additionally, the standard deviations for both maximum pressure and IMEP are low, with values of 0.96 bar (3.2% of the mean) and 0.04 bar (0.7%), respectively. Regarding the mass

6.3. CYCLE-BY-CYCLE ANALYSES

fraction burned, the same pattern of clear distinction between fast and slow cycles during the early combustion phase, followed by divergence around CA50, can be observed. The standard deviations for CA10 and CA50 are also low, at 0.76 CAD (5% of the mean) and 1.05 CAD (4.6%), respectively.

In Figure 6.16, the same analysis is performed for the lower equivalence ratio case (0.7). In this case, the operating condition is near the lower misfire limit. This is evident from the misfire case among the 100 cycles, as shown in Figure 6.16a, where the pressure trace resembles motoring conditions, with no noticeable pressure increase due to combustion. This operating condition exhibits high variability in in-cylinder pressure, especially in the slowest cycles, due to poor combustion efficiency and even misfire. In these cases, combustion can vary significantly, leading to higher maximum pressure variability, as indicated by the standard deviation of 1.53 bar (10.2% of the mean). This variability also has a significant impact on IMEP and overall performance. As highlighted previously, the standard deviation of 0.47 bar represents 12.7% of the mean, indicating high operational variability, which compromises the stability of the condition.

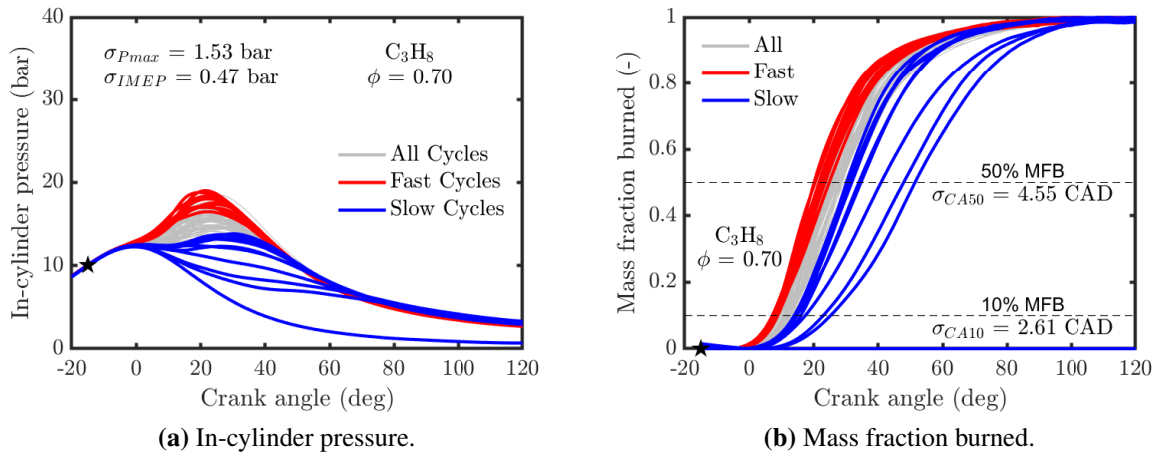


Figure 6.16: Heat release analysis parameters for a propane/air flame with an intake fuel-air equivalence ratio of 0.70. All 100 cycles are plotted in gray, with the 10 fastest cycles in red and the 10 slowest cycles in blue.

The MFB behavior in the in-cylinder pressure trace under this condition (Figure 6.16b) confirms the variability in combustion, especially in the slowest cycles. As shown, the primary difference in combustion progress stems from the slowest cycles (and misfires). In these cases, the flame can take up to twice as long as the average cycle to reach 10% or 50% MFB, which, as previously discussed, affects the pressure trace. Since the mixture is mostly homogeneous in this engine configuration, the likely cause of this behavior is the interaction between the flame and the aerodynamics near the spark timing and spark plug. This interaction could push the flame towards the combustion chamber wall or back to the spark plug, increasing heat exchange and causing flame quenching, thus slowing combustion, or in extreme cases, extinguishing the flame entirely, as shown by Welch et al. [164] with homogeneous iso-octane/air flames.

Figure 6.17 illustrates the flame development behavior for both equivalence ratios as a function of crank angle. The fast and slow cycles, as defined earlier, correspond to the cycles with the largest and smallest flames at a given crank angle, respectively, for both cases. Moreover,

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for a given flame radius, the slower flames exhibit greater fluctuation in crank angle, with higher variability at $\phi_{int} = 0.70$ compared to $\phi_{int} = 1.00$. This indicates that flame development speed significantly influences the in-cylinder pressure trace in propane/air mixtures. Slower flames tend to exhibit longer combustion durations and, therefore, greater pressure trace variability due to the extended time required to achieve complete combustion. In contrast, faster flames, with shorter combustion durations, allow less time for cycle-to-cycle variation, leading to lower pressure trace variability. This phenomenon was also observed for propane/air flames in a LES study [71].

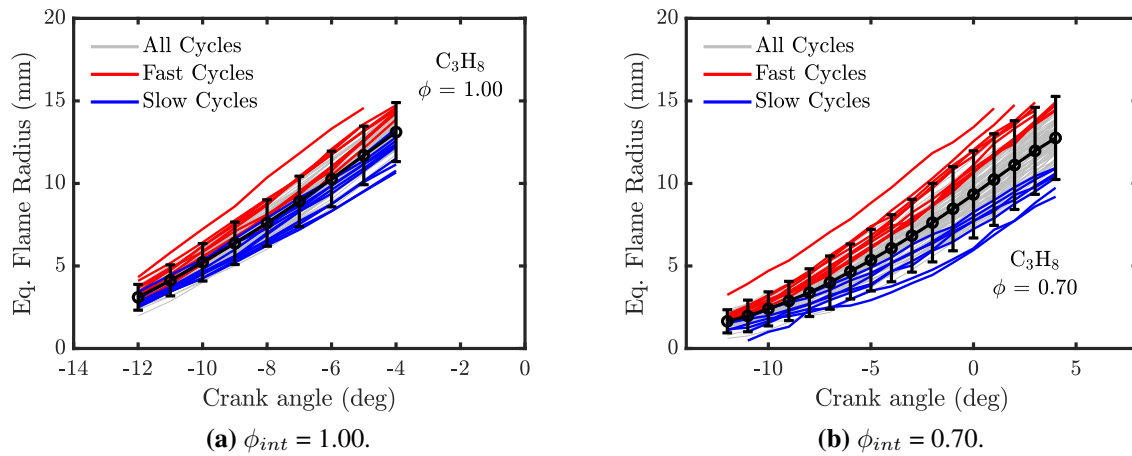


Figure 6.17: Equivalent flame radius as a function of the crank angle. The black line with dots represents the mean value, and the error bars represent two times the standard deviation. All 100 cycles are plotted in gray, with the 10 fastest cycles in red and the 10 slowest cycles in blue.

To further investigate flame variability, the flame probability density function is compared across all, fast, and slow cycles. Figure 6.18 shows the flame PDF for 9 crank angle degrees, ranging from 12 to 4 °bTDC. These PDFs are generated by calculating the probability of flame appearance at each pixel over 100 cycles (all), and separately over the 10 fastest and 10 slowest cycles. The general flame PDF reveals an ellipsoidal flame shape that develops consistently without significant changes until it reaches the field of view. The PDF of the fastest flames also displays an ellipsoidal shape, with faster development than the mean flame, as expected. Flame variability, represented by the gray-scale within the figure, is visible to some extent; however, it does not provide a clear view of the flame shape for individual cycles. The slowest flames show behavior similar to the fastest flames, but with a slower development compared to the mean and a slightly higher degree of variability. The difference in flame size in relation to crank angle timing between the fastest and slowest cycles is approximately 1 to 2°.

Figure 6.19 shows the 50% probability flame contour for all, the fastest, and the slowest cycles as a function of crank angle. Even at the first measurable angle, the flame size is distinct for each condition, though the shape remains similar across all three cases. As the flame develops, the difference in size between the fast and slow cycles compared to the mean becomes more pronounced. This indicates that not only was the initial flame size different, but the flame speed also varied, further increasing the discrepancy as the flame progressed.

The flame PDF of the lower equivalence ratio mixture cycles was also analyzed. Although its development is slower, as shown by the crank angle degrees in Figure 6.20, the flame shape

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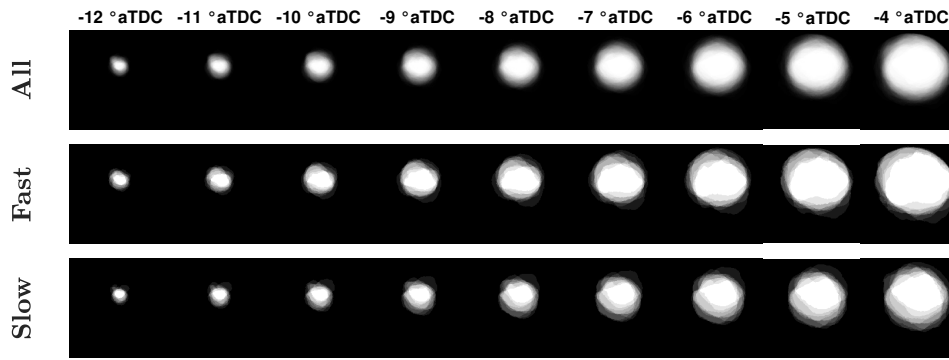


Figure 6.18: Flame PDF for all 100 cycles (top), the 10 fastest cycles (middle), and the 10 slowest cycles (bottom) for a propane/air flame with an equivalence ratio of 1.00.

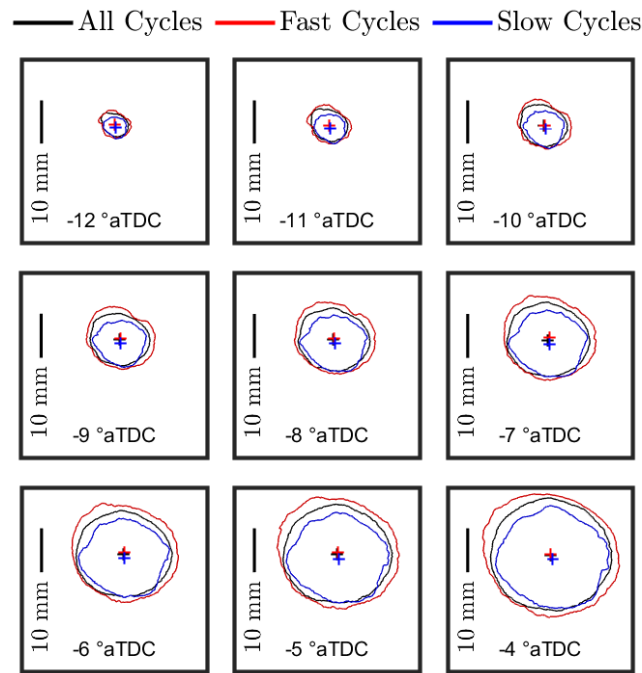


Figure 6.19: Flame contour at the 50% probability level for all 100 cycles (top), the 10 fastest cycles (middle), and the 10 slowest cycles (bottom) for a propane/air flame with an equivalence ratio of 1.00.

in the PDF for all cycles is similar to that of the stoichiometric condition. However, the fastest and slowest cycles display distinct behaviors. For the fast cycles, the PDF gray-scale reveals significant differences between individual cycles, making it possible to almost visualize the individual flame shape of each cycle, i.e. each contour development is different. This suggests that the fast cycles vary greatly in flame development, resulting in a highly divergent PDF. The slowest cycles exhibit even more variability. Initially, the flame shape is much smaller than in the mean and fast cycles and develops in different directions, leading to a lower probability of

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flames occupying the same region. As the flame grows, its speed, as also indicated in the MFB figure for this condition, and its path differ between cycles, further increasing the variation. This results in a PDF that is significantly different from the mean and fast cycles.

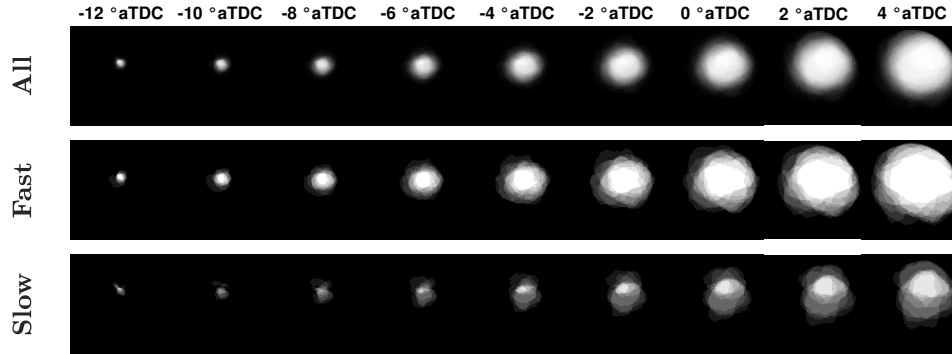


Figure 6.20: Flame PDF for all 100 cycles (top), the 10 fastest cycles (middle), and the 10 slowest cycles (bottom) for a propane/air flame with an equivalence ratio of 0.70.

Based on the previous discussion, Figure 6.21 illustrates the difference between the mean, fast, and slow cycles using the 50% probability flame contour. The flame contour for all cycles presents a more circular shape compared to the others. The fastest cycles show a larger, elliptical flame contour until reaching TDC, after which it becomes more circular. As with the case for $\phi_{int} = 1.00$, the size difference between the fastest and mean flames increases as the flame progresses. The slowest flame contours are significantly smaller than the mean, not only due to misfires (which reduce the overall PDF by 10%) but also because of the variability in both flame size and trajectory. This results in a deformed shape, neither circular nor elliptical, caused by these fluctuations. The fast flame contour is 2 to 4 CAD ahead of the mean contour, while the slow flame contour lags by about 6 CAD.

Hydrogen

The same analysis was conducted for both hydrogen conditions. Figure 6.22 shows the in-cylinder pressure trace and mass fraction burned as a function of the crank angle for an equivalence ratio of 0.50. Statistics are calculated over 500 cycles for all cycles, and 50 for both fast and slow cycles. Unlike propane/air flames, in this condition, the fastest and slowest cycles maintain their respective behaviors until the end of combustion, meaning that the initial stage of combustion determines the cycle's performance throughout. This is evident in both the pressure trace and the MFB curve. The standard deviation of the pressure trace is 0.51 bar, half of the value for propane/air at stoichiometry. Additionally, the IMEP variability is practically the same, but for half the mean value, suggesting that hydrogen can achieve a more stable operating condition at lower loads. Furthermore, the variability in combustion progress is also lower for hydrogen/air flames at an equivalence ratio of 0.50. The crank angle degrees required to reach 10 and 50% of MFB vary by only 0.43 and 0.65 CAD, respectively - two-thirds of the values for the stoichiometric propane flame. This indicates that the hydrogen flame exhibits less variability in CAD to reach a given flame radius, which is further explored in the flame imaging analysis.

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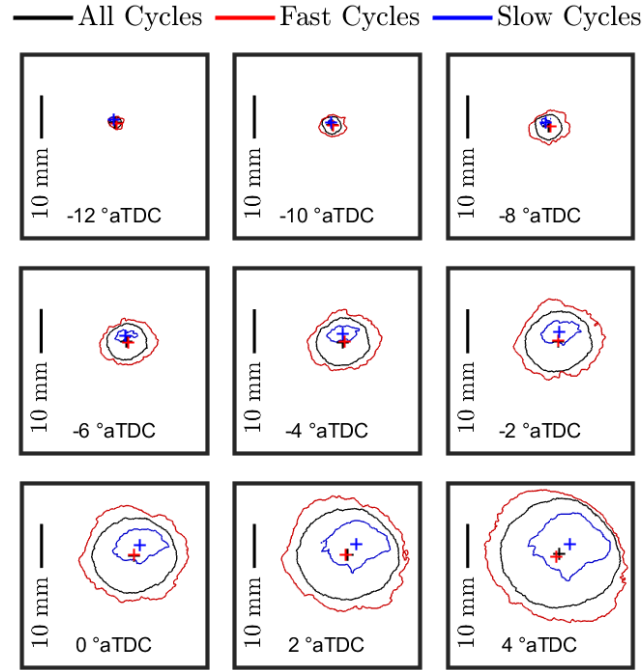


Figure 6.21: Flame contour at the 50% probability level for all 100 cycles (black), the 10 fastest cycles (red), and the 10 slowest cycles (blue) for a propane/air flame with an equivalence ratio of 0.70.

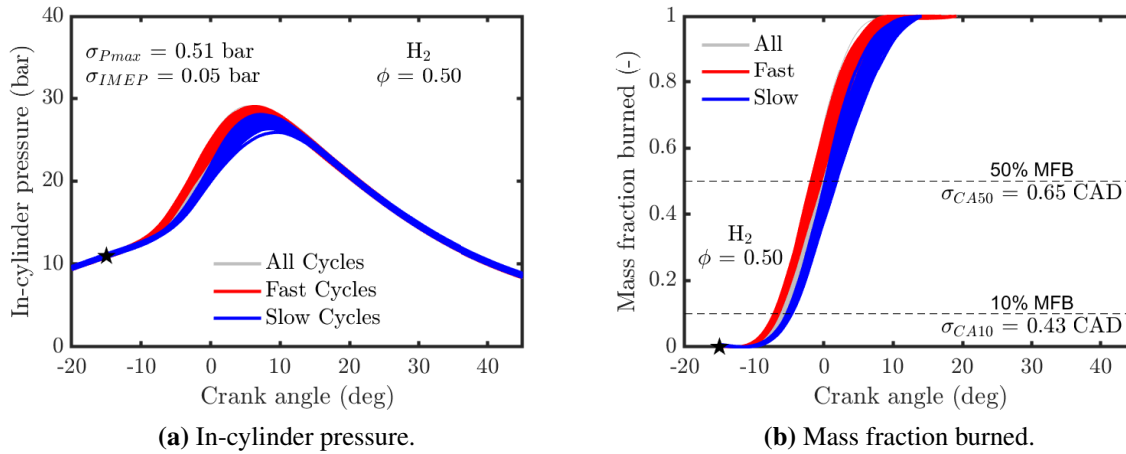


Figure 6.22: Heat release analysis parameters for a hydrogen/air flame with an intake fuel-air equivalence ratio of 0.50. All 500 cycles are plotted in gray, with the 50 fastest cycles in red and the 50 slowest cycles in blue.

