

Direct numerical simulation of flame-wall interaction and flame-cooling air interaction

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Abstract

The interaction of a flame with a relatively cold combustor wall with or without cooling air jets, i.e. flame-wall interaction (FWI) and flame-cooling air interaction (FCAI) influences emissions and fuel consumption. In particular, with the current trend towards increasing the power density in energy-producing systems, these phenomena become even more important in the new generation of modern gas turbines. As a result, a full understanding of FWI and FCAI and their impact on the produced emissions is a topic of interest. In this thesis, a preheated, premixed methane/air flame is studied in the context of FWI and FCAI using direct numerical simulation (DNS).

First, two-dimensional (2D) DNSs are performed to study the impact of unsteady, laminar flame-wall interaction on flame dynamics, wall heat transfer and near-wall *CO* emissions. The flame is excited by imposing velocity perturbations at the inlet to the flow for several forcing frequencies. The flame dynamics over a forcing cycle is investigated for low, intermediate and high forcing frequencies. The significance of low-activation energy radical recombination reactions near the wall is also analysed. These reactions contribute to about 50% of the overall heat release rate at the wall at the quenching instant. An investigation of the near-wall *CO* transport mechanisms revealed that the near-wall *CO* transport close to the flame tip is dominated by convection and diffusion.

Second, a parametric study of flame-cooling air interaction (FCAI) is performed using 2D DNSs of forced laminar flames. The effects of injection of coolant jets through the wall on the flame dynamics, the near-wall *CO* and the wall heat flux are explored. The forcing frequency, the coolant mass flux, the position of the cooling hole and the coolant type are varied in this analysis. Several factors including

the dilution of the flame tip by the coolant, variations in the trajectory of the cooling jet are found to impact the flame and *CO* behaviours. Furthermore, a modelling framework to predict near-wall *CO* due to FCAI based on one-dimensional unstrained laminar freely propagating flame simulations is proposed.

Third, analysis of FWI and FCAI under turbulent flow conditions are performed in a three-dimensional computational domain. Under FWI conditions, vorticity-induced flame structures are found to impact the wall heat flux and *CO* at the wall. Under FWI and FCAI conditions, the *CO* characteristics are investigated using the thermochemical states of *CO*. Finally, the performance of the model proposed to predict near-wall *CO* due to FCAI in the 2D flames is evaluated under the turbulent flow conditions and showed promising results.

Declaration

This is to certify that:

1. the thesis comprises only my original work towards the Ph.D. except where indicated,
2. due acknowledgment has been made in the text to all other material used,
3. the thesis is less than 100,000 words in length, exclusive of tables, maps, bibliographies and appendices.

Signed,

Rahul Palulli

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Nomenclature

α	Thermal diffusivity
ΔH	Heat of reaction
δ_L	Diffusive flame thickness
δ_Q	Quenching distance
δ_{th}	Thermal flame thickness
Λ	Pre-exponential factor
λ_g	Thermal conductivity of gas mixture
ω	Reaction rate
Φ	Wall heat flux (dimensional)
ϕ	Equivalence ratio
Φ_Σ	Flame power (dimensional) = $\rho_1 Y_f s_L \Delta H$
ϕ_{wall}	Wall heat flux (non-dimensional)
ρ_u	Density of unburnt gas
ξ	Modified mixture fraction
c_{CO_2}	Progress variable based on Y_{CO_2}
$c_{p,g}$	specific heat of gas mixture
D_{mass}	Mass diffusivity
E_a	Activation energy of reaction(s)

HRR	Heat release rate
L_{ref}	Reference length
Le	Lewis number ($=\alpha/D_{mass}$)
Pe	Peclet number
Pe_{min} or Pe_Q	Quenching (i.e. minimum) Peclet number
R_u	Universal gas constant
Re_{ac}	Acoustic Reynolds number ($= \frac{a_{ref}\rho_{ref}L_{ref}}{\mu_{ref}}$)
s_L	Laminar flame speed
T_b	Burnt gas temperature
T_u	Unburnt gas temperature
T_{wall}	Wall temperature
X^+	Streamwise coordinate (non-dimensional)
X_{fuel}	Mole fraction of fuel
Y^+	Wall-normal coordinate (non-dimensional)
Y_f	Fuel mass fraction
Y_k	Mass fraction of the species k
Z^+	Spanwise coordinate (non-dimensional)

Chapter 1

Introduction

1.1 Background and motivation

According to the International Energy Agency (IEA), a more than 25% increase in the global energy demand is expected by 2040 [1], and renewable energy sources are likely to meet about 40% of the energy demand by then [1, 2]. Despite the growth of renewable resources, the consumption of natural gas is also expected to increase by 45% to 2040 [1, 2]. One of the reasons for this is that natural gas, due to its higher hydrogen to carbon ratio, produces less CO_2 emission per unit power produced, compared to conventional fuels [3]. Furthermore, natural gas is a common fuel in gas turbines for power production. The ability of gas turbines to quickly change load thereby aiding frequency control of the grids makes them able counterparts to variable renewable power sources [3]. Therefore, natural gas powered gas turbines are expected to become increasingly relevant in the coming decades.

1.1.1 Gas turbine emissions

The emissions resulting from combustion processes, including those in gas turbines, pose health and environmental hazards [4] and are rigorously legislated. Exposure to carbon monoxide (CO) emissions reduces the oxygen absorption capability of blood and exposure can be fatal. The oxides of nitrogen, collectively called NO_x , causes effects such as photochemical smog [4]. The control of these emissions is complicated. Decrease of one emission may lead to an increase in another. For in-