Figure 6.23 presents the results for an equivalence ratio of 0.25, where the mean IMEP value (load) is much smaller, around 1.0 bar. In this case, the in-cylinder maximum pressure has a standard deviation of only 0.14 bar. Since the combustion timing is not optimized and CA50 is located at 30 °aTDC, the pressure rise occurs later in the power stroke, as discussed previously.

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The maximum pressure is either due to compression in the slow cycles or combustion in the fast cycles, but it is not much higher than the compression peak and occurs 5 to 10 °aTDC. Additionally, since all cycles exhibit stable ignition despite the low equivalence ratio, the IMEP variation, at 0.11 bar, is similar to that of the higher equivalence ratio case. This behavior contrasts with propane/air flames, where the standard deviation increased more than tenfold at lower equivalence ratios. This is even more noteworthy considering the lower load, which typically allows for more combustion variability.

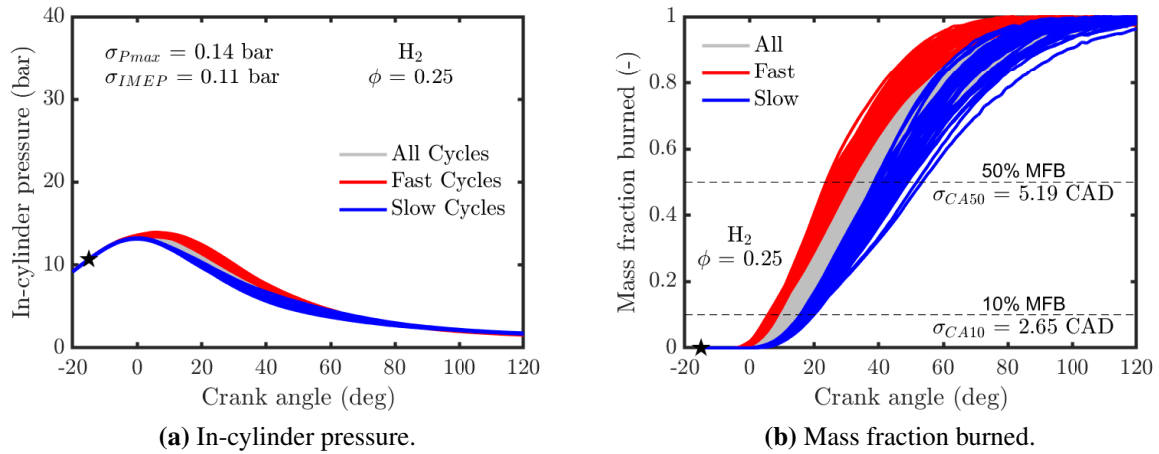


Figure 6.23: Heat release analysis parameters for a hydrogen/air flame with an intake fuel-air equivalence ratio of 0.25. All 500 cycles are plotted in gray, with the 50 fastest cycles in red and the 50 slowest cycles in blue.

The mass fraction burned, shown in Figure 6.23b, highlights the slow combustion in this operating condition and the variability resulting from it. The variability in combustion progress is similar to that of low equivalence ratio propane/air flames, as seen in the overall analysis. The variability in combustion duration increases by about 6 to 8 times compared to $\phi_{int} = 0.50$, even though the in-cylinder maximum pressure and IMEP variation remain nearly the same. This behavior is addressed further in the next subsection.

The equivalent flame radius development for both equivalence ratios is shown in Figure 6.24. As with propane, higher in-cylinder pressure and faster MFB are associated with quicker flame development in the combustion chamber. However, the variability at each crank angle degree appears to increase much more gradually than in propane flames. This suggests that the hydrogen flame, at both equivalence ratios, develops in a more uniform manner, and that the differences between slow, mean, and fast cycles are less pronounced compared to propane flames. This would also explain the lower variability in both in-cylinder maximum pressure and IMEP.

Figure 6.25 displays the flame PDF for all 500 cycles, as well as for the 50 fastest and slowest cycles, for a hydrogen/air mixture with an equivalence ratio of 0.50. The flame PDFs are circular and very similar in both shape and intensity. From these experiments, it can be observed that the overall shape of the fastest cycles resembles that of the mean cycles but is shifted 1 CAD earlier, whereas for the slowest flames, it is shifted 1 CAD later to reach a given flame radius. This shift appears consistent from the first to the last measurable crank angle.

Figure 6.26 displays the 50% flame probability contours for the three cases. The first image

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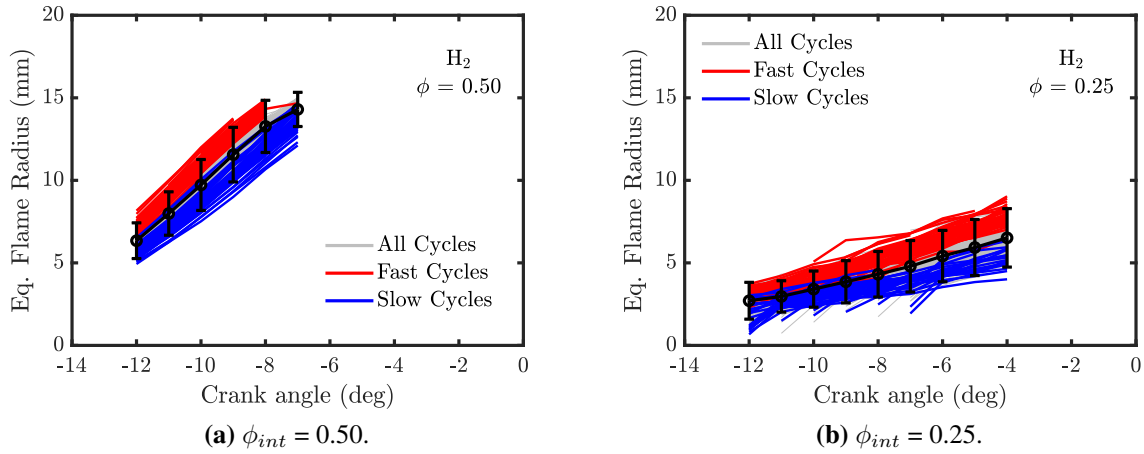


Figure 6.24: Equivalent flame radius as a function of the crank angle. The black line with dots represents the mean value, and the error bars represent two times the standard deviation. All 500 cycles are plotted in gray, with the 50 fastest cycles in red and the 50 slowest cycles in blue.

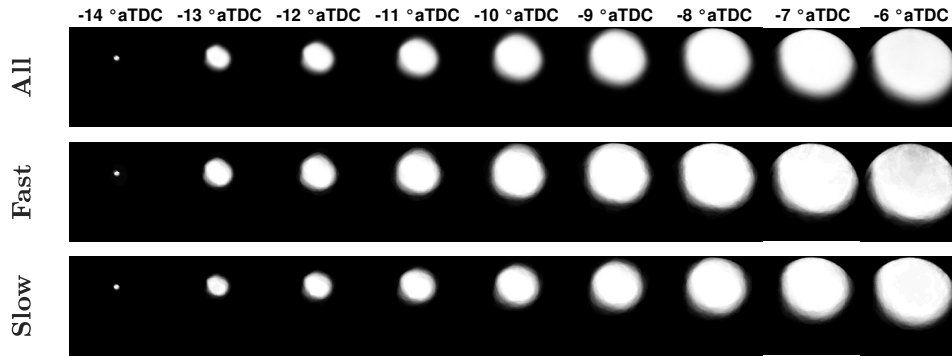
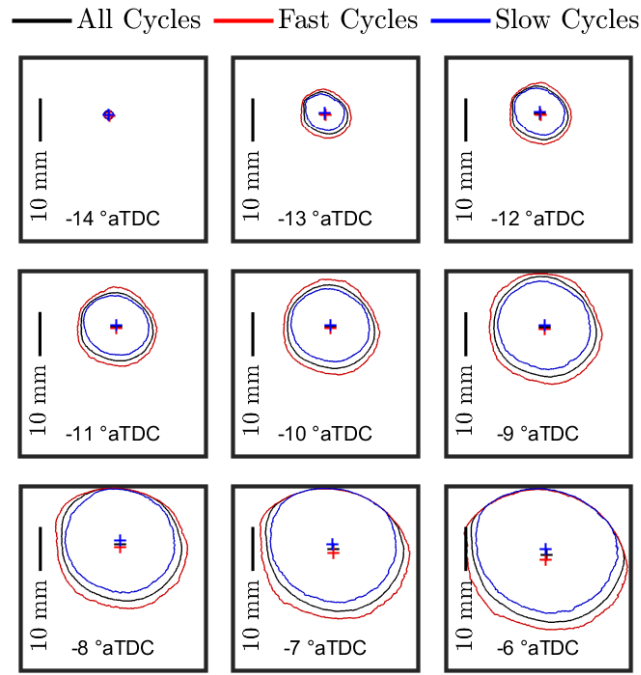


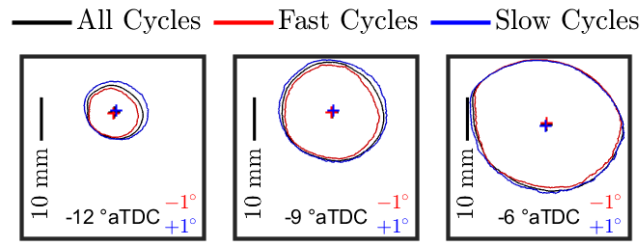
Figure 6.25: Flame PDF for all 500 cycles (top), the 50 fastest cycles (middle), and the 50 slowest cycles (bottom) for a hydrogen/air flame with an equivalence ratio of 0.50.

is captured 1 CAD after spark timing, while the spark is still visible on the high-speed camera. This initial stage is repetitive, as the flame size and location are similar across all cases. At the first measurable crank angle, the flame contours already show distinctions, with the fastest flames having a larger size and the slowest flames a smaller size, as expected. As the crank angle increases and the flames develop, the growth in each case remains consistent, with the differences between them not changing significantly. As observed previously, the fast and slow cycles can be related to a shift of -1 or +1 CAD from the mean, respectively, as illustrated in Figure 6.26b.

Finally, the comparison is made for the low equivalence ratio condition, where the flame is considerably slower. Figure 6.27 illustrates the flame PDF for all cycles, as well as the fastest and slowest cycles, over a wide range of crank angles. In this condition, the flame shape and behavior remain similar across cases. The flame starts with an elliptical shape, which gradually transforms into a circular shape as combustion progresses. Comparing both the fast and slow cycles to the mean, a shift of 2 to 4 CAD can be observed, with fast cycles showing a negative



(a) Normal crank angle degrees.



(b) Shifted crank angle degrees for fast and slow cycles.

Figure 6.26: Flame contour at the 50% probability level for all 500 cycles (black), the 50 fastest cycles (red), and the 50 slowest cycles (blue) for a hydrogen/air flame with an equivalence ratio of 0.50.

shift and slow cycles showing a positive one. This aligns with the decrease in combustion speed and the increase in combustion duration, which are approximately one-third and three times the values of the parameters at an equivalence ratio of 0.50, respectively.

The 50% probability contours for this condition are shown in Figure 6.28. In the first flame image for all three cases, differences between the fast and slow cycles are already noticeable, with the fast cycles developing slightly quicker on the right side of the figure compared to the slow cycles. This difference becomes more pronounced as the crank angle increases, initially in the tumble direction (from left to right) and then in the counter-tumble direction (from 2 °bTDC onward). The variation between fast and slow cycles is more significant in this condition than in the other hydrogen equivalence ratio, although the overall flame contour shape remains similar. The disparity between fast and slow cycles becomes more evident at the last measurable crank angle, especially for the fastest cycles. Moreover, the lower flame temperatures of ultra-lean hydrogen-air flames reduce heat loss to the spark plug and other surfaces due to the smaller

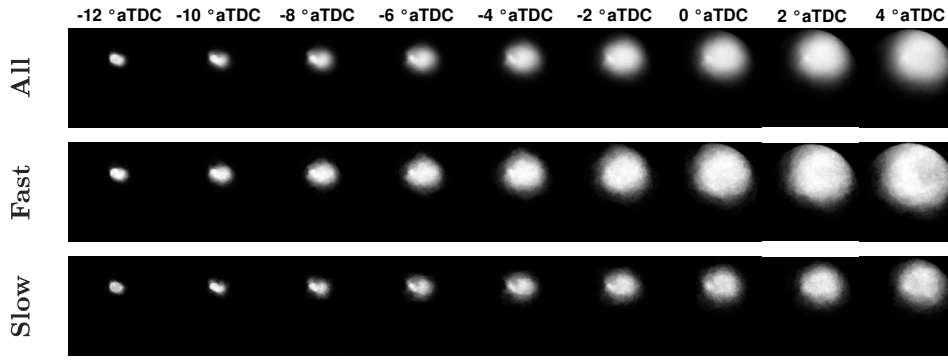


Figure 6.27: Flame PDF for all 500 cycles (top), the 50 fastest cycles (middle), and the 50 slowest cycles (bottom) for a hydrogen/air flame with an equivalence ratio of 0.25.

temperature difference. This could lessen the influence of heat loss on flame development variability, thereby reducing the impact of flow field variability as well. This hypothesis is supported by Figure 3.3, which shows that colder spark plugs - where heat loss is higher - exhibit greater variability compared to hotter spark plugs.

6.3.2 In-cylinder flames and associated velocity fields

Further experiments were conducted using simultaneous PIV and chemiluminescence to investigate the impact of flow variability in hydrogen/air flames and to better understand the low operating variability in this homogeneous charge H₂ICE.

Vertical chemiluminescence measurements

Figure 6.29 presents an image of a hydrogen/air flame with an equivalence ratio of 0.5, captured by the high-speed camera in the experimental setup, which includes a dichroic mirror and band-pass filter. The first panel shows the raw image, followed by the extracted flame contour, and finally the position of the flame's right and left extremes. From these extremes, various flame parameters can be calculated, such as equivalent flame radius, centroid position, flame speed, and more.

Figure 6.30 illustrates key parameters for a specific operating condition: $P_{int} = 0.7$ bar, $N = 1200$ rpm, and $\phi_{int} = 0.40$. This equivalence ratio enables longer measurement times than $\phi_{int} = 0.50$. Moreover, the flame appears to be less spherical, allowing for the exhibition of the tumble flow effect on flame development for a longer time before the end of the measurement. The flame contour as a function of the crank angle over 100 cycles is displayed in Figure 6.30a. As expected, the right flame extreme develops faster than the left due to the tumble motion, reaching the right side of the field of view (FoV) as early as 7 crank angle degrees (CAD) after ignition. The left flame extreme develops more slowly because it moves against the flow field and must achieve a higher velocity than the flow to progress in that direction, reaching the left side of the FoV 15 CAD after ignition. Additionally, the mean value and two times the standard deviation represent the overall flame behavior well.

From the flame contour extremes, the equivalent flame radius was calculated as half the distance between the left and right extremes. This parameter is shown in Figure 6.30b, which

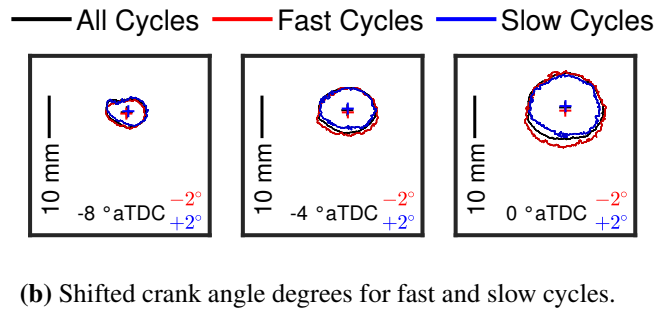
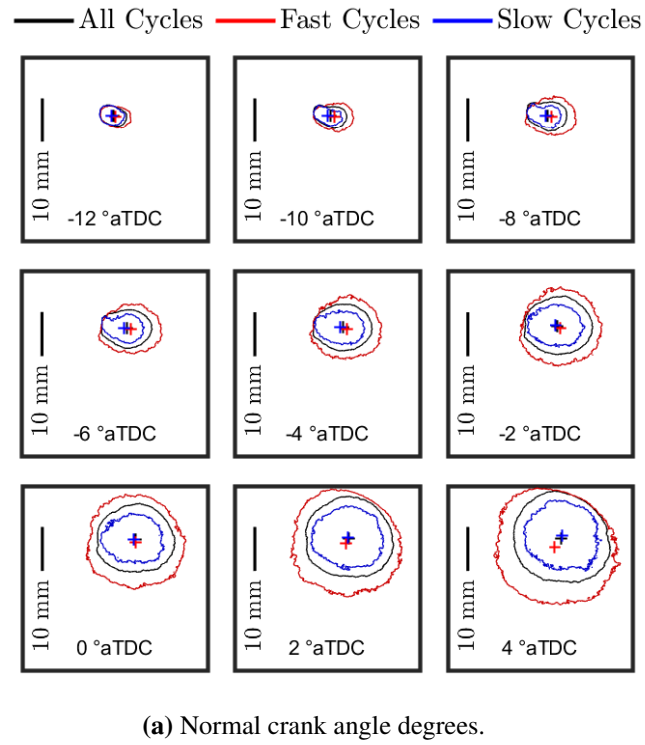


Figure 6.28: Flame contour at the 50% probability level for all 500 cycles (black), the 50 fastest cycles (red), and the 50 slowest cycles (blue) for a hydrogen/air flame with an equivalence ratio of 0.25.