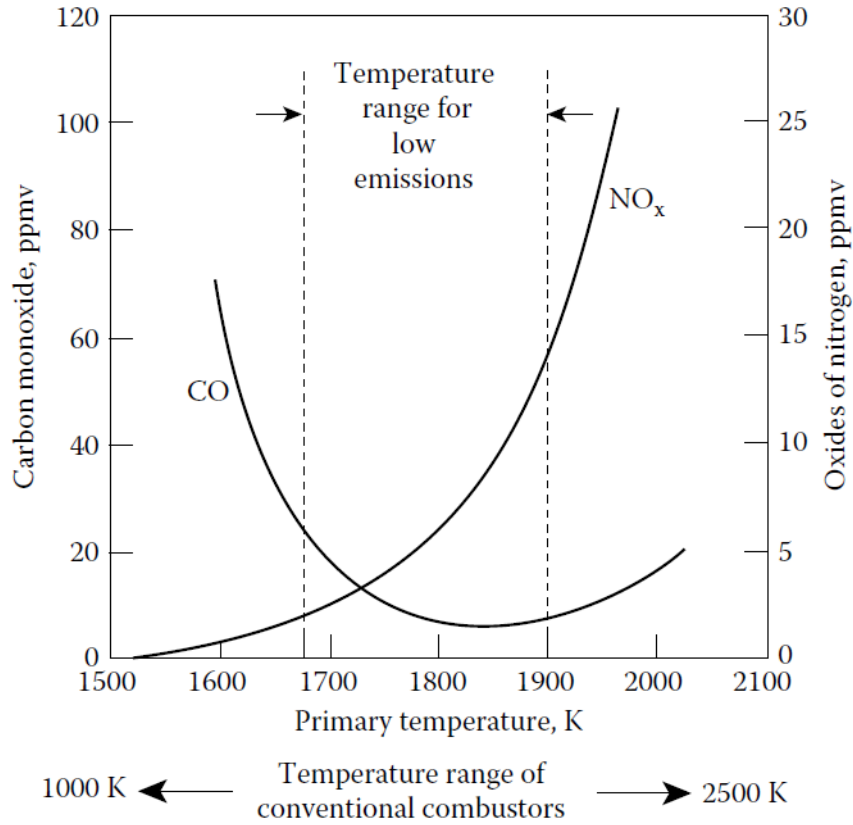


Figure 1.1: The variation of carbon monoxide (CO) and oxides of nitrogen (NO_x) with primary combustor temperature [4].

stance, Figure 1.1 illustrates the inverse behaviour of CO and NO_x with an increase in primary combustor temperature. One of the major mechanisms of NO_x production is highly temperature dependent. This thermal NO_x , which is produced by the oxidation of atmospheric nitrogen at high temperatures, increases exponentially with temperature. Therefore, the various efforts to reduce NO_x have focussed on the reduction of the flame temperature. However, reduction in primary combustor flame temperature increases the CO emission [4]. This could be due to incomplete combustion and/or reduced CO oxidation rates at lower temperatures.

Incomplete combustion is the major cause of significant CO emission [4]. Some of the reasons for incomplete combustion are as follows:

- Extremely low fuel/air ratio and/or insufficient residence time [4].
- Improper mixing of fuel and oxidiser leading to pockets of rich mixtures [4].
- Quenching of a flame in the presence of a wall which acts as a heat and radical

sink [5].

- Entrainment of burned products into wall-cooling air [4]. The oxidation rate of CO would reduce in this low-temperature, lean region.

A detailed understanding of each of these mechanisms facilitates further control of the emission. The formation of CO due to interaction of the flame with a wall (flame - wall interaction, FWI) and cooling air (flame - cooling air interaction, FCAI) are investigated in this thesis.

1.1.2 Gas turbine wall heat flux

The near-wall behaviour of the flame affects the combustor wall heat flux as well. The thermal stress experienced by gas turbine combustor walls is extremely high. The hot gases released by the combustion process are generally at temperatures over $2100^{\circ}C$ [4]. Also, there is a constant effort to increase the maximum temperature of the gas turbine cycle, as this improves the thermal efficiency. However, the melting point of the combustor walls is less than the temperature of hot gases [4]. Therefore, it is important to cool the combustor walls, which is generally done with a fraction of the inlet air. Using a larger amount of cooling air then reduces the performance of the combustor. The maximum wall heat flux influences the longevity of the combustor wall while the mean wall heat flux is used in estimating the cooling load requirement [6]. Improved insights regarding the near-wall behaviour of a flame is therefore important in the design of combustor walls.

1.1.3 Flame-wall interaction (FWI)

Flame-wall interaction impacts emissions and fuel consumption. An attempt to improve engine efficiency and to reduce emissions has triggered a trend towards downsizing. Downsizing refers to increasing the power density of the combustion engines by reducing the dimensions for a given power output. This leads to a higher surface to volume ratio, and as a result phenomena like flame-wall interaction become more significant. Therefore, the importance of flame-wall interaction is increasing [7].

The fundamental concept of flame-wall interaction is as follows. As a flame ap-

proaches a cold wall, the heat loss through the wall increases. This is because of the high gradient generated between the hot flame and the cold wall. At the instant when the heat loss through the wall increases beyond the energy required to sustain the flame, the flame stops propagating. This phenomenon, where the flame ‘quenches’ at a certain distance away from the wall, is called flame-wall interaction. The various quenching configurations are explained in Section 2.2.

1.2 Research goals

The review of FWI related literature, as detailed in Chapter 2, identifies the study of *CO* emission characteristics, wall heat flux and flame dynamics near a combustor wall as some of the important areas of research which require further investigation. The overall objective of this project is to investigate the flame dynamics, wall heat flux and near-wall *CO* characteristics of preheated, premixed methane/air flames interacting with walls, with or without cooling air jets, using direct numerical simulations (DNS). Laminar and turbulent flow conditions will be studied.

Chapter 2

Literature Review

2.1 Introduction

The literature review is structured as follows. The fundamentals of flame-wall interaction are reviewed in Section 2.2 where the effect of several parameters on quenching parameters and wall heat flux are discussed. The effect of flame-wall interaction on CO is reviewed in Section 2.3 while the CO due to interaction of a flame with cooling air jets is discussed in Section 2.4. Turbulent flame-wall interaction studies reported in the literature are discussed in Section 2.5. The major learnings from the literature are then summarised and the research questions are presented in Section 2.6.

2.2 Fundamentals of flame-wall interaction (FWI)

The various flame quenching configurations and the basic parameters related to FWI are introduced in Section 2.2.1. The effects of pressure, wall temperature, Lewis number and surface chemistry on the quenching parameters and wall heat flux are then discussed in Sections 2.2.2 to 2.2.5. The concept of low-activation, exothermic radical recombination reactions is reviewed in Section 2.2.6.

2.2.1 Basic parameters

The interaction of a flame with a relatively cold wall affects both the wall heat transfer as well as the flame behaviour. Due to the temperature difference between the wall and the flame, heat is transferred from the flame to the wall. When the wall heat loss increases beyond the energy required to sustain the flame, the flame quenches. The minimum distance between the flame and the wall is called the quenching distance (δ_Q).

There are two common types of quenching, namely, head-on quenching (HOQ) and side-wall quenching (SWQ). In the HOQ configuration, the flame propagates normal to the wall. It moves parallel to the wall during SWQ. Schematics of these quenching configurations are shown in Figure 2.1. The flame is pushed closer to the wall during HOQ, compared to the SWQ configuration, and hence features a higher wall heat flux. A numerical study of the two configurations demonstrated that the quenching distance during HOQ could be less than 50% of that during SWQ [8].

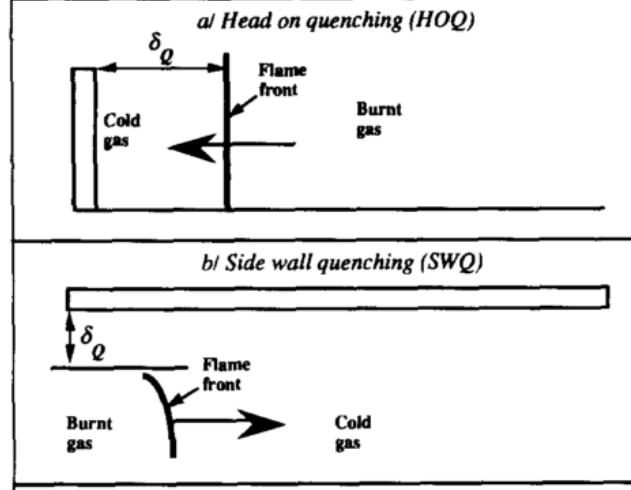


Figure 2.1: Various FWI configurations: (a) Head-on quenching (HOQ), and (b) Side-wall quenching (SWQ) [8].

In the context of FWI, two parameters are used in the literature: the minimum distance of the flame from the wall (δ_Q); and the maximum wall heat flux (ϕ_{max}). The distance of the flame from the wall is commonly non-dimensionalised by the flame thickness to obtain the local Peclet number (Pe). The limiting (minimum) value of Pe , i.e. $Pe_{min} = \delta_Q/\delta_L$, indicates the quenching distance non-dimensionalised

by the diffusive flame thickness (δ_L) [8]. The dimensional wall heat flux (Φ_{wall}) is normalised by the reference laminar flame power (Φ_Σ) to get the non-dimensional wall heat flux (ϕ_{wall}).

$$\Phi_\Sigma = \rho_u Y_f s_L \Delta H \quad [8], \quad (2.2.1)$$

where ρ_u , Y_f , s_L and ΔH refer to the unburnt gas density, fuel mass fraction, unstretched laminar flame speed and the heat of reaction, respectively. The maximum and mean (time-averaged) values of the wall heat flux are practically important as the former influences the combustor lifetime while the latter determines the cooling load requirement [6].

A simple correlation between the minimum Pe (Pe_{min}) and the maximum non-dimensional wall heat flux at the quenching instant was proposed for laminar flames in Ref. [8]. It was assumed that heat conduction in the quenching layer is the only contributor to the wall heat flux, leading to,

$$\phi_{max} = \left(\frac{T_b - T_{wall}}{T_b - T_u} \right) \frac{1}{Pe_{min}}. \quad (2.2.2)$$

The quenching distance (δ_Q) is closely related to the maximum wall heat flux (Φ_{wall}) as well. Fundamentally, a flame quenches when the heat transferred to the wall exceeds the energy required to sustain the flame. Sotton et al. [9] expressed δ_Q in terms of the wall heat flux (see Equation 2.2.3). The variables λ_g , X_{fuel} , and $c_{p,g}$ denote the thermal conductivity of the gas mixture, fuel mole fraction and specific heat of the gas mixture. Equation 2.2.4 defines the reaction rate (ω) in terms of pre-exponential factor (Λ), activation energy (E_a), universal gas constant (R_u) and temperature (T). Coefficients a and b are dependent on the reaction mechanism:

$$\delta_Q^2 = k_2 \left(1 - \frac{\Phi_{wall}}{\Phi_\Sigma} \right) \frac{\lambda_g \cdot X_{fuel}}{c_{p,g} \cdot \omega} \quad (2.2.3)$$

$$\omega = \Lambda \cdot \exp\left(\frac{-E_a}{R_u T}\right) \cdot [\text{Fuel}]^a \cdot [\text{Oxidiser}]^b \quad (2.2.4)$$

This correlation between δ_Q and Φ_{wall} can be useful to estimate the quenching distance in some cases. For instance, due to experimental constraints, the quenching distance at higher pressures cannot be measured directly [9]. Under such conditions, δ_Q can be determined from Φ_{wall} .

2.2.2 Effect of pressure

Several experimental studies have investigated the effect of pressure on the quenching distance [9–12]. In early 50s, measuring quenching distance between two plane parallel plates revealed an inverse relationship between the pressure and the quenching distance [10, 11]. This is a power-law relation where δ_Q is inversely proportional to the n^{th} power of pressure. This relation has been reported in the literature for various fuels including propane [10], n-heptane, iso-octane, benzene, ethyl ether [11] and methane [9]. The value of n for several fuels are compiled in Table 2.1.

Table 2.1: Power law relation ($\delta_Q \propto p^{-n}$) for various fuels

Fuel	n	Reference
Propane	0.91	Friedman and Johnston, 1950 [10]
n-heptane	0.92	Friedman and Johnston, 1952 [11]
iso-octane	0.91	
Benzene	0.91	
Ethyl ether	0.87	
Methane (for 0.05-0.2 MPa)	1.27	Sotton et al., 2005 [9]

The variation of δ_Q with pressure, studied in one of the above works is displayed in Figure 2.2, as an example. The quenching distance of a propane/air flame propagating between two parallel plates was measured. The minimum distance between two parallel plates when flashback can happen was considered as the quenching distance in this setup. The variation of the quenching distance, for various pressures and air/fuel ratios, is shown in Figure 2.2. The inverse relationship between δ_Q and p

observed is likely to be linked to the inverse relationship between pressure and the flame thickness.

The minimum value of the quenching distance for a given pressure occurs at slightly less than the stoichiometric air-fuel ratio. This trend is similar to that of the flame thickness suggesting that the flame thickness plays an important role in the observed behaviour. Similar trends have been reported for methane [13], methanol [13], propane [10], n-heptane [11] and iso-octane [11].

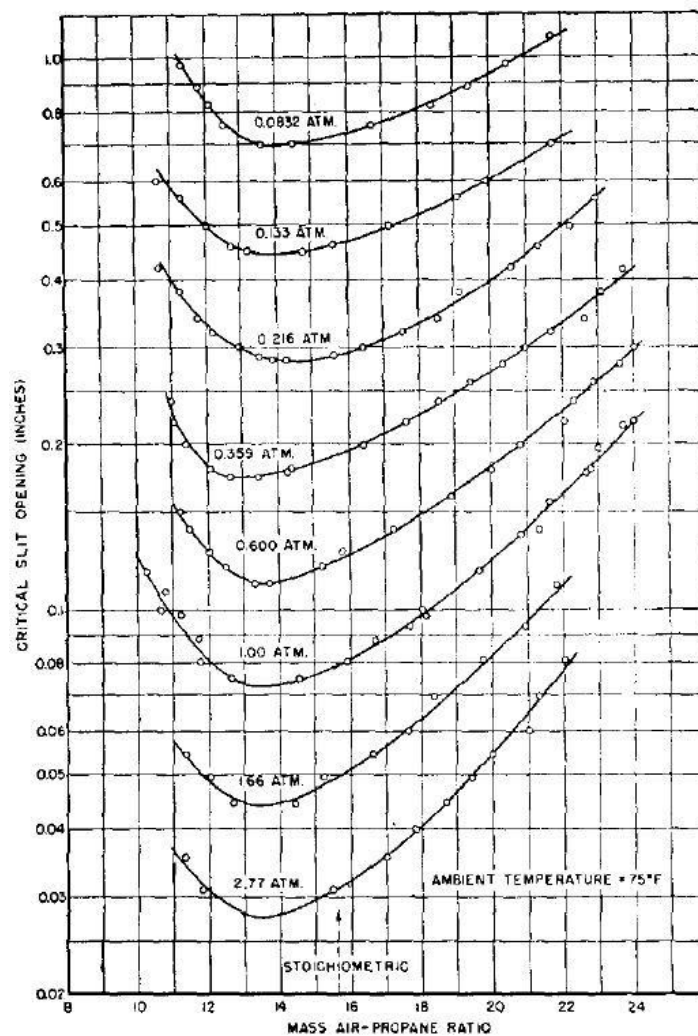


Figure 2.2: Quenching distance versus air/fuel ratio (propane fuel) at different pressures [10].