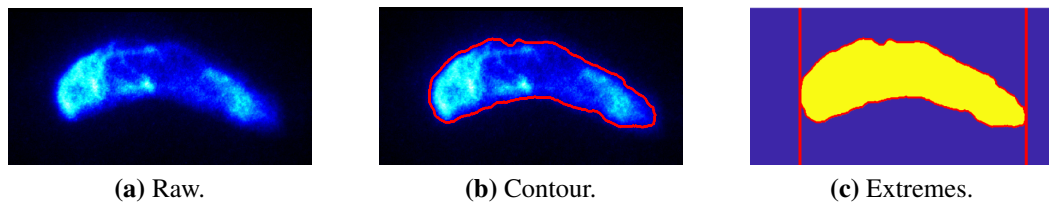


Figure 6.29: Chemiluminescence flame methodology for extracting the extremes position from a hydrogen/air flame with an equivalence ratio of 0.50, viewed through the vertical optical access to the combustion chamber.

displays all cycles, as well as the 10 fastest and 10 slowest cycles. The flames that start larger generally remain larger throughout the FoV and combustion duration, as observed in the in-cylinder pressures for hydrogen flames. The fastest and slowest cycles were defined by the

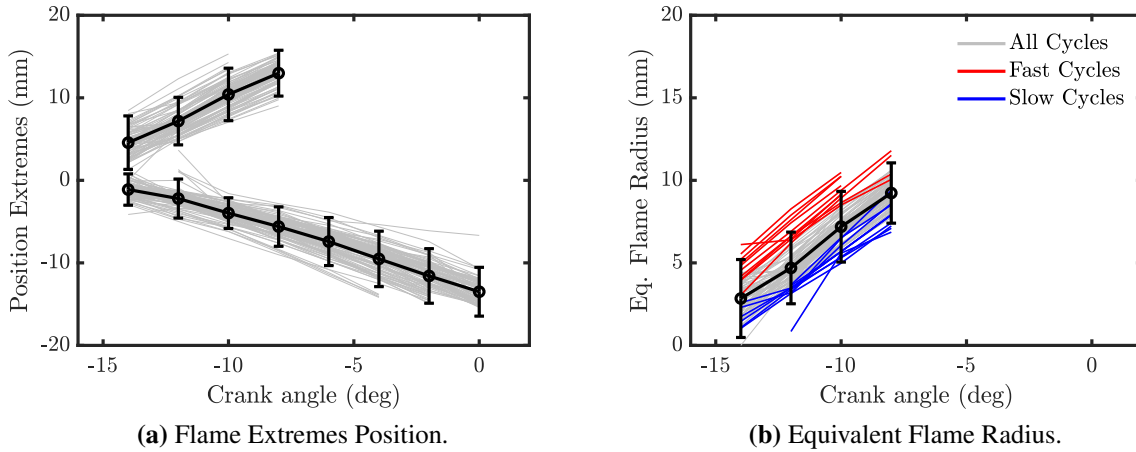


Figure 6.30: Position of flame extremes for all cycles and equivalent flame radius with indication of the 10 fastest and 10 slowest cycles as a function of the crank angle for a hydrogen/air flame with $\phi_{int} = 0.40$.

largest and smallest flame sizes at 12 °bTDC, and these flames consistently remain, indeed, the largest and smallest throughout the entire flame measurement and combustion duration.

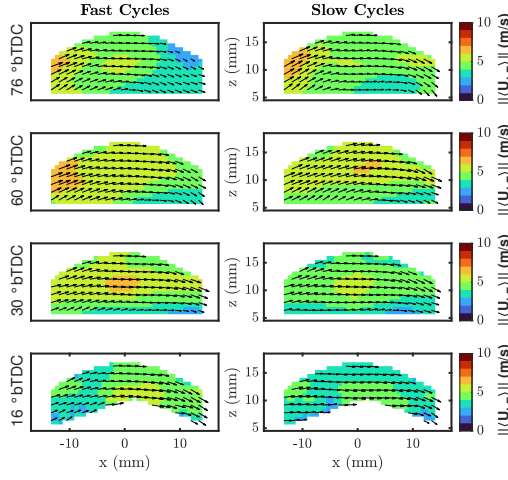
Simultaneous PIV and Chemiluminescence

Figure 6.31 shows the mean in-cylinder flow for the 10 fastest and slowest cycles before and after combustion, along with the hydrogen/air flame at 50% probability for three different equivalence ratios (0.30, 0.40, and 0.50) at the same engine speed (1200 rpm) and intake pressure (0.7 bar). The comparison between the flow of fast and slow cycles reveals a distinct flow speed near the spark plug center ($-5 < x < 5$ mm and $8 < z < 13$ mm) at 30 and 16 °bTDC, which corresponds to 15 and 1 CAD before spark timing. The stronger flow near the spark plug during ignition in the fast cycles and weaker flow in the slow cycles suggest that flow characteristics influence combustion development across multiple equivalence ratios.

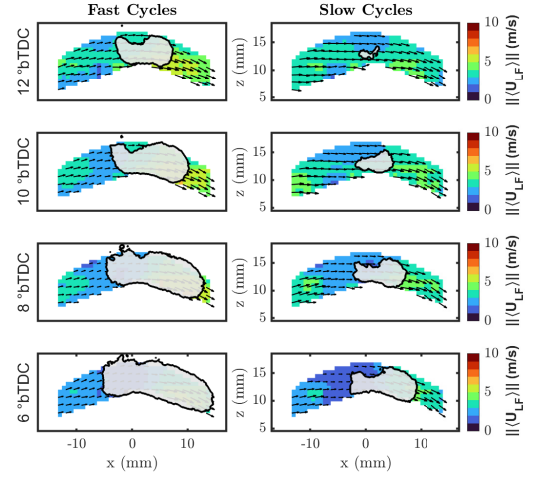
As previously discussed, this initial interaction between the flow and the flame during early flame development is critical and may determine the entire combustion event. In this type of engine, stronger flow in the positive x -direction accelerates the flame's movement away from the spark gap. As it moves away from surfaces, the heat transfer becomes less important and the flame is less subject by quenching, making the flame development faster, which is not the case if it is pushed towards the cylinder head in the early flame phase by the flow. Even during combustion, in the early crank angles, faster flows are noticeable near the flame, particularly along the right contour, for all cases. This supports the hypothesis that variations in flow near the spark plug at the start of combustion contribute to fast and slow cycles.

To delve deeper into the influence of the flow pattern on flame development, an analysis of the flow structures near the spark plug and the flame itself was conducted. Figure 6.32 presents four correlations between pairs of variables for a flame with an equivalence ratio of 0.40, under conditions of 1200 rpm and 0.7 bar of intake pressure. The Pearson's correlation coefficient, denoted as r , is displayed for each variable pair, quantifying the strength and direction of their linear relationship. The coefficient is calculated using Equation 6.1 and ranges from -1 to +1.

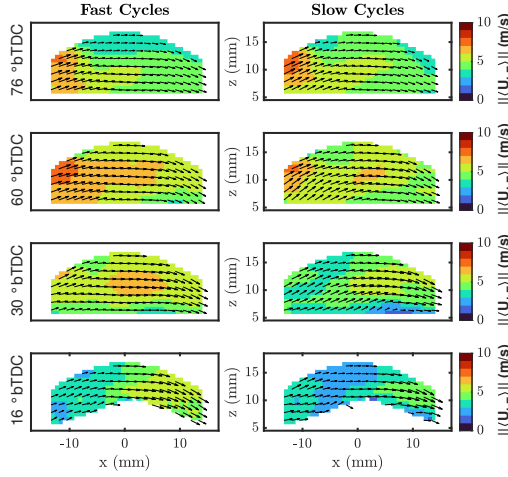
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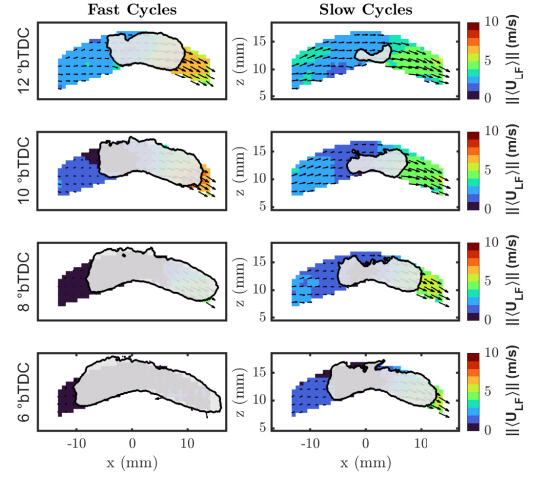
(a) Flow before spark ignition ($\phi_{int} = 0.30$).



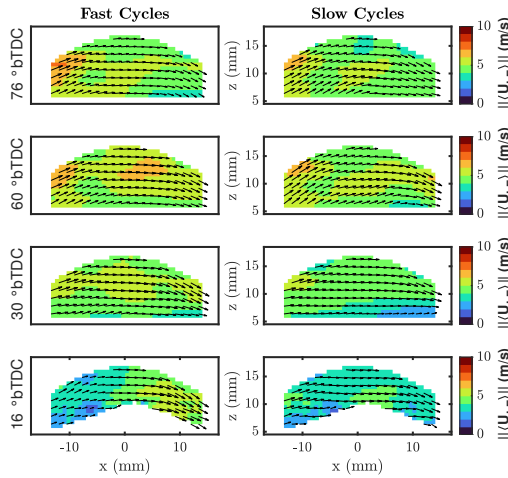
(b) Flow and flame after spark ignition ($\phi_{int} = 0.30$).



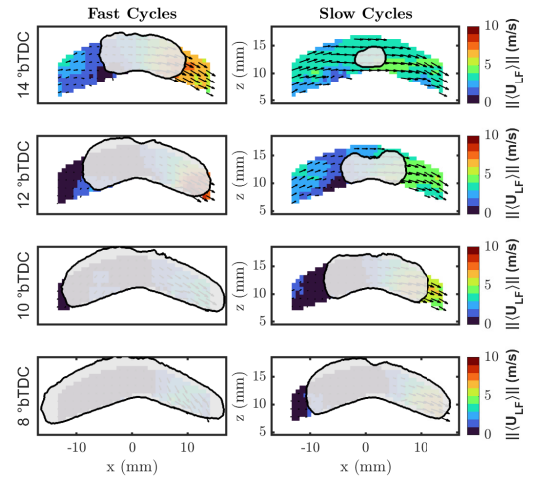
(c) Flow before spark ignition ($\phi_{int} = 0.40$).



(d) Flow and flame after spark ignition ($\phi_{int} = 0.40$).



(e) Flow before spark ignition ($\phi_{int} = 0.50$).



(f) Flow and flame after spark ignition ($\phi_{int} = 0.50$).

Figure 6.31: Simultaneous PIV and chemiluminescence measurements of hydrogen/air mixtures.

$$r = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^n (X_i - \bar{X})^2 \cdot \sum_{i=1}^n (Y_i - \bar{Y})^2}} \quad (6.1)$$

Here, X_i and Y_i represent individual data points, while $\bar{X}$ and $\bar{Y}$ are the means of X and Y , respectively. A value of $|r|$ between 0 and 0.3 indicates a weak linear correlation, values between 0.3 and 0.5 indicate a moderate correlation, and values greater than 0.5 signify a strong linear relationship.

Figure 6.32a presents a scatter plot of 100 cycles, showing the relationship between the rightmost extreme position of the flame, x_R , and the equivalent flame radius, $r_F = (x_R - x_L)/2$, measured 5 CAD after ignition. The plot reveals a clear linear relationship between these two variables: flames with a rightmost extreme located farther from the spark plug generally have a larger equivalent flame radius. Additionally, the fast cycles (in red) and slow cycles (in blue) are consistently distributed in the scatter plot, indicating that a faster development of the right extreme of the flame corresponds to a larger flame radius (i.e., the average distance between the right and left extremes). This qualitative observation is quantitatively confirmed by the Pearson coefficient of 91.8%, indicating a strong positive correlation.

Figure 6.32b explores the correlation between low-frequency (LF) and high-frequency (HF) velocity components within a cycle, calculated using the EMD method to capture variations in the flow field. The LF velocity is computed as the mean flow-field velocity near the spark plug (within $x = -5$ – $+5$ mm and $y = 8$ – 13 mm), representing the low-frequency flow structure that interacts with the flame during its early stages. The data from -30 to -16 °bTDC are used in the computation of the average in order to provide a robust spatial and time average of the LF flow. For the HF velocity, the same spatial region and crank angle range are used, but instead of calculating the mean (which would approach zero due to the isotropic and homogeneous nature of turbulence near TDC), the root-mean-square (RMS) is computed. This highlights HF fluctuations just before spark timing, reflecting the turbulence level near the spark plug that the flame encounters. These two variables exhibit a weak linear correlation ($r \approx 22\%$), suggesting that under these experimental conditions, the LF flow is not strongly linked to HF turbulence.

Figure 6.32c examines the relationship between the LF velocity component and the equivalent flame radius. The analysis reveals a moderate linear correlation ($r = 32.2\%$), indicating that LF flow structures positively and moderately influence flame development – i.e., faster LF flows near the spark plug before ignition lead to higher flame speeds. This trend is further evidenced by the distribution of fast and slow cycles in the scatter plot. Slow cycles are concentrated in zones where U_{LF} ranges from 2 to 6 m/s, whereas fast cycles are associated with LF velocities between 4 and 8 m/s.

Conversely, Figure 6.32d investigates the impact of HF turbulence near the spark plug center electrode on flame development speed. The Pearson coefficient here is lower than for the LF velocity field, indicating that the LF component has a more direct influence on flame size than the HF component. This difference is also apparent in the scatter plot: the fast and slow cycles show no clear organization, unlike in Figure 6.32c, underscoring the weak correlation between HF turbulence and flame radius under this condition.

The sensitivity of this analysis was tested for variations in the spatial region of the flow field (e.g., near the spark plug versus the entire combustion chamber), the timing of flame characteristic measurements (e.g., 5 – 10° after ignition), the historical flow data range (e.g., -30 to -16 °bTDC versus only -16 °bTDC), and the flame characteristic used (e.g., equivalent flame

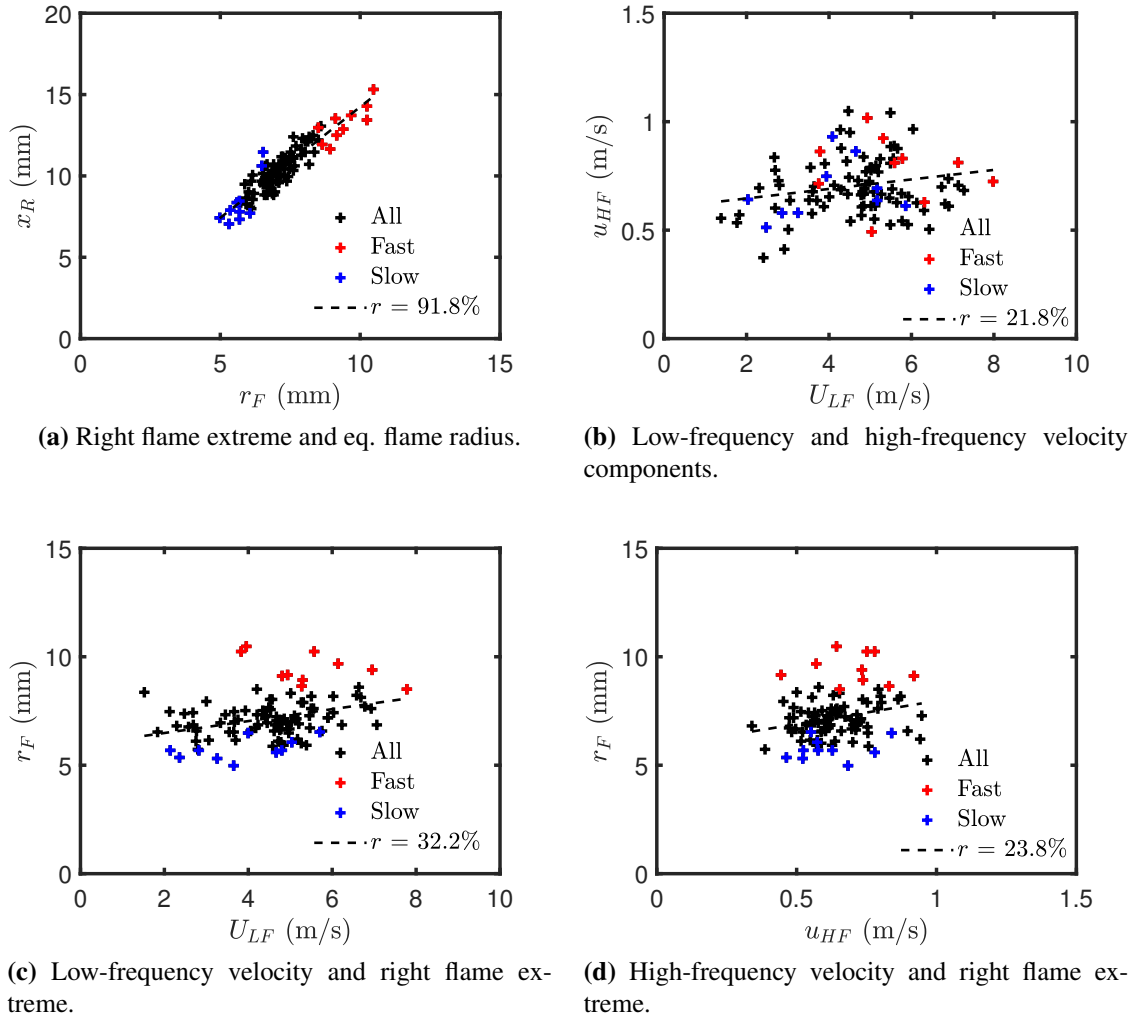


Figure 6.32: Scatter plots of 100 cycles from simultaneous PIV-Chemiluminescence measurements of a hydrogen/air flame with an equivalence ratio of 0.40, recorded at 1200 rpm and 0.7 bar intake pressure. All cycles are shown in black, fast cycles in red, and slow cycles in blue. A dashed line represents the linear regression, and the Pearson correlation coefficient is provided in the legend.

radius versus individual flame extremes). The results indicate that correlation coefficients are relatively insensitive to the chosen flow-field region, with changes affecting the coefficient by up to 2% in absolute percentage. Similarly, the timing of flame measurements has little impact, provided the flame extremes are within the field of view (FoV) and can still develop further. Including historical flow data increases correlation coefficients by up to 3%, enhancing the robustness of the analysis – hence the decision to retain historical flow information in subsequent studies.