Equation 2.2.3 can be used to test the validity of the power law correlation discussed earlier. The quenching distance in the HOQ configuration deduced using three different methods, are shown at different pressures in Figure 2.3 [9]. The minimum

δ_Q is determined by (i) direct photography (shown by black circles in Figure 2.3), (ii) from the power law correlation (shown by dotted line), and (iii) from Equation 2.2.3. Experimental data is reported for pressure ranging from 0.05 MPa to 0.2 MPa. The power law prediction of δ_Q matched with the experimental and calculated results in this range of pressure, see Figure 2.3 (a). Authors noted that there were no experimental methods to directly measure quenching distance at high pressures. A comparison of the quenching distances calculated using methods (ii) and (iii) showed a mismatch at high pressures, see Figure 2.3 (b).

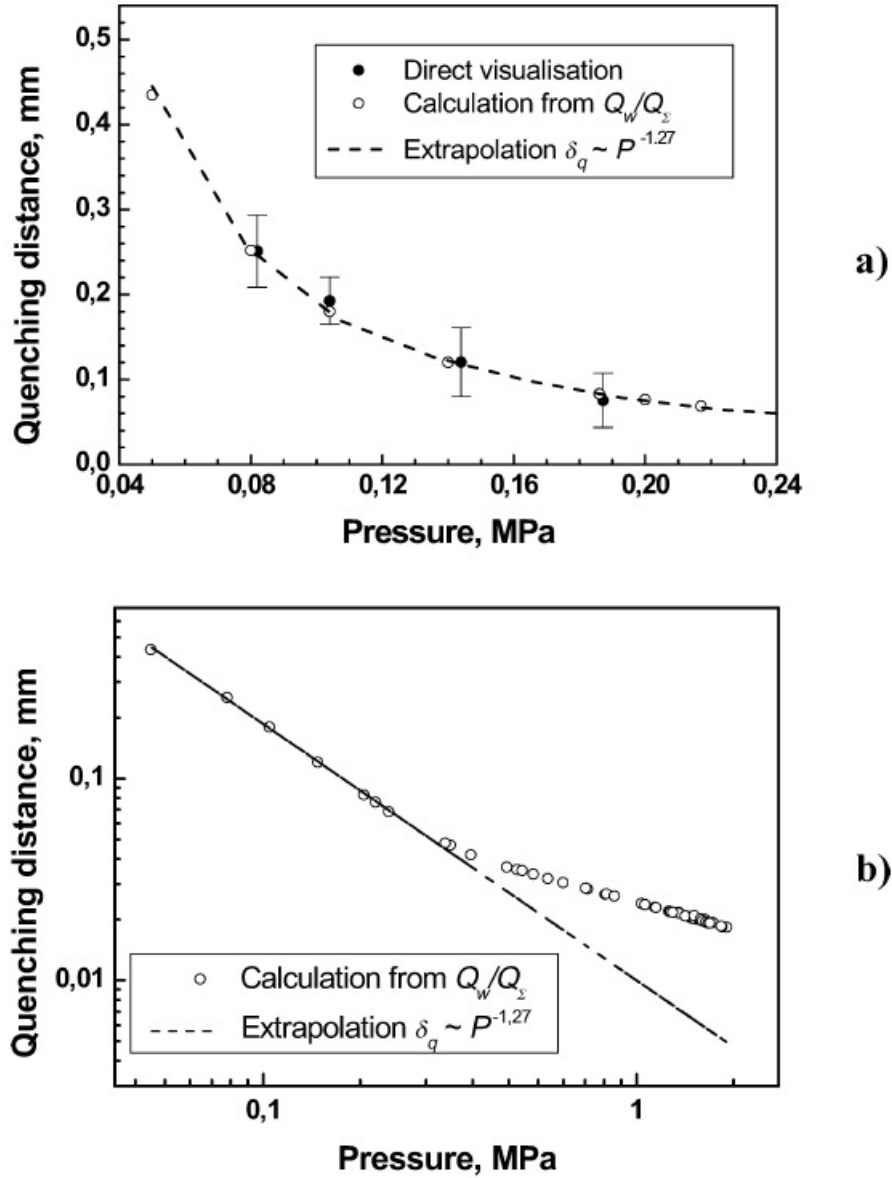


Figure 2.3: Quenching distance over a range of pressures: (a) 0.05-0.24 MPa and (b) 0.05-1.7 MPa [9]. ($Q_w \equiv \Phi_{max}$, $Q_\Sigma \equiv \Phi_\Sigma$.)

2.2.3 Effect of wall temperature

An increase in the wall temperature (T_{wall}) heats up the unburnt gas adjacent to the wall. This preheating increases the flame speed and the flame power, thereby reducing δ_Q . As a result, the wall heat flux increases, provided the wall temperature is much less than the adiabatic flame temperature. Computational results of stoichiometric methane/air and propane/air flames interacting with a wall, shown in Figure 2.4, demonstrate this relation. The effects of wall surface chemistry and cross-diffusion (Soret effect) on the wall heat flux are also elucidated therein.

Surface chemistry and Soret effects are negligible at low temperatures (≤ 400 K) for methane/air flames. However, at higher wall temperatures (> 400 K), the maximum Φ_{wall} of a methane/air flame is higher when both surface chemistry and Soret effects are neglected (see Figure 2.4) [14]. Of these two effects, surface chemistry is found to influence the wall heat flux more. Up to 18% reduction in the maximum Φ_{wall} was observed when Soret effect and surface chemistry were included in the analysis [14]. Furthermore, surface chemistry becomes more important at a lower temperature for a propane/air flame (see Figure 2.4). This is expected as propane/air mixtures ignite at lower temperatures compared to methane [14]. As the reactions initiate, more reactive radical species will be formed, some of which may be adsorbed by the reactive wall.