Using alternative flame characteristics, such as individual flame extremes, also affects the correlations. The right flame extreme is generally more correlated with flow variables than the equivalent flame radius, with differences of up to 7%. At higher equivalence ratios ($\phi = 0.50$), the right flame extreme is strongly correlated with the equivalent flame radius ($r = 97\text{--}99\%$), while at lower equivalence ratios ($\phi = 0.30$), the correlation weakens (up to $r \approx 70\%$). This reduction probably occurs because the slower flame development at lower equivalence ratios

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allows the left extreme to behave differently from the right, decreasing the correlation between the radius and the extremes.

To evaluate the combined influence of LF and HF velocity components on hydrogen/air flames under various operating conditions, this analysis is extended across 12 conditions. The effect of the flow with variations in intake pressure, engine speed, and equivalence ratio are explored and discussed below.

Figure 6.33 presents the Pearson's correlation coefficient between the equivalent flame radius and the flow velocity components: (a) low-frequency and (b) high-frequency, over 100 cycles (145 in some cases), as a function of intake pressure. For both LF and HF velocity components, no strong linear relationship was observed, with the correlation coefficient consistently below 50%, which is a different behavior compared to conventional hydrocarbon fuels [124, 164]. Furthermore, a noticeable trend emerges with increasing intake pressure: the correlation with both LF and HF flow structures decreases as intake pressure rises. This indicates that combustion is less influenced by the flow field at higher intake pressures. It is important to note that, as shown in Chapter 4, variations in intake pressure between 0.7 and 0.9 bar do not significantly alter the engine flow field. Therefore, the observed trend is likely attributed to changes in combustion behavior. Variations in intake pressure affect the conditions at which the mixture ignites, directly influencing the flame speed. At higher pressures, the laminar flame speed decreases. Additionally, as pressure increases, hydrodynamic instabilities at the flame front also intensify, potentially leading to earlier formation of cellular structures. Consequently, the reduced correlation between flow velocity, specially with the HF component, and flame development at higher intake pressures may be due to the increased flame speed resulting from these instabilities, which are not directly related to the flow field. Conversely, at lower intake pressures, the slower flame development makes it more susceptible to the influence of the flow field.

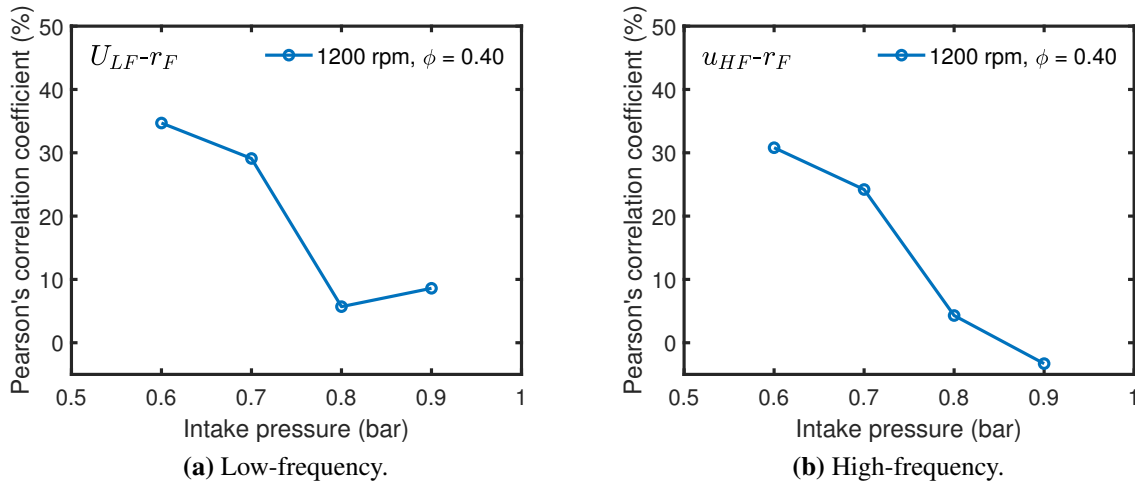


Figure 6.33: Correlation coefficient as a function of the intake pressure (from 0.6 to 0.9 bar) under 1200 rpm and $\phi_{int}^{H_2} = 0.40$.

Figure 6.34 illustrates the impact of engine speed on the correlation between the flow field (LF and HF components) and flame development (equivalent flame radius). The engine speed varies from 900 to 1500 rpm at two intake pressures (0.7 and 0.9 bar) with an equivalence ratio of 0.40. As demonstrated in Chapter 4, increasing engine speed is directly associated with

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higher ensemble-averaged velocity (U_{EA}) and velocity fluctuation (u'). Additionally, engine speed significantly influences both LF and HF velocity fields, which scale proportionally with engine speed variation.

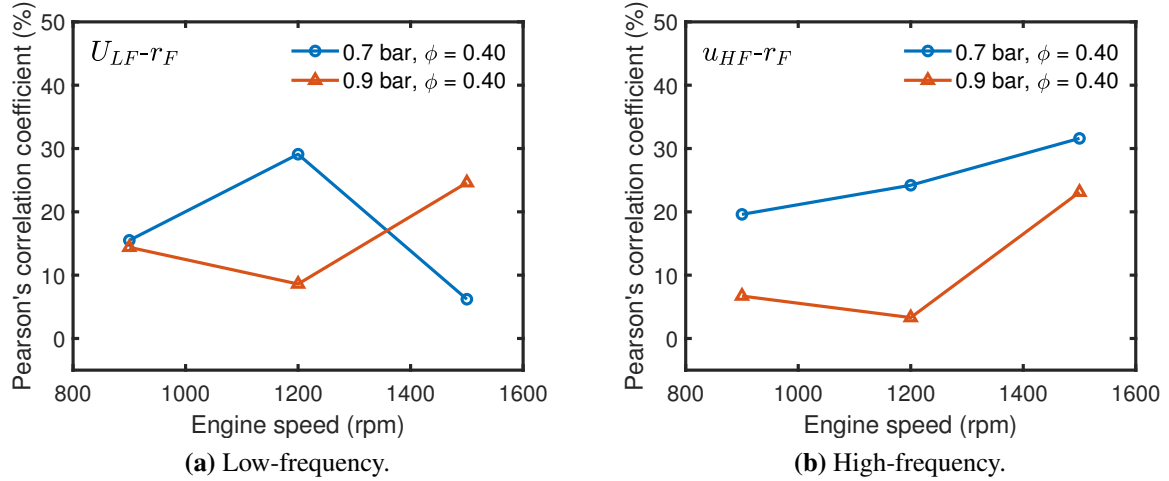


Figure 6.34: Correlation coefficient as a function of the engine speed (from 900 to 1500 rpm) under 0.7 and 0.9 bar of intake pressure and $\phi_{int}^{H_2} = 0.40$.

The correlation coefficients for the LF flow and flame development are presented in Figure 6.34a. At an intake pressure of 0.7 bar, the correlation coefficient ranges from 8% to 30%, showing a non-monotonic trend with no clear dependence on engine speed. Similarly, for an intake pressure of 0.9 bar, the correlation remains weak, varying between 18% and 27% across the tested engine speeds, indicating minimal influence of engine speed on the LF flow-flame correlation. In contrast, the Pearson's correlation coefficients for the HF velocity components, shown in Figure 6.34b, reveal a more noticeable trend. At an intake pressure of 0.7 bar, the correlation coefficient increases with engine speed, rising from 19% at 900 rpm to 32% at 1500 rpm, transitioning from weak to moderate correlation. This suggests that flames are more strongly influenced by the turbulent cycles as engine speed increases and enhances turbulence levels. At an intake pressure of 0.9 bar, the influence of HF turbulence on flame development is less pronounced. At lower engine speeds, the correlation coefficient remains close to 0%, indicating no apparent relationship. Only at the highest engine speed, 1500 rpm, does a weak correlation emerge. This aligns with the earlier observation that higher intake pressures tend to decouple the flow field from flame development.

The effect of equivalence ratio on the flow-flame correlation is analyzed in Figure 6.35. Two operating conditions are considered: $P_{int} = 0.7$ bar (at 1200 and 1500 rpm) and $P_{int} = 0.9$ bar (at 1500 rpm). The equivalence ratio is varied from 0.30 to 0.50. Figure 6.35a indicates that as the equivalence ratio increases, the flame becomes less correlated with the LF flow field. This suggests that at higher equivalence ratios, where flame speed is greater, the flame is less influenced by LF flow structures. As noted in Chapter 5, richer mixtures tend to develop more spherical flames, which are less affected by internal aerodynamics. Conversely, at lower equivalence ratios, the correlation coefficient increases, indicating a greater influence of LF flow structures on flame development.

For the HF flow component, Figure 6.35b reveals the opposite trend. Unlike the LF velocity component, the correlation with HF turbulence increases as the equivalence ratio rises. This

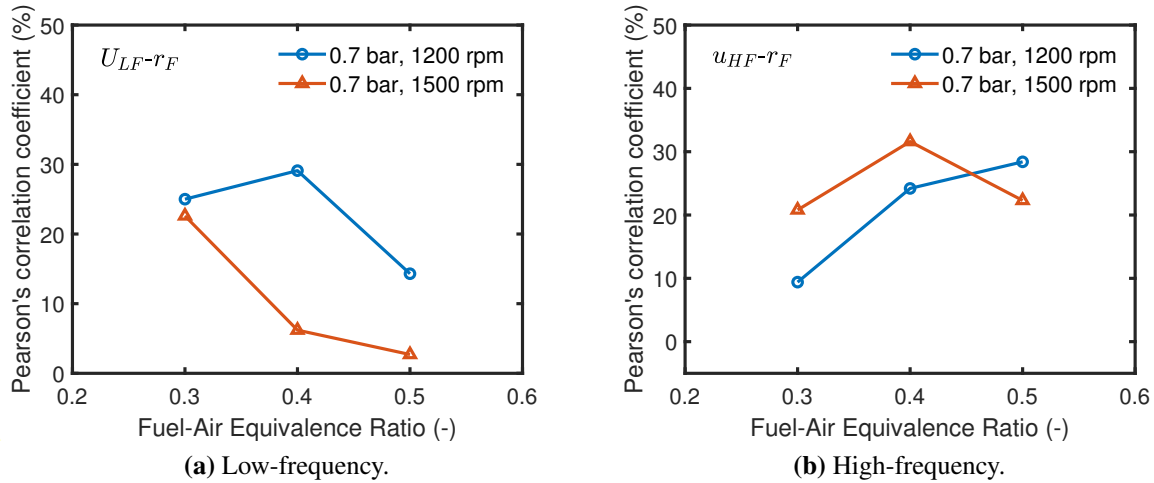


Figure 6.35: Correlation coefficient as a function of the equivalence ratio (from 0.30 to 0.50 rpm) for two operating conditions.

suggests that at higher equivalence ratios, turbulence plays a more significant role in determining the speed of individual cycles than LF flow structures. This behavior is present over two engine speeds (1200 and 1500 rpm), further emphasizing the effect of turbulence over different equivalence ratios.

Conclusion

In this chapter, the operating performance and flame parameter variability of hydrogen flames were compared to those of propane to better understand the key factors influencing each, with a focus on ultra-lean hydrogen as a fuel for internal combustion engines. Both in-cylinder pressure and flame parameters were analyzed as overall metrics and on a cycle-by-cycle basis to grasp the fundamental differences between fast and slow cycles. Additionally, the impact of multiple parameters on variability was investigated.

Hydrogen combustion in an ICE exhibits overall stable behavior in terms of in-cylinder pressure, particularly in the variability of maximum pressure, which differs significantly from propane. The variability in IMEP for both fuels showed similar values, although the mean IMEP for hydrogen was lower due to its reduced energy density. However, hydrogen displayed minimal variability, even at ultra-lean equivalence ratios (as lean as $\phi_{cyl} = 0.17$), without compromising stability. This is likely due to hydrogen's low minimum ignition energy, wide flammability range and low energy density (in a volume basis). Furthermore, the standard deviation of combustion durations for both hydrogen and propane was largely a function of laminar flame speed, with an inverse relationship observed.

When comparing flame behavior at a given crank angle, no significant impact of equivalence ratio on flame variability was observed for either hydrogen or propane. However, for a given flame radius, higher flame speeds resulted in lower flame variability, consistent with the combustion duration analysis. Engine speed primarily impacted flame speed variability for hydrogen flames at lower equivalence ratios. Conversely, intake pressure variation mostly affected higher equivalence ratio mixtures, and no definitive conclusions could be drawn regarding the

effect of ignition dwell time variation.

Fast and slow cycles were analyzed using both in-cylinder pressure and equivalent flame radius. Faster flame development corresponded to higher in-cylinder pressure cycles, a trend observed for both fuels. For hydrogen, fast cycles were linked to a more intense flow field near the spark plug at ignition timing. Hydrogen flame cycles exhibited less variation between extremes compared to propane flame cycles. Overall, a moderate correlation between the flow field and flame development was observed. Increased intake pressure reduced the correlation of both low-frequency and high-frequency velocity components, likely due to faster flame propagation. Higher engine speeds resulted in stronger correlations between high-frequency velocity components and flame development. Finally, flames with higher equivalence ratios were less influenced by the low-frequency flow field and more affected by the high-frequency (turbulent) velocity components. Further investigation with varying spark timing would be beneficial to study conditions closer to real applications.

The analysis in this chapter was used in the following conference paper:

- C. Ramalho Leite, P. Brequigny, J. Borée, F. Foucher, "Comparative Analysis Of Cycle-To-Cycle Variabilities And Combustion Development In An Optical Spark-Ignition Engine Fueled By Pure Hydrogen And Propane: Insights From Chemiluminescence and PIV", 21st International Symposium on Applications of Laser and Imaging Techniques to Fluid Mechanics, 2024.

Chapter 7

Conclusions and Perspectives

Contents

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General remarks

In recent years, the growing urgency to address environmental degradation and climate change has been driven by rising greenhouse gas concentrations, particularly carbon dioxide (CO₂). This has underscored the critical need for sustainable alternative energy sources. Among these, decarbonized hydrogen has gained attention as a promising energy carrier, particularly for reducing CO₂ emissions in the transport sector through its use as a fuel in internal combustion engines (ICEs). However, the unique properties of hydrogen differ significantly from those of conventional fuels, necessitating a thorough understanding of its behavior in ICE applications. Hydrogen’s distinct physical and chemical characteristics influence various aspects of engine performance, including energy density, air-fuel mixing, turbulence, combustion dynamics, flame instabilities, and emissions. Notably, flame behavior has become a key area of focus, emphasizing the urgent need to develop hydrogen combustion models to support hydrogen-fueled ICEs (H₂ICE) and align with European net-zero emissions targets by 2050.

To meet these standards and improve combustion efficiency, a range of advanced combustion strategies has been proposed. These include exhaust gas recirculation (EGR), homogeneous charge compression ignition (HCCI), highly dilute spark-ignition, ultra-lean spark-ignition combustion, and stratified combustion – each of which is being studied for H₂ICEs. However, implementing these strategies increases the sensitivity of the combustion process to in-cylinder flow dynamics, which can result in significant cycle-to-cycle variability. To accurately predict engine performance and capture this variability, high-fidelity data and numerical simulations, such as Large-Eddy Simulations (LES), are crucial. Such simulations enable the modeling of complex interactions within the combustion chamber, which is essential for predicting combustion behavior and optimizing engine performance.

Hydrogen, with its wide flammability range and low ignition energy, poses additional challenges for engine operation, particularly with the risk of pre-ignition, knock, and backfiring.

These phenomena can arise due to locally rich mixture zones or hot spots within the combustion chamber. To mitigate these issues, precise control of injection parameters and optimization of internal aerodynamics are key to ensuring stable combustion. Despite these efforts, current models still struggle to fully capture the turbulent combustion interactions under engine conditions. Recent studies also highlight the importance of considering thermodiffusive and stretch effects on flame behavior, particularly for hydrogen and hydrogen-based fuels, to reflect trends observed in real engine operations. Given hydrogen's properties, a significant redesign of internal combustion engines to enable their effective application is considered.

7.1 Key findings

Given the importance of characterizing hydrogen/air flames under engine conditions and the need for high-fidelity data, this thesis focuses on studying homogeneous charge ultra-lean hydrogen/air flames in an optical spark-ignition engine. The research prioritizes understanding the combustion development of a well-mixed homogeneous charge and the influence of flow fields on turbulent flame behavior. By excluding the complexity of mixture preparation, the study ensures that all variability and sensitivity analyses are attributed solely to the interaction of flow and flame dynamics. Particle Image Velocimetry (PIV) measurements are conducted in conjunction with three decomposition techniques: Reynolds Decomposition, Empirical Mode Decomposition (EMD), and Triple Decomposition. These methods provide a comprehensive analysis of the flow field, capturing the ensemble-averaged component and distinguishing between low-frequency (large-scale) and high-frequency (small-scale) turbulent structures. This decomposition approach aligns closely with Large-Eddy Simulation (LES) frameworks, which inherently separate flow dynamics into resolved (low-frequency) and sub-grid-scale (high-frequency) components. Additionally, the EMD method offers insights into identifying the "natural" cut-off frequency by utilizing intrinsic mode functions (IMFs), which reflect fundamental flow structures.