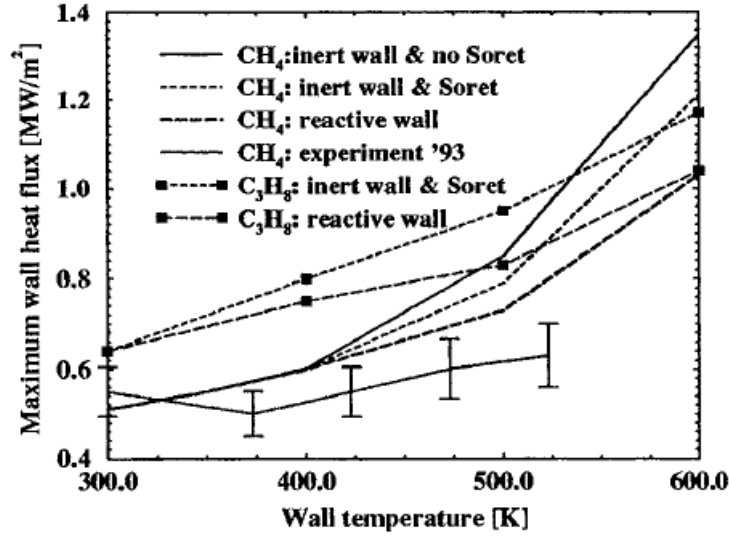


Figure 2.4: The variation of maximum wall heat flux (Φ_{max}) with wall temperature (T_{wall}) for methane/air and propane/air flames [14]. Computational results obtained for methane (with and without wall surface chemistry and Soret effects) are compared to the corresponding experimental findings [15].

The qualitative trend of Φ_{wall} as a function of T_{wall} , captured by the computational studies is different from that in the experimental results where no discernible variation in Φ_{wall} with T_{wall} is observed. Also, in general, the computational results over-predict the wall heat flux compared to the experimental findings. This is because the heat loss to the surroundings (except for the wall) is not included in the computational studies.

2.2.4 Effect of Lewis number (Le)

The relative importance of mass diffusivity (D_{mass}) of each species relative to the thermal diffusivity (α) is quantified by the Lewis number ($Le = \alpha/D_{mass}$). The mass diffusivity of the fuel affects the transport of the fuel near the wall. This influences the fuel concentration in the quenching zone. As fuel trapped in the quenching zone does not undergo combustion, this can affect fuel consumption and emissions. It can also locally alter flame speed and quenching distance.

In a turbulent flame, Le affects the local flame speed depending on the local flame curvature [16, 17]. Figure 2.5 shows this effect in a premixed, turbulent flame simulated in a two-dimensional domain with a single-step chemical mechanism [16]. Figures 2.5(a)-(c) show the results for $Le = 0.8$, 1 and 1.2, respectively. A positive

value of curvature in Figure 2.5 indicates that the flame is convex in shape towards reactants. In this region, the local flame speed increases with a decrease in Le . One may explain this trend as follows. For $Le < 1$, the mass diffusion is faster than the thermal diffusion. As a result, the reactant species reach the convex region of the flame faster thereby increasing the reaction rate and the local flame speed. Conversely, the local flame speed decreases in the negative curvature region, i.e. a concave shaped (towards reactants) flame, with a decrease for $Le < 1$. For concave shaped flame, the reactant species diffuse in a larger region, therefore reducing the flame speed.

Lai et al. [18] investigated the effects of Lewis number on head on quenching of turbulent premixed flames using a three-dimensional DNS under turbulent conditions with single-step chemistry. They showed the observed trends for the flame speed as a function of curvature and Lewis number in a turbulent flame can affect the minimum Pe .

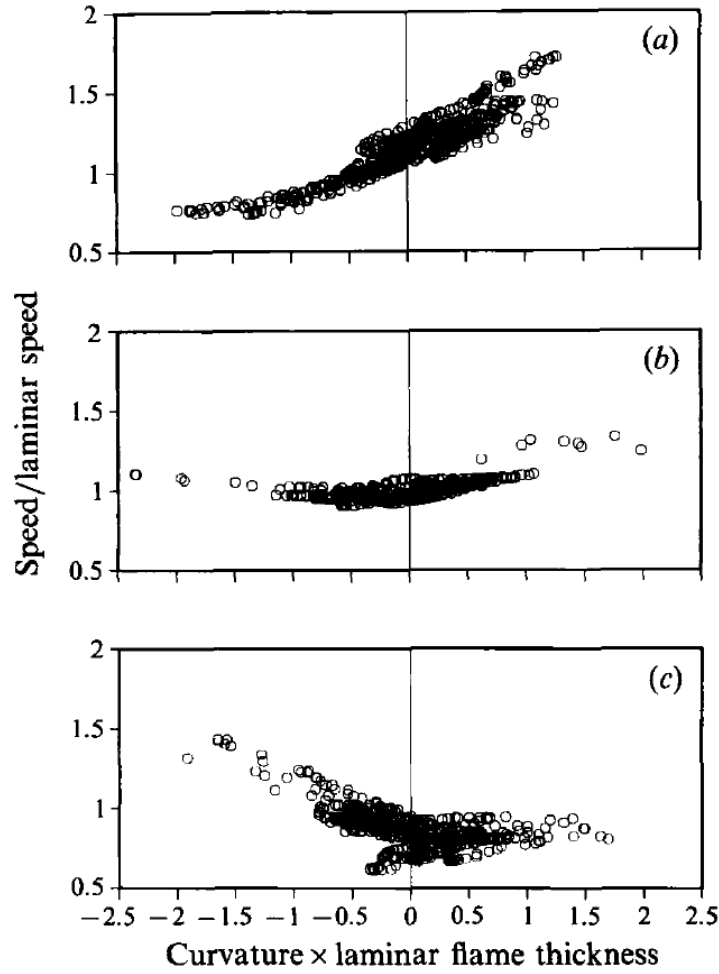


Figure 2.5: Scatter plots of local flamelet speed (normalised by laminar flame speed) varying with the normalised local flame curvature for different Le [16]. Curvature, which is the reciprocal of the radius of curvature, is normalised by the reciprocal of laminar flame thickness. (a) $Le = 0.8$, (b) $Le = 1.0$, (c) $Le = 1.2$.

2.2.5 Effects of surface coatings

Modification of the wall surface properties, due to the presence of surface coatings and/or due to the use of different surface materials, influences the flame quenching properties. The thermal conductivity of the wall influences the wall heat transfer which in turn can affect the quenching distance. For instance, low heat loss through an insulating wall delays the flame extinction, thereby decreasing the quenching distance. The adsorbing and/or catalytic characteristics of the wall can influence the near-wall chemistry. Adsorption can affect the availability of various species for reactions and catalysis may accelerate the near-wall chemical reactions.

Figure 2.6 shows the effect of wall material in SWQ and HOQ configurations. In a

pressure range of 0.05 - 0.15 MPa, the quenching distance with an insulating wall material like ceramic was lower than that with a steel wall by a factor of 1.1 - 1.8 in a SWQ configuration (see Figure 2.6(a)). Also, the quenching distance was found to change for an unchanged wall material with an additional covering of soot. The quenching distance was reduced by a factor of 1.1 - 1.5 when a steel wall was coated with a layer of soot [12]. Figure 2.6(b) shows the effect of wall material in a HOQ configuration. The quenching distance observed in SWQ, discussed above, is plotted as a reference. As expected, the quenching distance is lower in a HOQ configuration. For polished steel, the quenching distance in the HOQ configuration is lower than that in the SWQ configuration by a factor of 1.4 - 2.5 when the pressure ranges from 0.08 - 0.19 MPa [12]. In a HOQ configuration also, the quenching distance decreased by a factor of 1.25 - 1.45 relative to that observed in a steel wall, in the pressure range of 0.08 - 0.12 MPa when an insulating wall material (ceramics) was used.

An experimental uncertainty of 0.05 mm, noted in Ref. [12], is shown in Figure 2.6. Considering the possibility of erroneous measurements within this range of uncertainty, one may infer that the effect of wall material may not be that significant. This is further explained in Ref. [19].

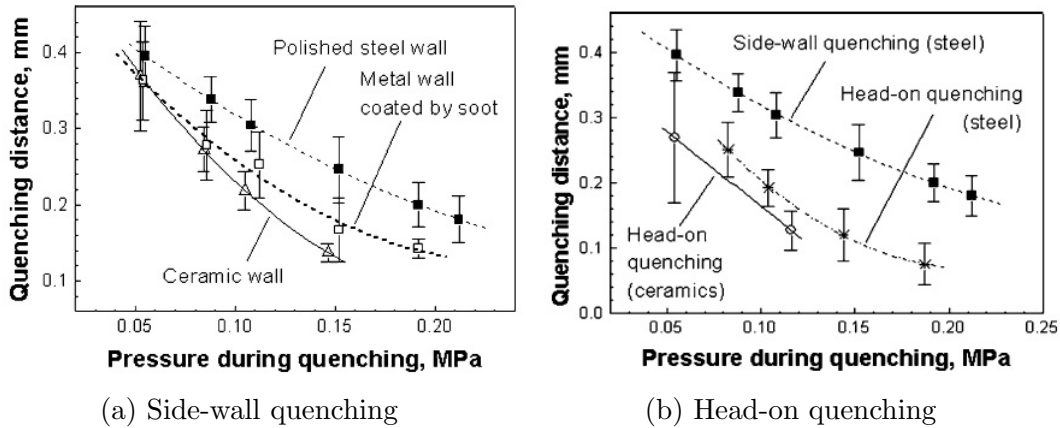


Figure 2.6: Quenching distance with various wall materials for varying pressure [12]

Haber and Suntut [19] observed that ceramic coating affected quenching distance in a SWQ configuration. The authors were cautious of drawing conclusions, as the difference in the quenching distance for different cases was comparable to the experimental uncertainty of 84 μm . Figure 2.7 shows the quenching distance for

methane/air and propane/air flames over a range of equivalence ratios. In general, the quenching distance decreased with an increase in the thickness of the ceramic coating. This is clearly seen for propane/air flames (Figure 2.7(b)), while a different trend is observed for lean methane/air flames.

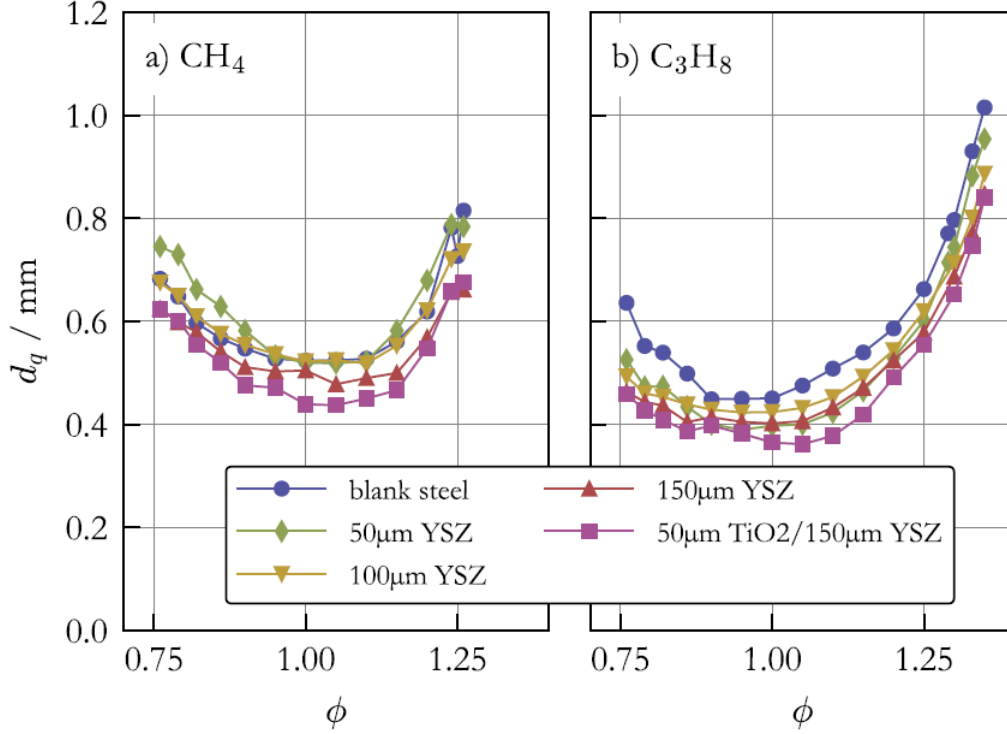


Figure 2.7: The variation of quenching distance with different ceramic coating thickness for laminar premixed methane/air and propane/air flames over a range of equivalence ratios [19]. Ceramic materials shown are yttrium-stabilised zirconium-dioxide (YSZ) and titanium dioxide (TiO₂).

Saffman studied the catalytic and adsorption characteristics of a wall in a SWQ configuration [20]. The temperature and fuel mass fraction profiles of a propane/air flame in the quenching layer for different wall materials, namely copper, Teflon and platinum were noted. The observed differences in temperature and fuel mass fraction were again within the experimental uncertainties [20].

Owston et al. [21] numerically investigated the influence of wall surface chemistry on the wall heat flux. The wall surface chemistry influences the concentration of radical species near the wall. One of the effects of a chemically active surface is to adsorb radicals thereby reducing their concentration near the wall. This effect was simulated in Ref. [21] by defining a recombination wall where the concentration of

radicals H , O and OH were set to zero in the near-wall cell. This is referred to as the radical sink methodology. The mass fractions of these radicals were added to that of water to ensure a sum of unity. A 750-K isothermal wall and a n-heptane/air flame were considered. The peak wall heat flux was about 16% lower with a recombination wall (Figure 2.8) as opposed to a chemically inert wall. However, the significance of surface chemistry on the quenching distance and thus on the wall heat flux depends on the wall temperature and wall material [22].