Using turbulence parameters such as turbulent intensity and integral length scale – calculated from high-frequency velocity fluctuations – the study evaluates the interaction between turbulent flow and laminar flame characteristics. This analysis reveals significant differences in turbulence-laminar flame ratios across various equivalence ratios, intake pressures, and engine speeds. While laminar flame parameters vary substantially with equivalence ratio, the flame development within the engine exhibits remarkable consistency. For instance, chemiluminescence images of flames with an initial radius as small as 4 mm strongly correlate with in-cylinder pressure increases due to combustion. This correlation persists from the early flame phase (2% mass fraction burned, ≈ 20 mm flame radius) to the end of the flame propagation phase (50% mass fraction burned). A classical Damköhler-based Wrinkled Flamelet model, incorporating turbulent intensity and laminar flame speeds, successfully predicts the overall combustion behavior across all test conditions, despite not fully capturing ultra-lean flame shapes or wrinkling effects ($\phi < 0.35$).

Comparative analysis of hydrogen/air ($\phi_{H_2} = 0.20 - 0.55$) and propane/air ($\phi_{C_3H_8} = 0.70 - 1.50$) flames presents key distinctions in flame development. Hydrogen flames exhibit a broader range of flame speeds due to the relatively stable laminar flame speed of propane near stoichiometry. Interestingly, despite the significant differences in laminar flame properties between the two fuels, their in-cylinder flame behavior and sensitivity to stretch during early flame development are notably similar under engine conditions. This contrasts with observations at ambient

pressure and temperature, where propane's shift from lean to rich mixtures significantly alters its laminar flame behavior due to Lewis number inversion. The findings suggest that elevated pressures, temperatures, and turbulence levels in engines diminish these disparities, underscoring the importance of engine conditions in moderating the influence of laminar flame properties on combustion events.

Regarding cycle-to-cycle variations (CCVs), hydrogen/air combustion under ultra-lean conditions demonstrates unexpectedly low variability in engine performance metrics, like maximum in-cylinder pressure and indicated mean effective pressure (IMEP), compared to propane. While hydrogen's lower energy density results in a reduced mean IMEP, its flame development variability is comparable to propane. This operational stability, even at low loads, highlights hydrogen's potential for reliable equivalence ratio-based load control – something that hydrocarbon fuels struggle to achieve due to their narrow flammability range and increased operation instability at low flame speeds and high dilution.

Cycle-resolved analyses show that faster combustion cycles correspond to higher in-cylinder pressures, with hydrogen flames showing less variation between extreme cycles than propane. The correlation between flame propagation and flow dynamics varies with operating conditions: higher engine speeds strengthen the influence of high-frequency velocity components, while low-frequency flow structures have a diminishing effect as equivalence ratios increase. Intake pressure primarily influences flame properties rather than flow dynamics, suggesting that thermodynamic conditions and flame instabilities are critical to hydrogen flame development. These findings emphasize the need for high-fidelity modeling of hydrogen flames to capture the complex interplay of turbulence, thermodynamics, and instabilities essential for advancing hydrogen internal combustion engines.

7.2 Perspectives for future research

The work presented in this manuscript opens a wide range of academic and industrial perspectives on fundamental aspects of ultra-lean hydrogen/air in-cylinder flames, their behavior in turbulent environments, and their modeling and manipulation for innovative industrial design concepts. From this foundation, several guidelines are proposed to address challenging research directions in the future.

The study of hydrogen combustion development across different equivalence ratios demonstrates that a single turbulent flame speed correlation can represent a broad range of turbulence-to-flame scales on the Peters-Borghi diagram. This finding suggests that the combustion regimes experienced by these flames are not intrinsically different, as the same model and its assumptions can explain their behavior. These results highlight intriguing paths for further exploration of hydrogen/air flames in both laminar and turbulent environments. Notably, unstretched laminar flame speeds – commonly used to model the initial stages of combustion for traditional fuels – are not well-defined properties for ultra-lean hydrogen flames. Instabilities, such as hydrodynamic, thermodiffusive, and gravitational effects, rapidly influence the flame after ignition, making robust measurement of "unstretched" laminar flame speeds impractical. Instead of applying correction factors to account for the effects of instabilities on flame speed, a redefinition of flame speed may be necessary to accurately study and model ultra-lean hydrogen flames. This is especially critical for turbulent flame measurements, which often rely on well-defined laminar flame properties as a foundation for understanding turbulence effects. Moreover, detailed investigations of flame instabilities, particularly thermodiffusive effects, in both ambient

and engine-like conditions are crucial for advancing knowledge of hydrogen-based fuel combustion.

Flame modeling is another vital area of research, encompassing everything from kinetic models for 0D/1D combustion simulations – often not validated under engine-like conditions but still widely used in internal combustion engine (ICE) modeling – to physical phenomena like ignition, turbulent combustion, heat transfer, and quenching effects. The experimental data provided in this thesis could significantly aid these efforts. For example, it could predict flame radius at specific crank angles and its variability across different operating conditions (e.g., equivalence ratio, engine speed, intake pressure) to refine ignition models. The developed turbulent combustion correlation could be extended to other configurations, incorporating thermodiffusive instabilities for improved in-cylinder turbulent flame modeling. Additionally, in-cylinder pressure data could be leveraged to enhance heat transfer and quenching models, particularly after CA50, potentially linking these effects to equivalence ratios. Advanced techniques, such as Mie-scattering for two-dimensional flame morphology measurements, could improve the modeling of turbulent wrinkling and stretch factors in both RANS and LES simulations of H₂ICEs. Such data would provide a more robust foundation than reliance on chemiluminescence-based projections alone.

Once these phenomena are well understood and modeled, expanding the scope to include configurations involving mixing effects becomes essential. For instance, exploring different mixing strategies, such as port-fuel versus direct injection and variations in injection pressure, can help analyze the impact of mixture stratification at spark timing. Research indicates that industrial applications are increasingly focusing on non-homogeneous mixtures to mitigate safety risks. Advanced optical techniques should be employed to validate mixing phenomena, providing a crucial link between inhomogeneous mixture effects and validated homogeneous turbulent flame models.

Finally, decoupling the contributions of turbulence and instabilities to the enhancement of hydrogen/air in-cylinder flame behavior represents an exciting avenue for advancing combustion science and sustainable propulsion technologies. High-fidelity experimental data from this study could complement existing DNS simulations under engine-like conditions, enabling deeper insights into flame behavior. Achieving agreement between DNS calculations and experimental results would allow access to extensive unmeasured data, improving predictions and understanding of flame properties. Adapting manifold or piston geometries to modify turbulent structures at spark timing, such as tumble strength or swirl, could yield valuable insights into turbulence effects on flame dynamics. Additionally, as a follow up of the ANR Alekcia project, Data Assimilation techniques could enhance high-fidelity numerical simulations, particularly for LES, enabling detailed investigations of hydrogen flame development during specific measured extreme cycles, such as abnormal combustion events, under well-known operating conditions.

Appendix A

Empirical Mode Decomposition

Empirical Mode Decomposition (EMD), first introduced by Huang et al. [165] for univariate time series, is a data-driven technique for analyzing nonlinear and non-stationary signals. It breaks down a signal into a series of oscillatory components known as intrinsic mode functions (IMFs), along with a residual term representing the trend. Over time, EMD was generalized to handle multivariate signals. This progression began with its application to complex signals [166, 167] and was later extended to bivariate (BEMD) [168], trivariate (TEMD) [169], and fully multivariate (MEMD) forms [170].

These multivariate extensions involve projecting the signal into multiple directions – for example, onto a circle for BEMD, a sphere for TEMD, or a hypersphere for MEMD. The projection facilitates the computation of an average envelope, which is essential for the iterative sifting process that characterizes EMD. This appendix provides an overview of the original EMD approach.

For a discrete signal $x[n]$, EMD decomposes it into a finite number of IMFs, $c_i[n]$, and a residual trend, $r[n]$, expressed mathematically as:

$$x[n] = \sum_{i=1}^m c_i[n] + r[n] \quad (\text{A.1})$$

The IMFs must meet two specific criteria, as outlined in [165]:

- The number of local extrema and zero-crossings must either match or differ by exactly one.
- At any point in the signal, the mean value of the envelope formed by the local maxima and the envelope formed by the local minima must be zero, ensuring symmetry.

Unlike classical harmonic functions, an intrinsic mode function can exhibit variability in both frequency and amplitude, making it inherently multi-scale. The EMD process is summarized below:

1. **Extrema Identification:** Identify the local maxima and minima of the signal $r_i[n]$ (initially equal to $x[n]$ for $i = 1$).
2. **Envelope Construction:** Construct upper ($e_u[n]$) and lower ($e_l[n]$) envelopes by interpolating the maxima and minima using cubic splines.

3. **Local Mean Calculation:** Compute the local mean as $m[n] = (e_u[n] + e_l[n])/2$.
4. **Oscillation Extraction:** Subtract the local mean from the signal to obtain $h_{ij}[n] = r_i[n] - m[n]$, representing the modulated oscillations.
5. **IMF Verification:** If $h_{ij}[n]$ meets the IMF criteria, designate it as $c_i[n]$; otherwise, repeat steps 1–4 with $r_i[n] = h_{ij}[n]$.
6. **Residual Update:** Subtract the derived IMF $c_i[n]$ from $r_i[n]$, yielding a new residual for further decomposition.
7. **Termination:** End the process when the residual becomes monotonic, indicating no remaining oscillatory components.

Step 5 ensures proper termination of the sifting process using criteria proposed in [146], involving parameters θ_1 , θ_2 , and α to balance global and local fluctuations in the mean envelope. The mode amplitude is computed as $a[n] = (e_u[n] - e_l[n])/2$, and the evaluation function $\sigma[n] = |m[n]/a[n]|$ guides the iteration process. Sifting continues until $\sigma[n] < \theta_1$ for a prescribed fraction $(1 - \alpha)$ of the signal length and $\sigma[n] < \theta_2$ for the remainder. Following the recommendations in [146], values of $\theta_1 = 0.05$, $\theta_2 = 0.5$, and $\alpha = 0.05$ are retained in this study.

To demonstrate the application of EMD, Ding [137] constructed a synthetic time series using the following expression:

$$x[n] = A_1 \sin(2\pi f_1 t[n]) + A_2 \sin(2\pi f_2 t[n]) + 2t[n], \quad (\text{A.2})$$

where $A_1 = 1$, $f_1 = 10$ Hz, $A_2 = 0.6$, $f_2 = 60$ Hz, and $t[n]$ spans from 0 to 0.2 seconds with 101 time steps. This series combines components with distinct frequencies (high and low) alongside a monotonic trend. Figure A.1 illustrates the results of the EMD process applied to this series. The decomposition separates the signal into intrinsic mode functions, starting with the highest frequency components and concluding with a residual representing the monotonic trend.

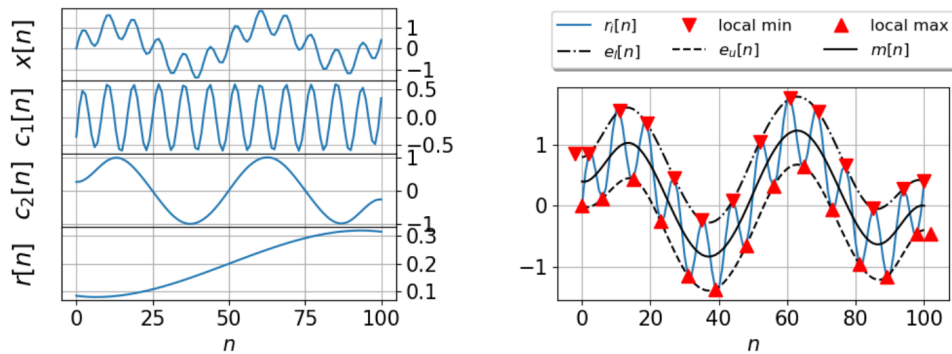


Figure A.1: Results of EMD applied to a 1D time series. Left: IMFs and residual extracted by EMD; Right: First iteration of the sifting process [137].

Appendix B

3D RANS study on hydrogen injection position

Preliminary study of three hydrogen injection positions for homogeneous mixture at spark timing, as illustrated in Figure 2.5 (except for the "Inside Plenum" configuration). Numerical study done in Converge CFD Software [171].

B.1 Numerical setup

- Number of cycles simulated = 6 – 8;
- Transient compressible solver with total energy formulation, multi-species (H_2 , O_2 , N_2) gas simulation, Redlich-Kwong equation of state, species-dependent critical conditions, mixture-averaged diffusion;
- Global transport parameters: turbulent Prandtl number is 0.9 and turbulent Schmidt is 0.78 (default);
- Density-based PISO algorithm with tolerance = $1e-03$, momentum in conservative form, Jacobi final iteration for conservation, Rhie-Chow interpolation, "pressure-ratio" relaxation at 0.5, segregated turbulence solver relaxation at 1.0, momentum algebraic solver is SOR with tolerance = $1e-05$ and relaxation 1.0, pressure solver is SOR with tolerance = $1e-08$ and relaxation 1.1, turbulence solver is SOR with tolerance = $1e-03$ and relaxation 0.7, solver for other transport equation is SOR with tolerance = $1e-04$ and relaxation 1.0 (default);
- 1st order implicit Euler time advancing, minimum time step = $1e-08$ s; maximum time step = $1e-05$ s. maximum convection CFL = 1.0 and maximum diffusion CFL = 2.0;
- Advection performed with a flux-bending of 0.5 fraction for FV scheme.
- RANS turbulence modeling with RNG $k-\epsilon$ closure, O'Rourke and Amsden (default) heat transfer model, near wall treatment with enhanced wall treatment;
- initialization: constant intake pressure of 0.7 bar at air inflow boundary (intake plenum) and constant mass flow of hydrogen to meet an equivalence ratio of 0.35 inside the cylinder at IVC.

B.2 Mesh

- Minimum volume ratio parameter in cut-cell algorithm is 0.2;
- Base grid is 4 mm (level 0), levels 1-3 corresponding to 2, 1 and 0.5 mm, respectively;
- Velocity Adaptive Mesh Refinement (AMR): sub-grid criterion = 1.0m/s, maximum embedding level = 2;
- Fixed embeddings: intake and exhaust valves regions (up to level 3), hydrogen injection (level 2), walls (level 1).

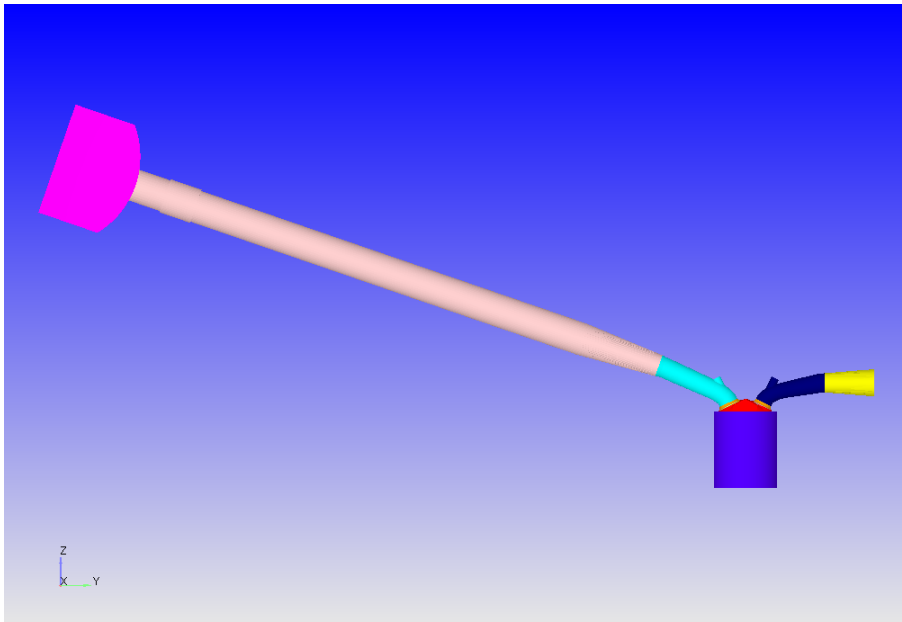


Figure B.1: Setup geometry.

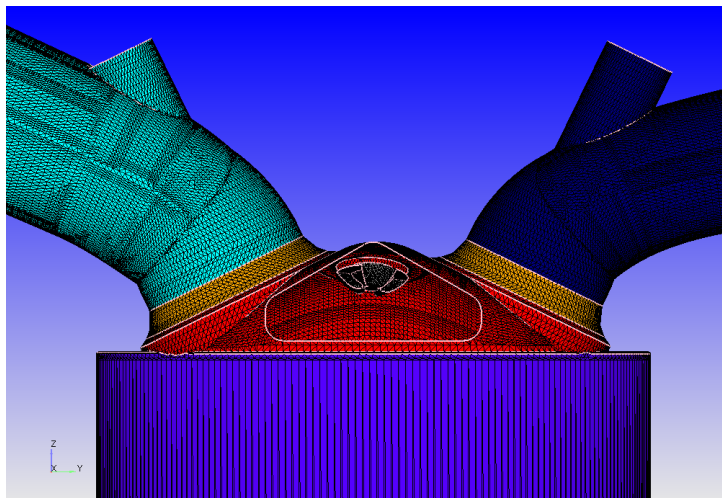


Figure B.2: Setup surface mesh: intake, exhaust and in-cylinder.