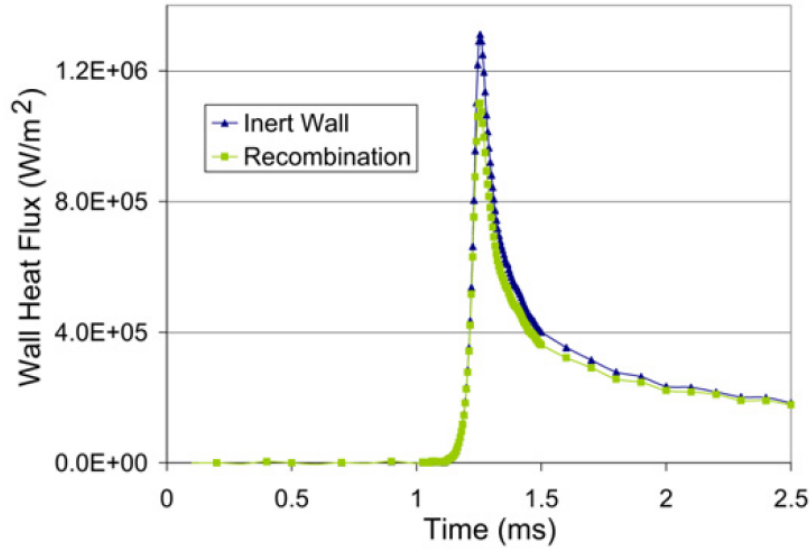


Figure 2.8: Wall heat fluxes at an isothermal (750 K) wall, with and without surface chemistry (‘recombination’ and ‘inert’, respectively) [21].

Kim et al. [22] experimentally studied the effects of surface chemistry over a range of wall temperatures using a slit burner in which a stoichiometric mixture of methane and air was burned and stabilised between two parallel plates behaving as the walls. The variations of quenching distance with temperature for inert and reactive walls made of stainless steel and quartz reported in [22] are shown in Figure 2.9. At low wall temperatures ($T_{wall} \leq 500^{\circ}C$), the quenching distances measured using reactive and inert quartz walls did not show a significant difference. This difference increased at higher temperatures. Similar observations were reported in [22] with an alumina wall (not shown in the figure). However, the effect of surface chemistry on the quenching distance was qualitatively different in the same temperature range when a stainless steel wall was used. The quenching distance measured with inert and reactive stainless steel walls showed a higher difference even at low temperatures.

Thus, one may infer that the effect of surface chemistry on quenching parameters depends on both wall temperature and wall material. Consideration of surface chemistry for a given wall material will limit the generality of the results as a number of wall materials may be used in practical combustors. Hence, high wall temperature (750 K) studies have also neglected surface chemistry deliberately [6].

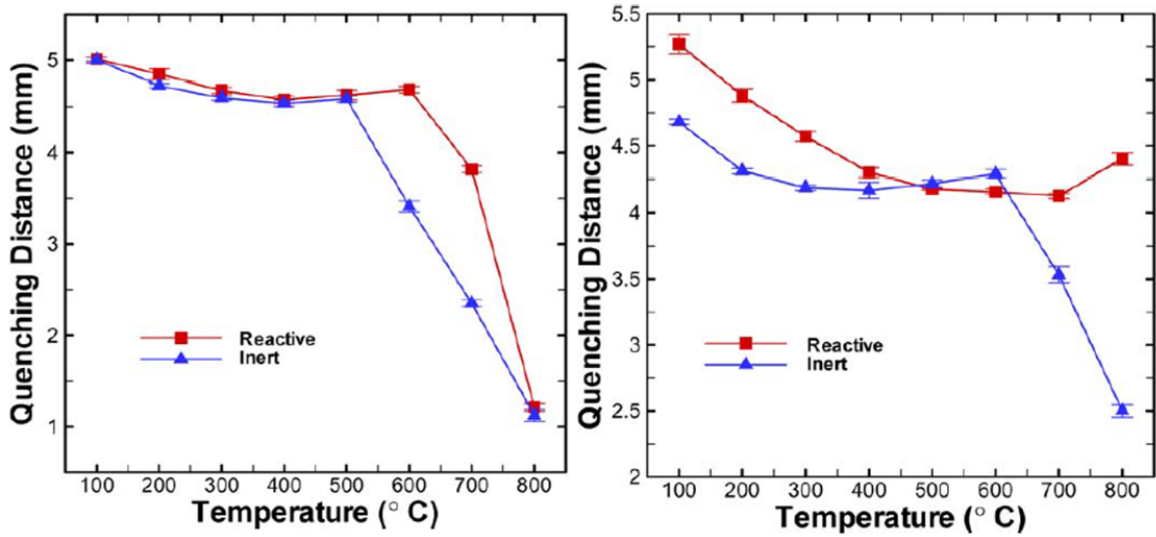


Figure 2.9: The effect of wall temperature on quenching distance with inert and reactive walls of quartz (left) and stainless steel (right) [22].

2.2.6 Radical recombination reactions

At or near a relatively cold wall, low temperature chemistry is activated, reason for which is as follows. The activation energy required to trigger major chemical reactions (e.g. fuel oxidation reactions) is generally high. Therefore, at low temperatures, these reactions do not occur. In this case, reactions with lower activation energy become more important. Radical species are chemically unstable and hence are chemically reactive. They react with each other or with other species to form more stable species. These reactions which are exothermic and have low-activation energy (or zero-activation energy, as defined in [6]) are called radical recombination reactions and are dominant in a certain temperature range (greater than 400 K [21, 23] and less than about 800 K [13]).

The radical recombination reactions consume most radicals near the wall. This can be observed in Figure 2.10 where the maximum mole fraction of the stable species such as CH_4 and O_2 are found near the wall while those of the radical species such

as H , O and OH are found at a distance from the wall [13]. More understanding of this concept requires a comparison of the major contributing reactions near and away from a wall, which was conducted by Owston et al. [21].