B.3 Results

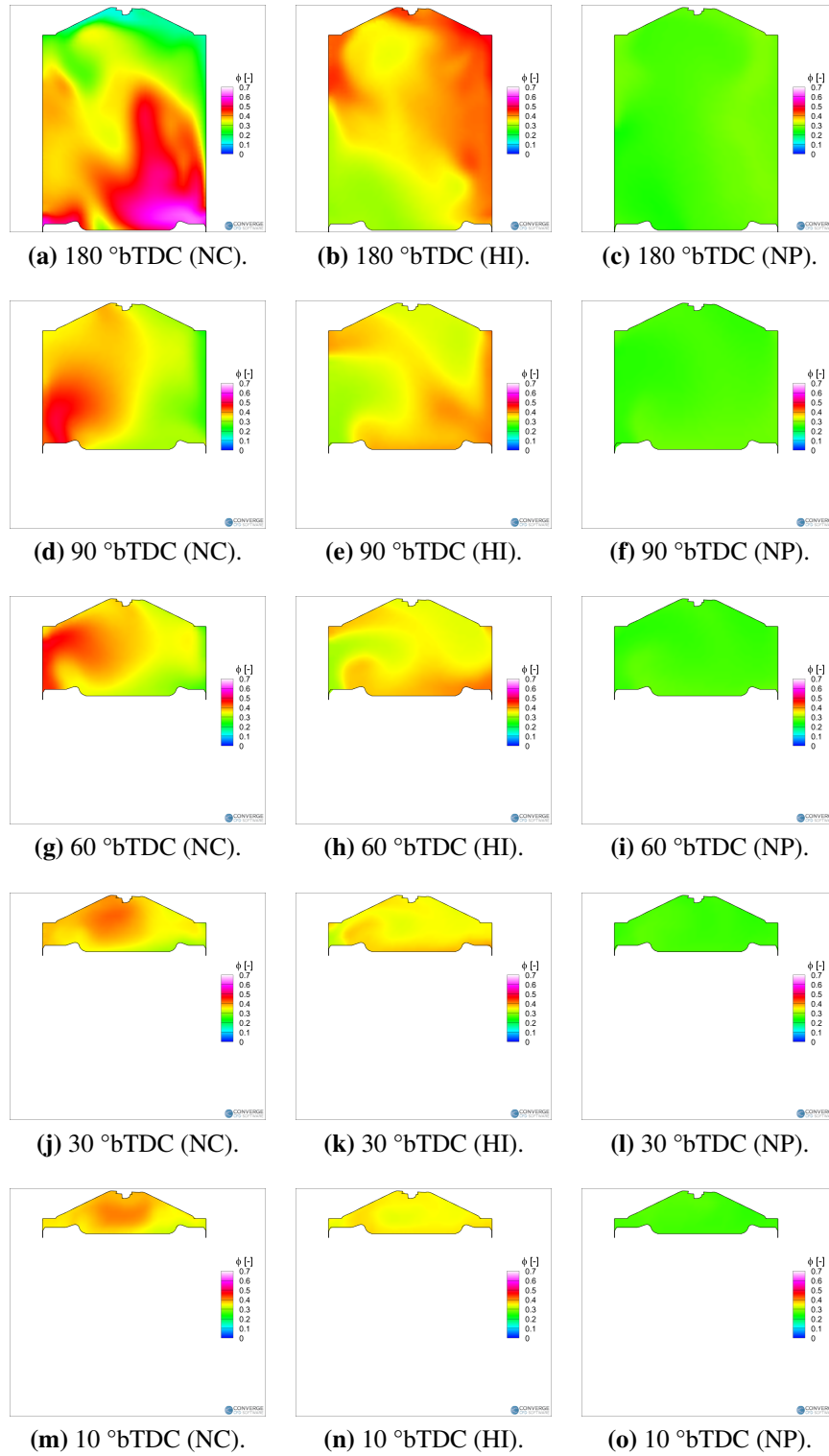


Figure B.3: Fuel-Air Equivalence Ratio map for the three tested hydrogen injection positions. P.S.: Lower final equivalence ratio at the NP configuration due to hydrogen slip at the intake plenum boundary.

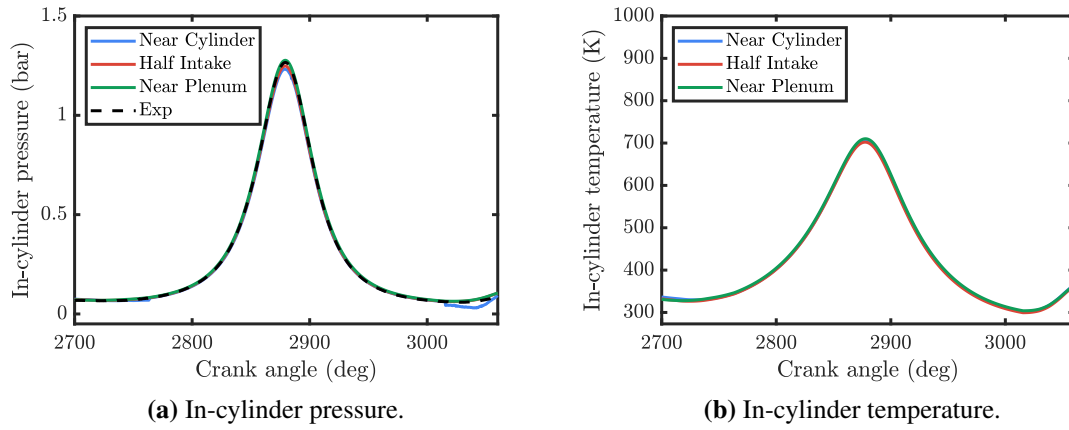


Figure B.4: Experimental results with simulated in-cylinder pressure and temperature.

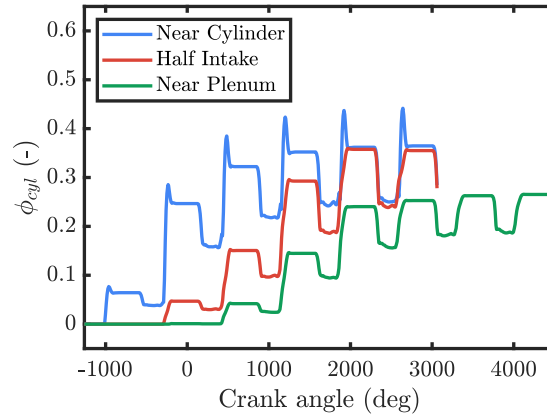


Figure B.5: Mean fuel-air equivalence ratio inside the combustion chamber as a function of the crank angle for the three hydrogen injection positions.

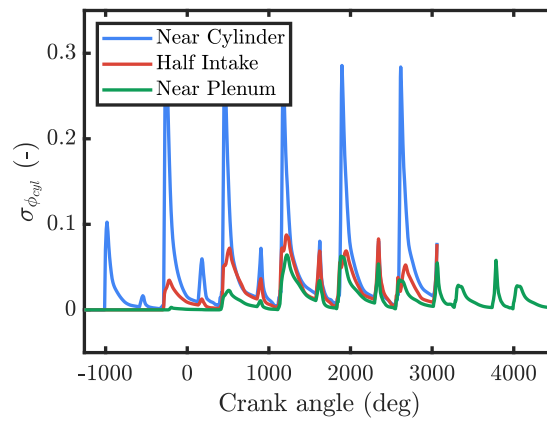


Figure B.6: Standard deviation of the fuel-air equivalence ratio inside the combustion chamber as a function of the crank angle for the three hydrogen injection positions.

Appendix C

PIV Measurements Data

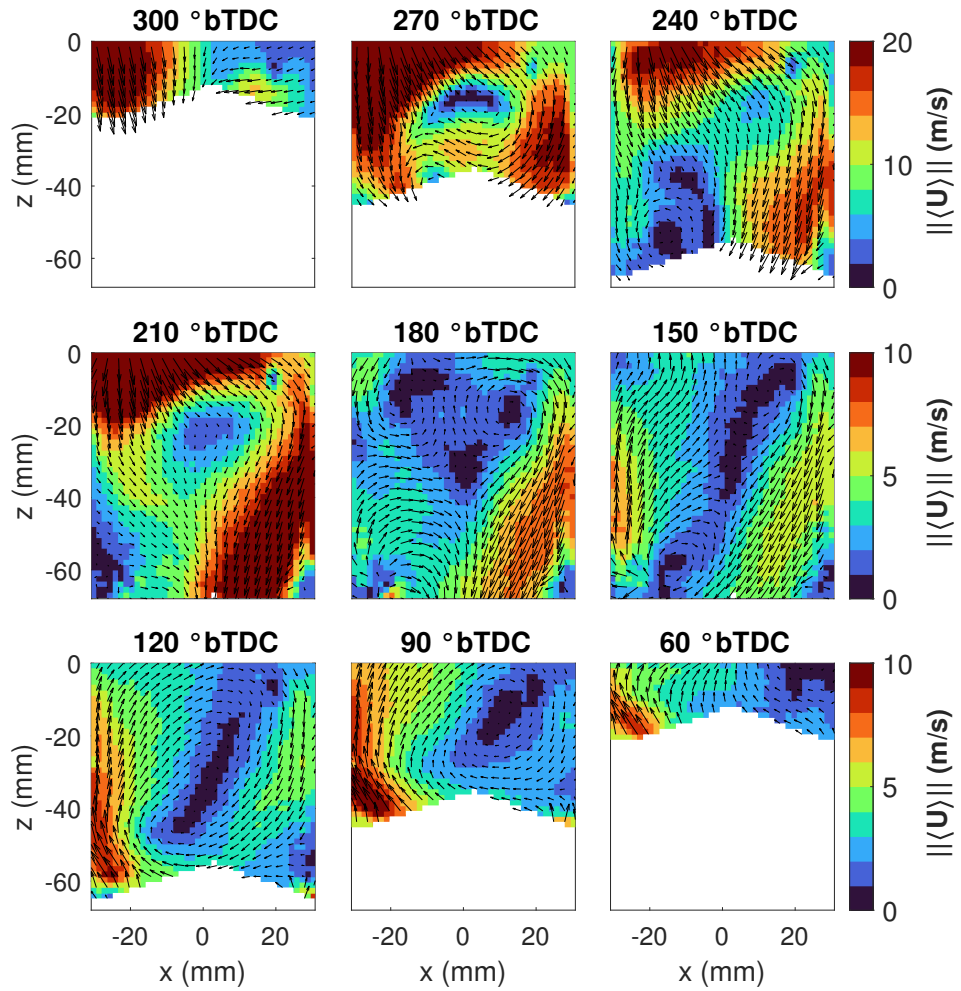


Figure C.1: Ensemble-averaged velocity components in the x and z directions (U and W , respectively) of the in-cylinder flow over 150 cycles, measured using high-speed PIV in the VC configuration. Measurements are shown at intervals of 30°, ranging from 300 (upper-left) to 60 °bTDC (bottom-right).

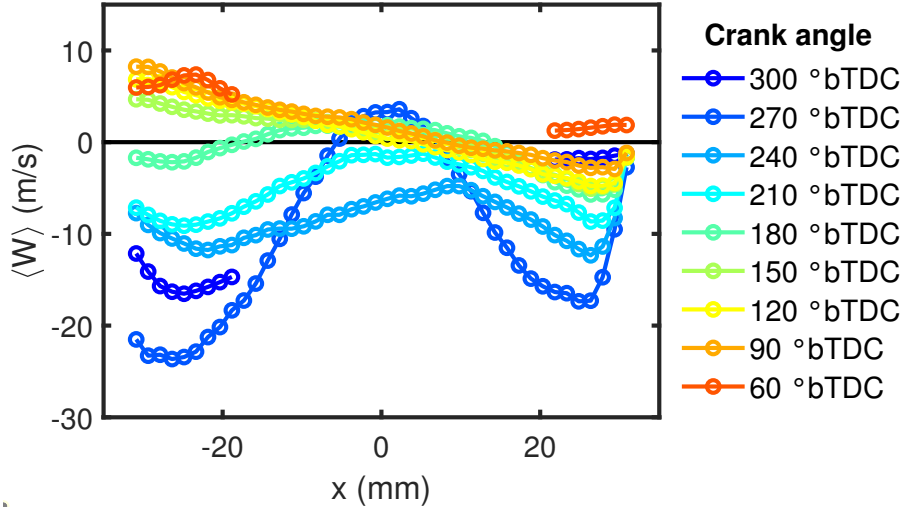


Figure C.2: Ensemble-averaged W velocity component over 150 cycles as a function of the x position at $z = -20$ mm, measured from 300° to 60° bTDC.

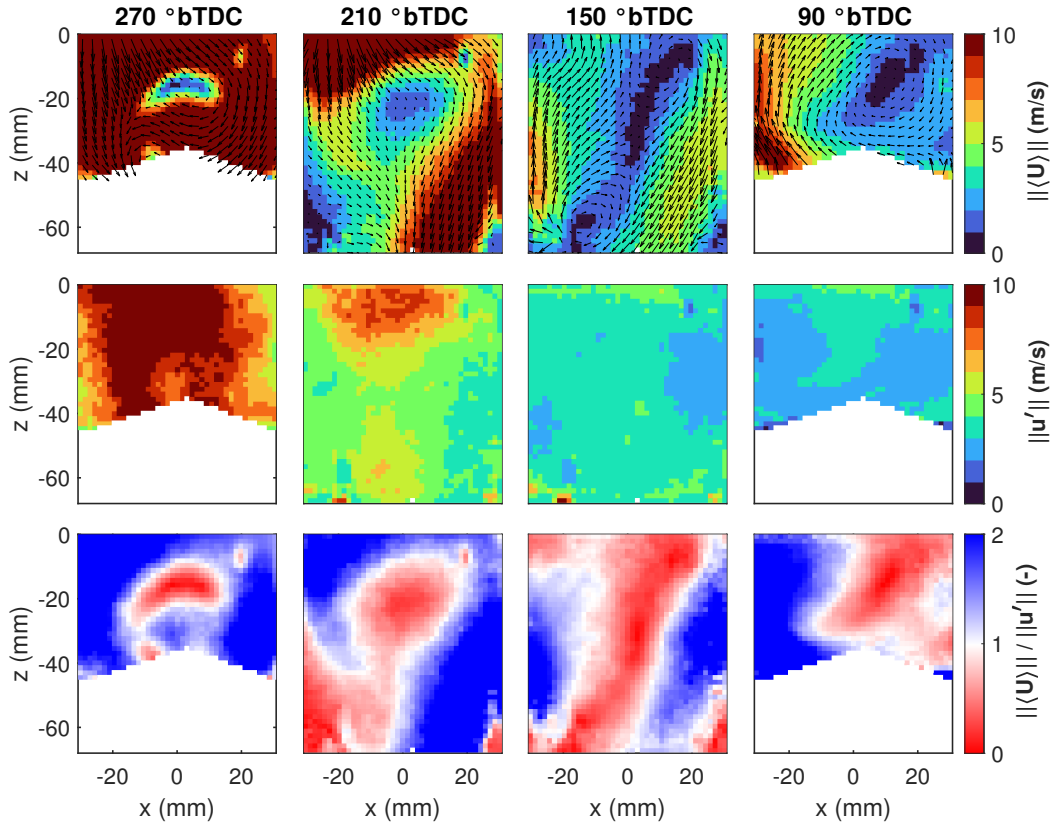


Figure C.3: Ensemble-averaged velocity magnitude (first row), turbulence intensity magnitude in the x and w directions, $\sqrt{u'^2 + w'^2}$ (second row), and their ratio (third row) at four crank angles: 270, 210, 150, and 90° bTDC.

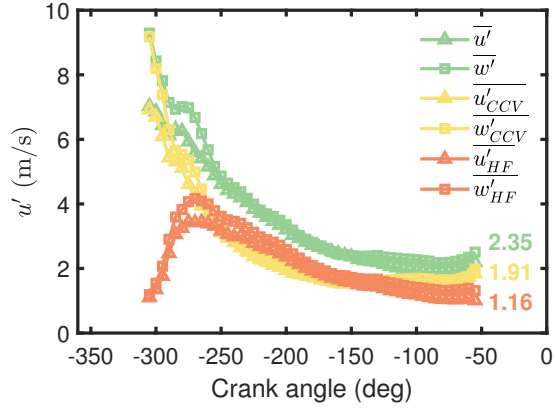
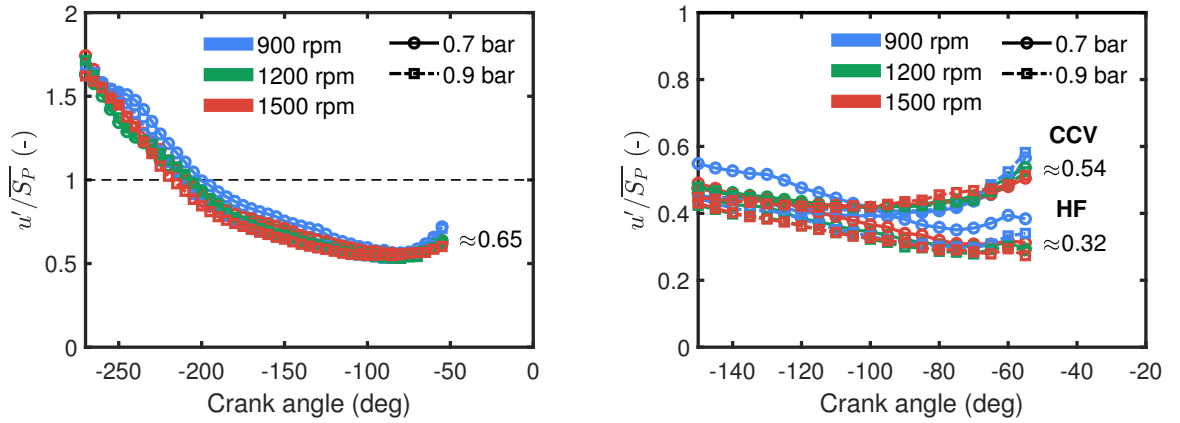


Figure C.4: Turbulent intensities of fluctuating velocities (F, CCV, and HF) as a function of crank angle.



(a) ReD fluctuating component normalized by the mean piston speed.

(b) TD fluctuating components (CCV and HF) normalized by the mean piston speed..

Figure C.5: Fluctuating turbulent intensities as a function of crank angle.

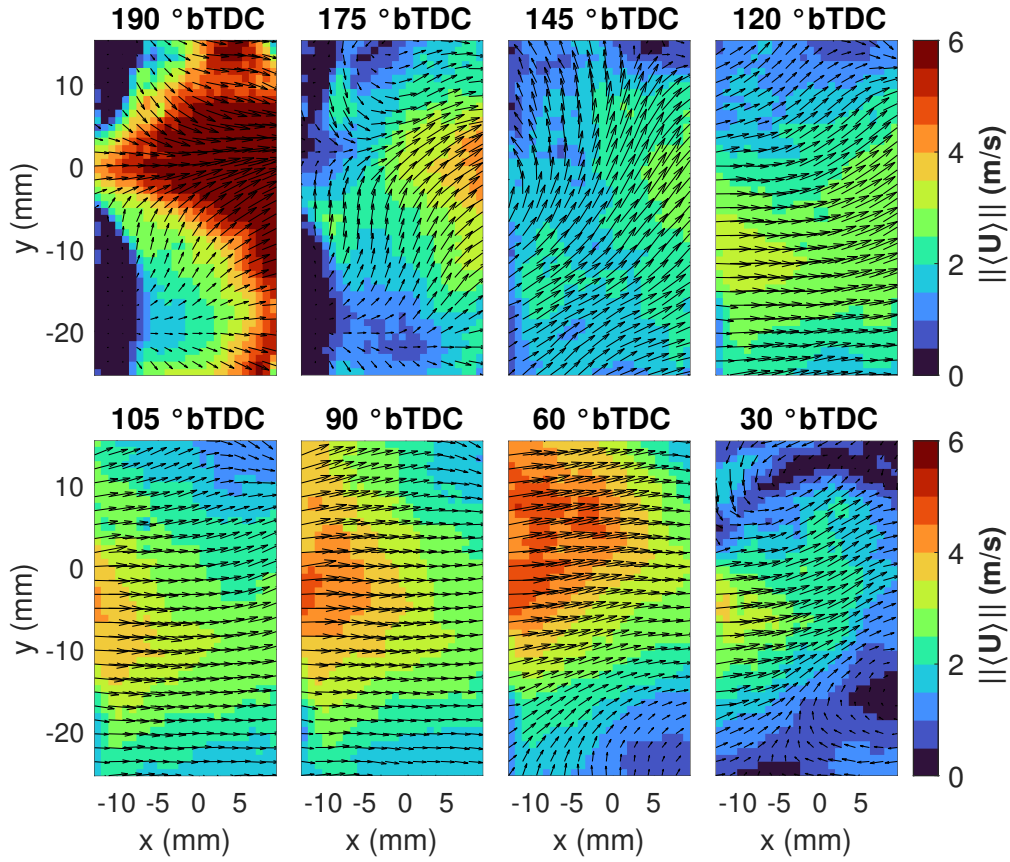


Figure C.6: Ensemble-averaged velocity components in the x and y directions (U and V , respectively) of the in-cylinder flow over 150 cycles, measured using high-speed PIV in the HCC configuration. Measurements are for eight crank angles ranging from 190° (upper-left) to 30° bTDC (bottom-right).

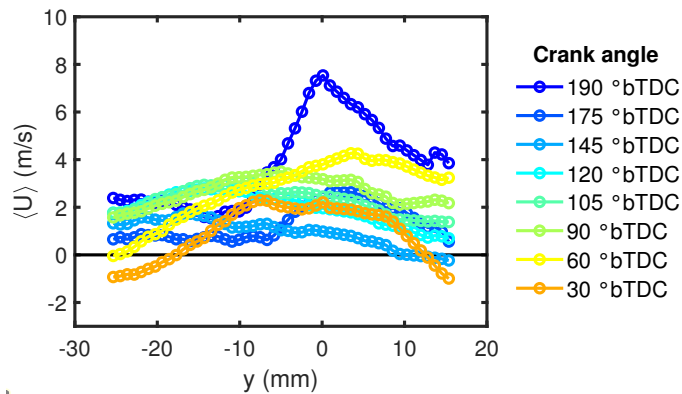


Figure C.7: Ensemble-averaged U velocity component over 150 cycles as a function of the y position at $x = 0$ mm, measured from 190° to 30° bTDC.

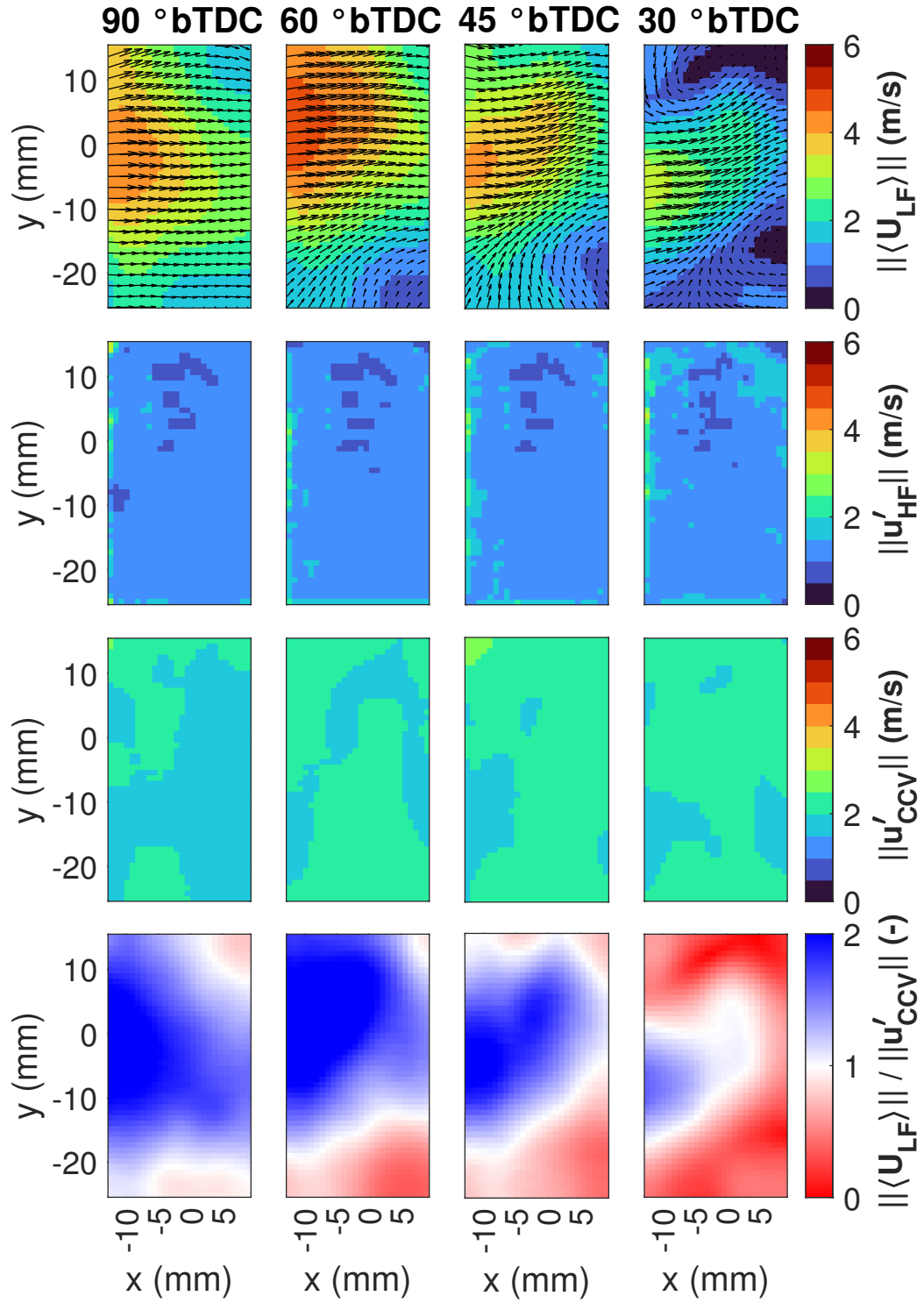
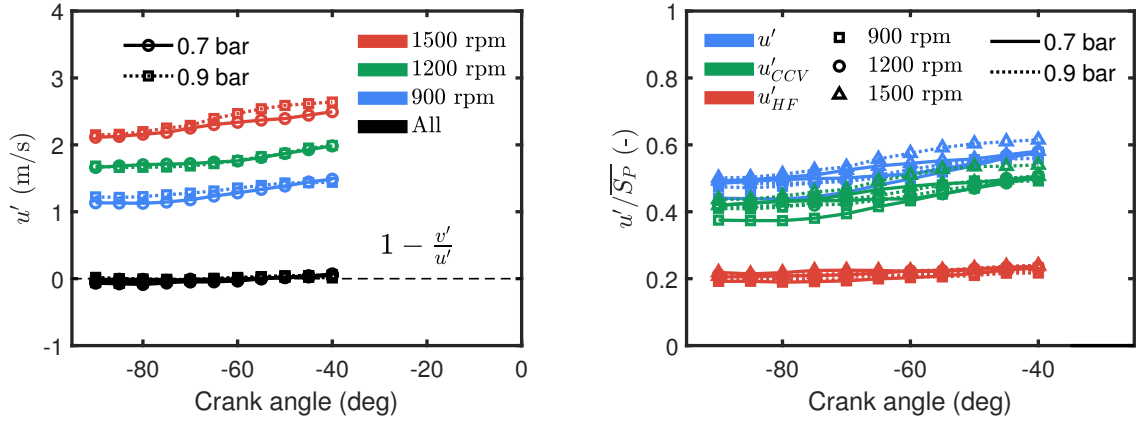


Figure C.8: Triple Decomposition analysis: Ensemble-averaged low-frequency (LFEA) velocity magnitude (first row), high-frequency fluctuating velocity turbulence intensity in the x and y directions, $\sqrt{u'^2_{HF} + v'^2_{HF}}$ (second row), low-frequency fluctuating (CCV) velocity turbulence intensity (third row), and the ratio between LFEA and CCV magnitudes (forth row) at four crank angles (90, 60, 45, and 30° bTDC).



(a) u' and v' as a function of crank angle for two intake pressures (0.7 and 0.9 bar) and three engine speeds (900, 1200, and 1500 rpm). (b) Turbulent intensities (F, CCV and HF) normalized by the mean piston speed as a function of crank angle.

Figure C.9: Effect of intake pressure and engine speed on turbulence intensities.

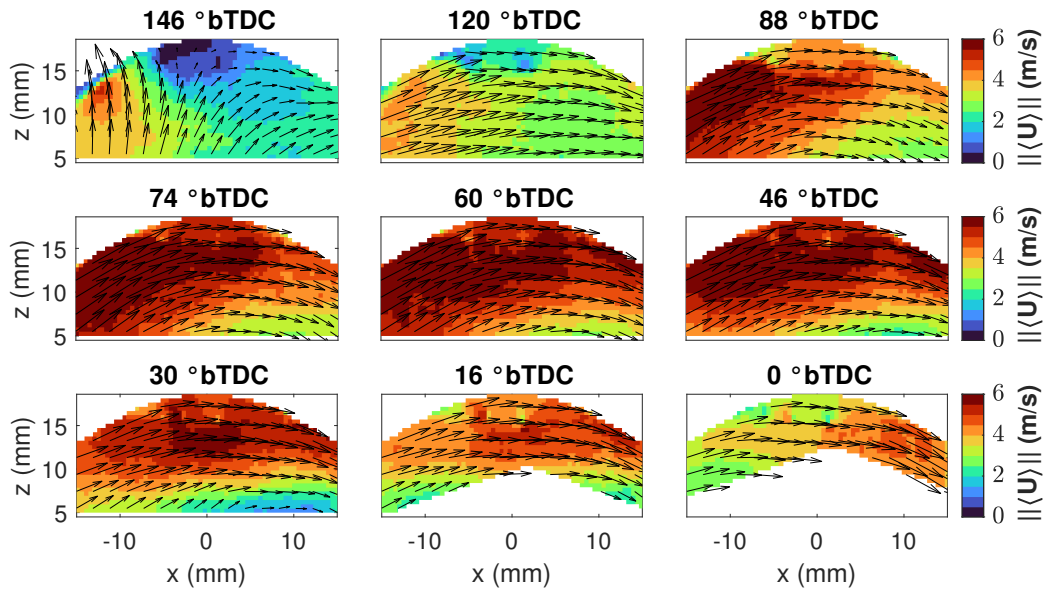


Figure C.10: Ensemble-averaged velocity components in the x and z directions (U and W , respectively) of the in-cylinder flow over 100 cycles in the VCC configuration. PIV measurements ranging from 146 (upper-left) to 0 °bTDC (bottom-right).

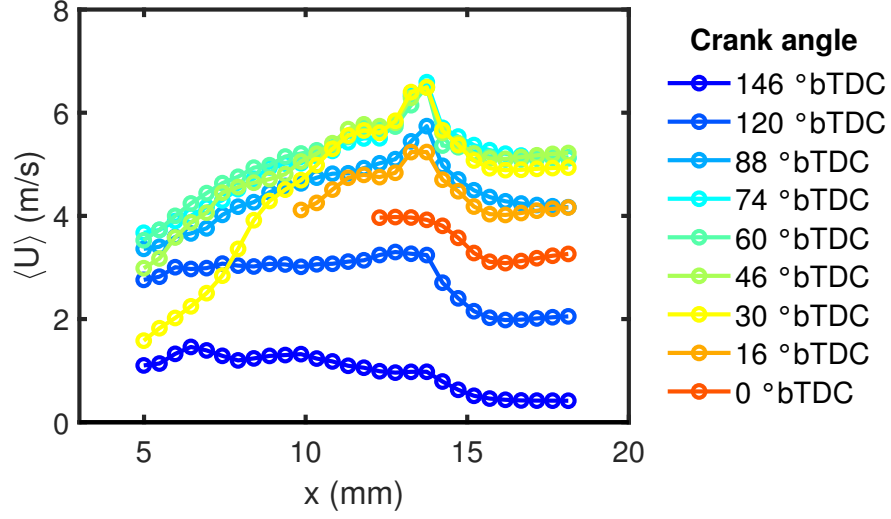


Figure C.11: Ensemble-averaged U velocity component over 100 cycles as a function of the y position at $x = 0$ mm, measured from 146° to 0° bTDC.

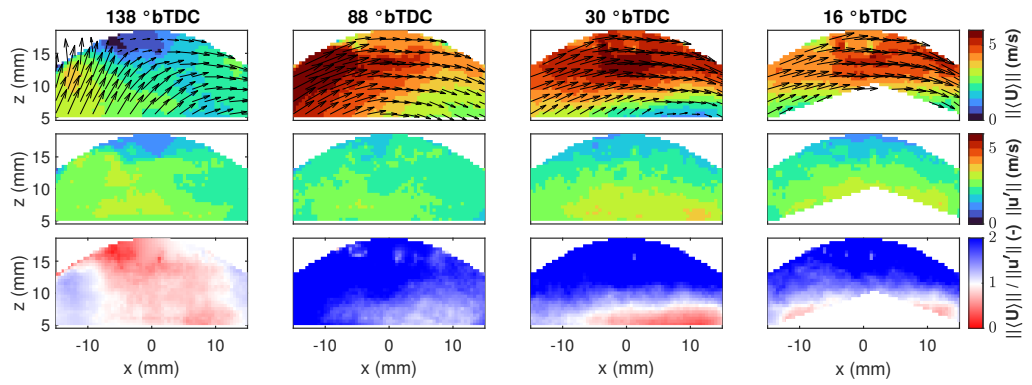


Figure C.12: Ensemble-averaged velocity magnitude (first row), turbulence intensity magnitude in the x and w directions, $\sqrt{u'^2 + w'^2}$ (second row), and their ratio (third row) at four crank angles: 138, 88, 30, and 16° bTDC.

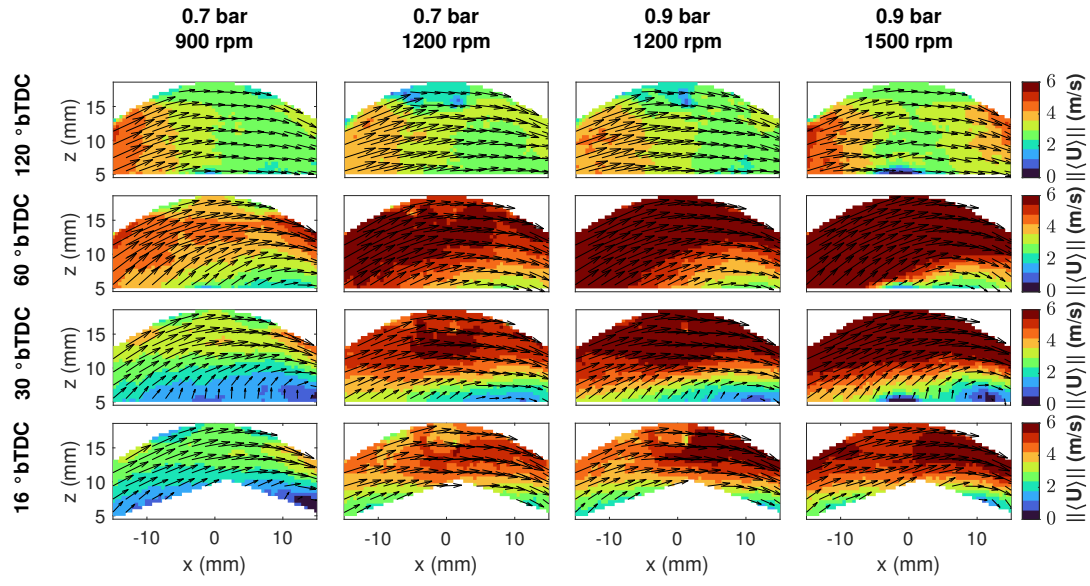


Figure C.13: Impact of engine speed and intake pressure on the flow field within the combustion chamber at four crank angles: 120, 60, 30, and 16 °bTDC.

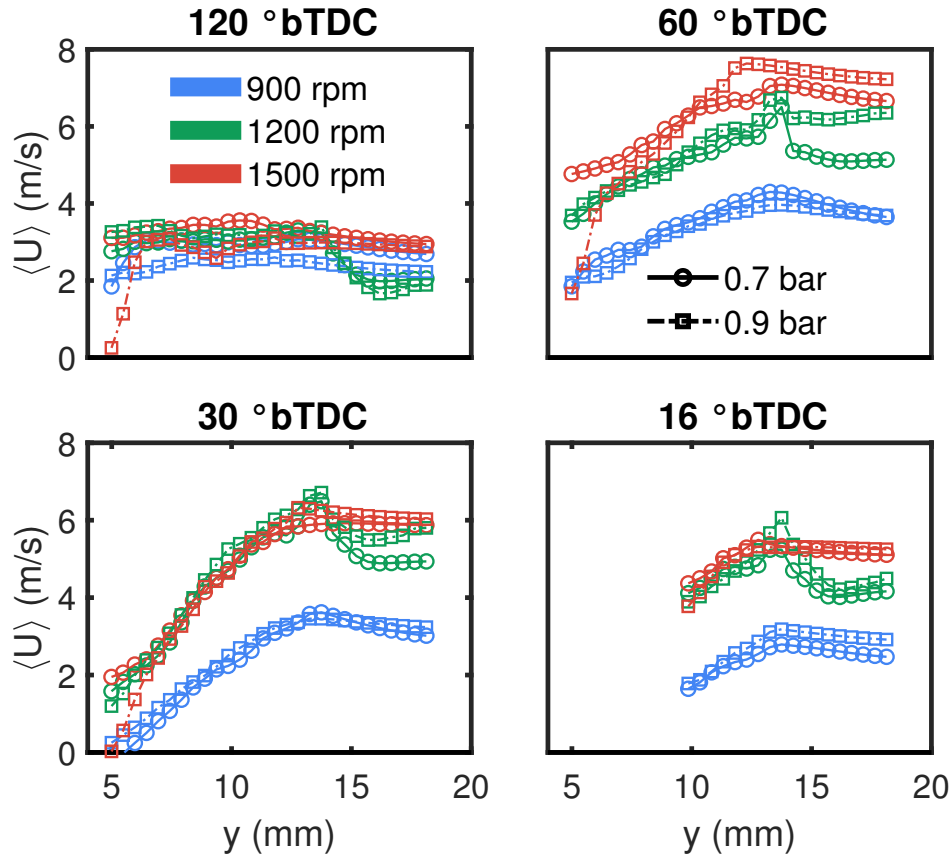


Figure C.14: U velocity at $x = 0$ mm for crank angles of 120, 60, 30, and 16 °bTDC, with two intake pressures (0.7 and 0.9 bar) and three engine speeds (900, 1200, and 1500 rpm).

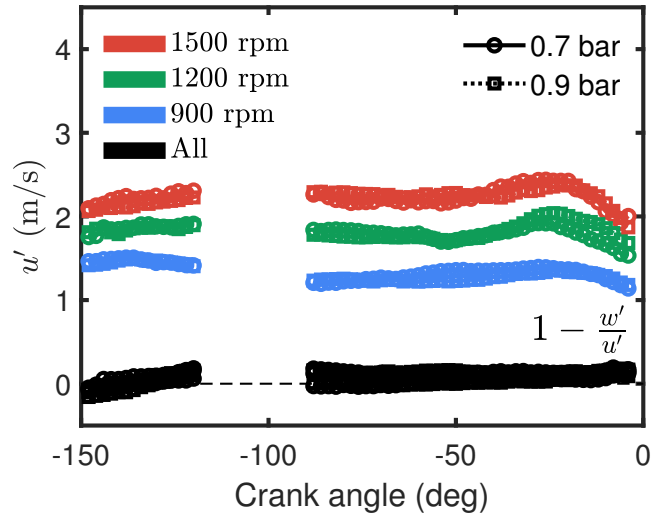


Figure C.15: Impact of engine speed and intake pressure on turbulent intensity as a function of crank angle.

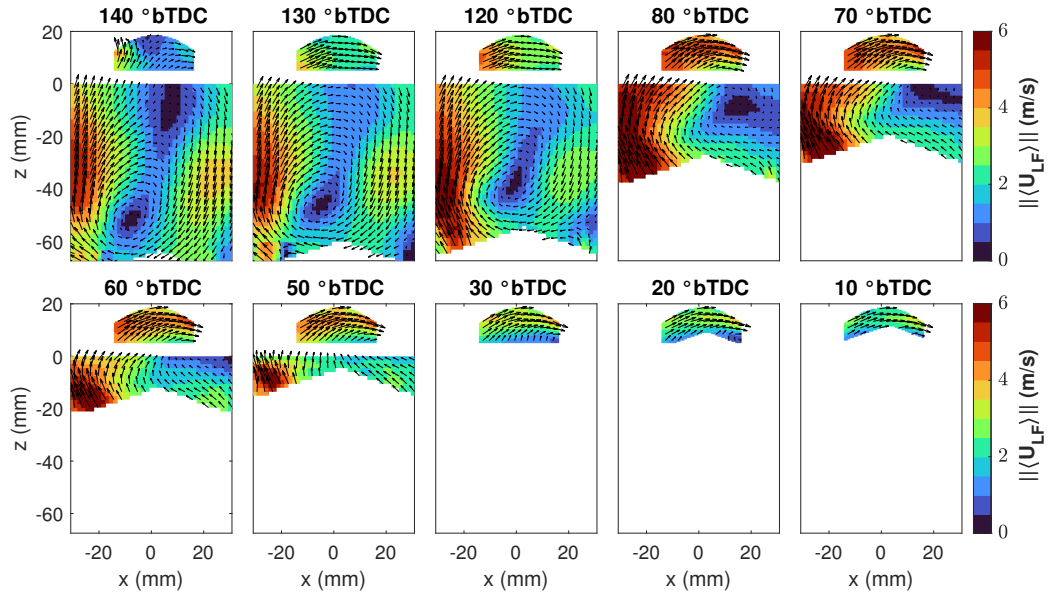


Figure C.16: Ensemble-averaged low-frequency velocity magnitude for the VC and VCC configurations at 0.7 bar intake pressure and 900 rpm across 10 different crank angles.

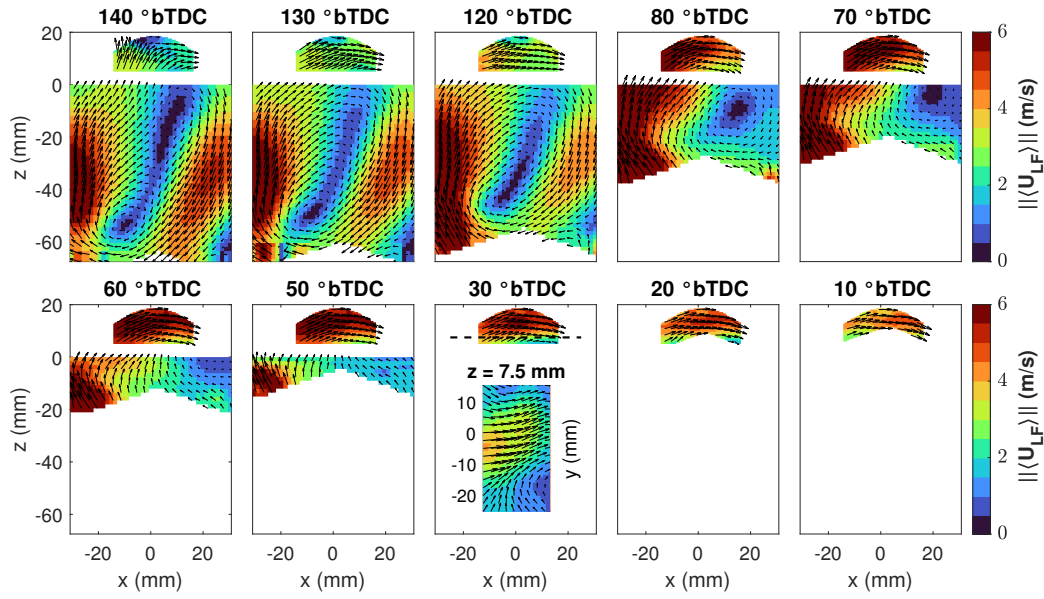


Figure C.17: Ensemble-averaged low-frequency velocity magnitude for the VC and VCC configurations at 0.7 bar intake pressure and 1200 rpm across 10 different crank angles.

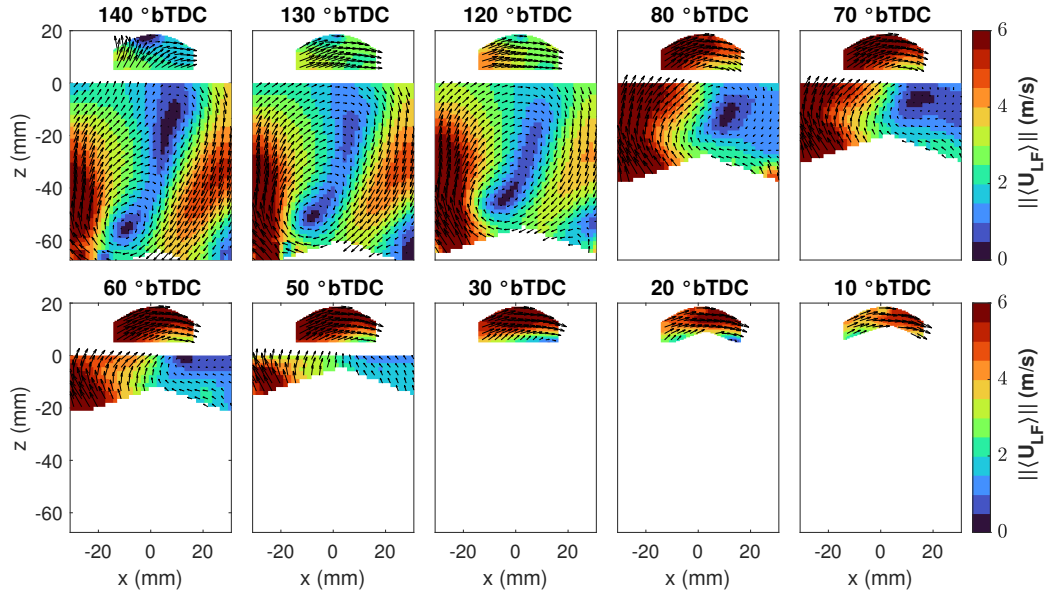


Figure C.18: Ensemble-averaged low-frequency velocity magnitude for the VC and VCC configurations at 0.9 bar intake pressure and 1200 rpm across 10 different crank angles.

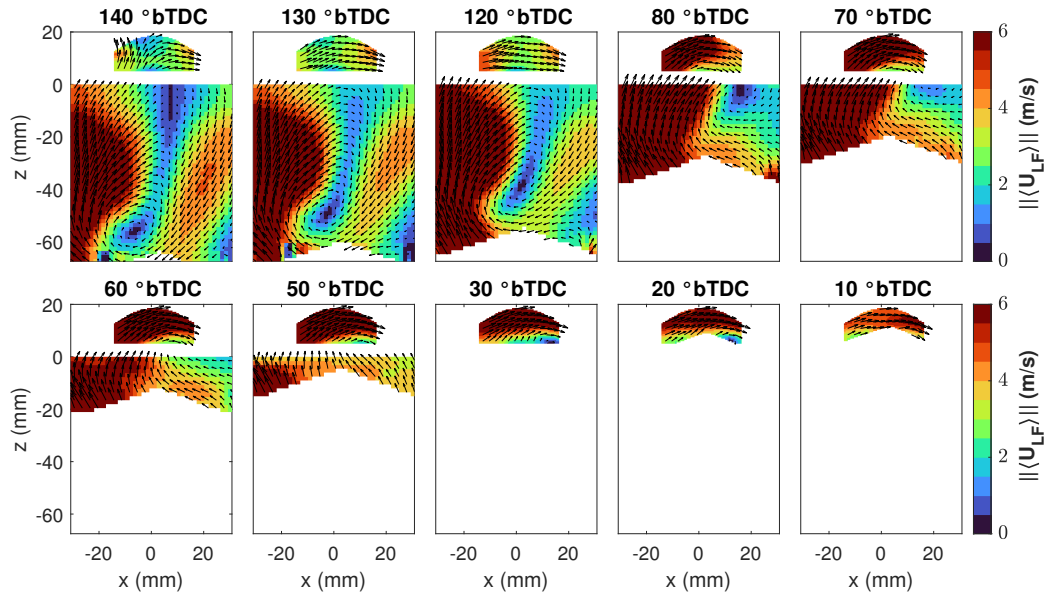


Figure C.19: Ensemble-averaged low-frequency velocity magnitude for the VC and VCC configurations at 0.9 bar intake pressure and 1500 rpm across 10 different crank angles.

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An experimental study on aerodynamics, combustion and cyclic variability in hydrogen-fueled spark-ignition engines under ultra-lean conditions

Hydrogen-fueled internal combustion engines (H_2 ICEs) hold promise for decarbonizing the transport sector. To advance this potential, research is essential on lean hydrogen/air combustion under engine-relevant conditions. This thesis investigates the behavior of very-lean to ultra-lean hydrogen/air flames ($0.20 < \phi < 0.55$) compared to propane/air flames ($0.70 < \phi < 1.50$) using an optical spark-ignition engine and provides enhanced data for the development of hydrogen combustion models in H_2 ICEs. Key flame characteristics are studied and discussed through heat release, chemiluminescence, and particle image velocimetry analyses. Turbulence, flame development, and cyclic variability are examined under varied conditions, including engine speed, intake pressure, and spark discharge duration. Findings highlight a strong relationship between heat release and flame structure. Notably, hydrogen flame development before 2% Mass Fraction Burned (MFB) strongly correlates with pressure-based metrics up to 50% MFB, underscoring the critical role of early flame phase behavior in predicting total combustion duration and in-cylinder pressure trends. A model for turbulent hydrogen flames in the initial combustion stages, based on the Zimont equation and supported by experimental data, demonstrates broad applicability within the Borghi-Peters diagram of turbulent combustion regimes. Additionally, flame chemiluminescence images across these turbulent regimes provide valuable insights into hydrogen flames' distinct characteristics. Ultra-lean hydrogen combustion exhibited greater stability and was less influenced by the flow compared to propane under low-load conditions, showing behavior uncommon in conventional fuels and advantageous for engine operation.

Keywords: *Spark-ignition engine, Combustion, Hydrogen, Ultra-lean mixtures, Aerodynamics, Cycle-to-cycle variations.*

Étude expérimentale de l'aérodynamique, de la combustion et des variabilités cycliques dans les moteurs à allumage commandé alimentés en hydrogène dans des mélanges ultra-pauvres

Les moteurs à combustion interne à l'hydrogène (H_2 ICEs) représentent un potentiel pour décarboner le secteur des transports. Afin de maximiser ce potentiel, des recherches sont essentielles sur la combustion des mélanges hydrogène/air pauvres dans des conditions moteurs. Cette thèse examine le comportement des flammes hydrogène/air très pauvres et ultra-pauvres ($0,20 < \phi < 0,55$) en comparaison avec les flammes propane/air ($0,70 < \phi < 1,50$) à l'aide d'un moteur optique à allumage commandé, fournissant des données haute fidélité pour le développement de modèles de combustion de l'hydrogène dans les H_2 ICEs. Les principales caractéristiques des flammes sont étudiées et discutées via des analyses de dégagement de chaleur, de chimiluminescence et de vélocimétrie par image de particules. La turbulence, le développement des flammes et la variabilité cyclique sont explorés dans des conditions variées, incluant la vitesse du moteur, la pression d'admission et la durée de décharge de l'étincelle. Les résultats mettent en évidence une relation étroite entre le dégagement de chaleur et la structure de la flamme. Notamment, le développement des flammes d'hydrogène avant 2% de la fraction de masse brûlée (MFB) montre une forte corrélation avec les mesures basées sur la pression jusqu'à 50% MFB, soulignant le rôle critique de la phase initiale de la flamme dans la prédiction de la durée totale de combustion et des courbes de pression cylindre. Un modèle pour les flammes turbulentes d'hydrogène dans les premières phases de la combustion, basé sur l'équation de Zimont et validé par les données expérimentales, démontre une large applicabilité dans le diagramme de Peters-Borghi des régimes de combustion turbulente. De plus, les images de chimiluminescence des flammes dans ces régimes turbulents fournissent des informations importantes sur les caractéristiques des flammes d'hydrogène. La combustion de l'hydrogène a également présenté une plus grande stabilité, étant moins influencée par l'écoulement, comparée à celle du propane, tant dans des conditions de faible charge qu'avec des mélanges ultra-pauvres, affichant un comportement atypique par rapport à des carburants conventionnels et avantageux pour le fonctionnement des moteurs.

Mots clés : *Moteur allumage commandé, Combustion, Hydrogène, Mélanges ultra-pauvres, Aérodynamique, Variabilités cycliques*