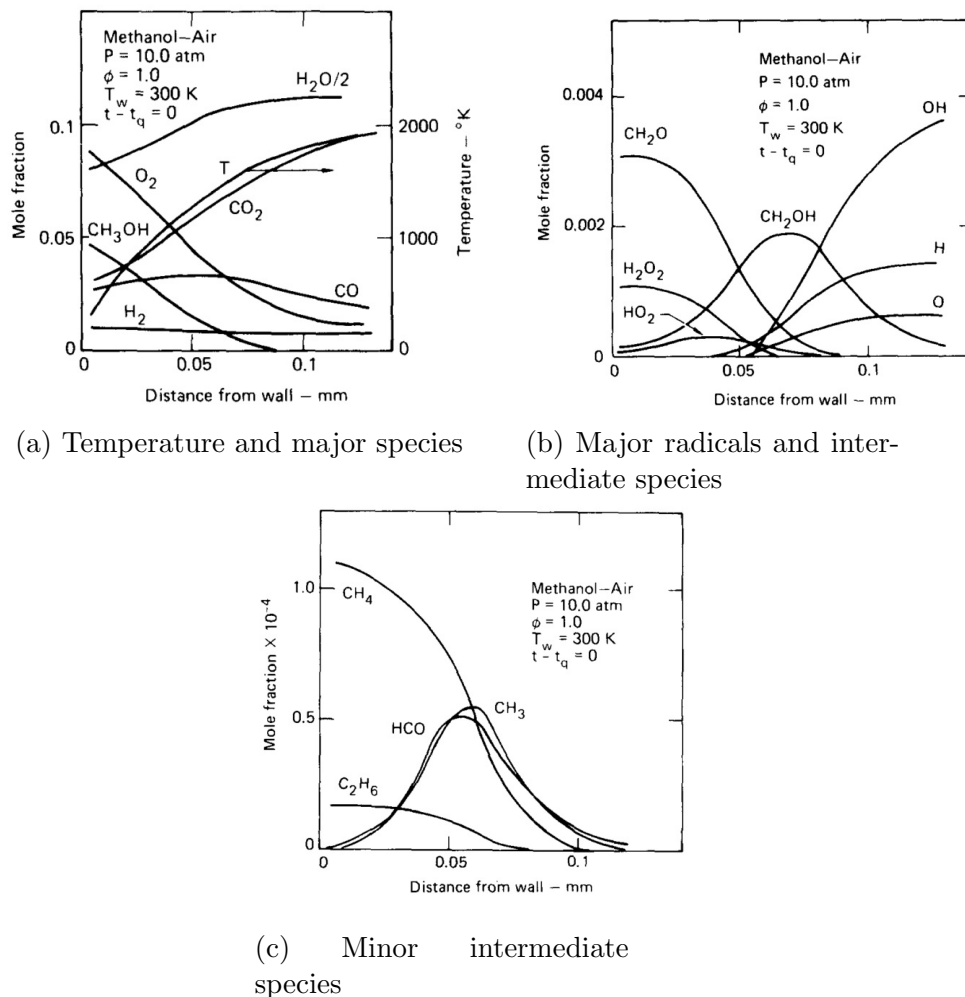


Figure 2.10: Temperature and species concentration during quenching [13]

Owston et al. [21] numerically investigated a one-dimensional, premixed n-heptane/air flame quenching against an isothermal (750 K), inert wall. A difference in heat release rate was observed between a freely-propagating flame and a quenching flame. They found that the major reactions contributing to the net heat release rate were different near the wall and away from the wall. Certain zero or low-activation energy reactions were found to release more heat near the wall, thereby underlining the increasing importance of radical recombination reaction in this region. For instance, the heat release rate of $CHO + H \rightarrow CO + H_2$, which has zero-activation energy, was 50% greater near the wall [21]. Also, the authors noted that four out of the

five reactions which released more than $7 \times 10^8 \text{W/m}^3$ in the near-wall region at the quenching instant involved consumption of H , O or OH radicals.

In a three-dimensional DNS of a rich ($\phi = 1.5$), preheated ($T_u = 750 \text{K}$) hydrogen/air flame with detailed chemical mechanism [6], the contribution of radical recombination reactions was quantified. The near-wall heat release rate due to each reaction was determined along with the overall heat release rate. It was identified that radical recombination reactions contributed to about 70% of the overall heat release rate. This result was established using a one-dimensional laminar simulation.

The contribution of different species to the overall heat release rate at the wall in turbulent premixed methane/air flames ($T_u = 300 \text{ K}$) was studied in Ref. [24] (see Figure 2.11). Authors reported that the species involved in the reaction steps $O_2 + H + M \rightarrow HO_2 + M$ and $2HO_2 \rightarrow H_2O_2 + O_2$ were the major contributors to the overall heat release rate at the wall and that these were low-temperature reactions. However, one may note from Figure 2.11 that the contributions of certain other species, e.g. CO_2 and H_2O , are at least as much as that of some of the above-mentioned species, e.g. HO_2 . An analysis of the overall heat release rate contributions of individual reactions instead of the species, at the wall may help to quantify the contribution of the low-temperature reactions in a premixed methane/air mixture. Such an analysis performed for a preheated flame will be more practically relevant.

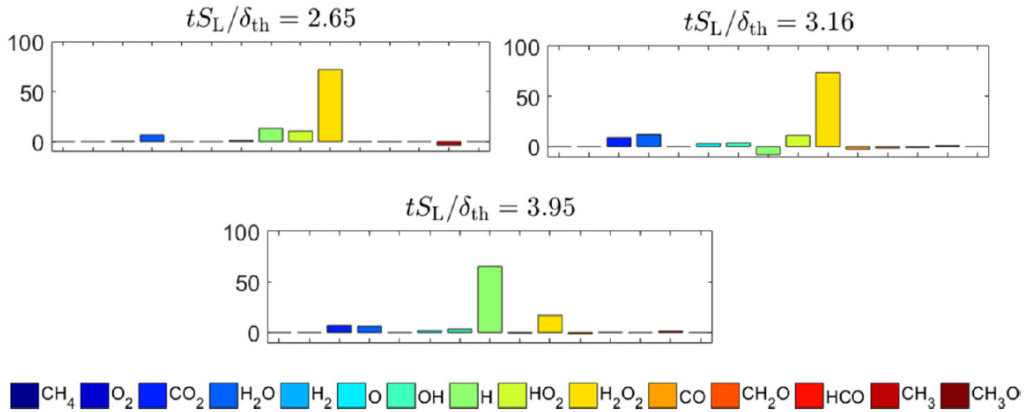


Figure 2.11: The percentage contribution of different species towards overall heat release rate at the wall at several instants during laminar HOQ [24]. These instants represent the flame away from the wall, in the influence zone and slightly after the quenching instant, respectively.

2.3 *CO* emissions

This section reviews the effect of flame-wall interaction on *CO* emissions. Section 2.3.1 discusses the experimental studies of *CO* due to FWI while the computational investigations of *CO* due to FWI are reviewed in Section 2.3.2.

2.3.1 Experimental studies

Although limited in number, several experimental studies have investigated *CO* emissions near a relatively cold wall [25–29] and have observed *CO* emissions in the near-wall region for different configurations. One such configuration, a HOQ-like configuration, has been studied in [25, 26] where a methane/air flame vertically impinges a wall. Statistically stationary flames [25, 26] and propagating flames [25] were considered to explore steady-state and transient effects, respectively. In a statistically stationary flame (see Figure 2.12(a)), the observed *CO* behaviour was categorised into three main branches: the flame front (1), post-flame zone (2) and the near-wall region (3). Unlike the flame front and the post-flame zone, the near-wall region, which is characterised by a massive heat transfer, shows approximately constant *CO* concentration. This high wall heat transfer is due to the strong wall cooling by a stream of cooling water to control the wall temperature. In turbulent conditions, the eddies push the reaction zone closer to the wall than that in a laminar flame [25]. As a result, many thermochemical states between the branches identified by a laminar flame are observed (see Figure 2.12(b)).

The near-wall *CO* branch does not exist in the case of a transient flame which is far away from the wall (see Figure 2.12(c)). In the vicinity of the wall, where the flame starts to quench, the flame and the post-flame branches converge (see Figure 2.12(d)). Figure 2.12(d) also shows that the near-wall *CO* concentration at the quenching instant is not negligible.

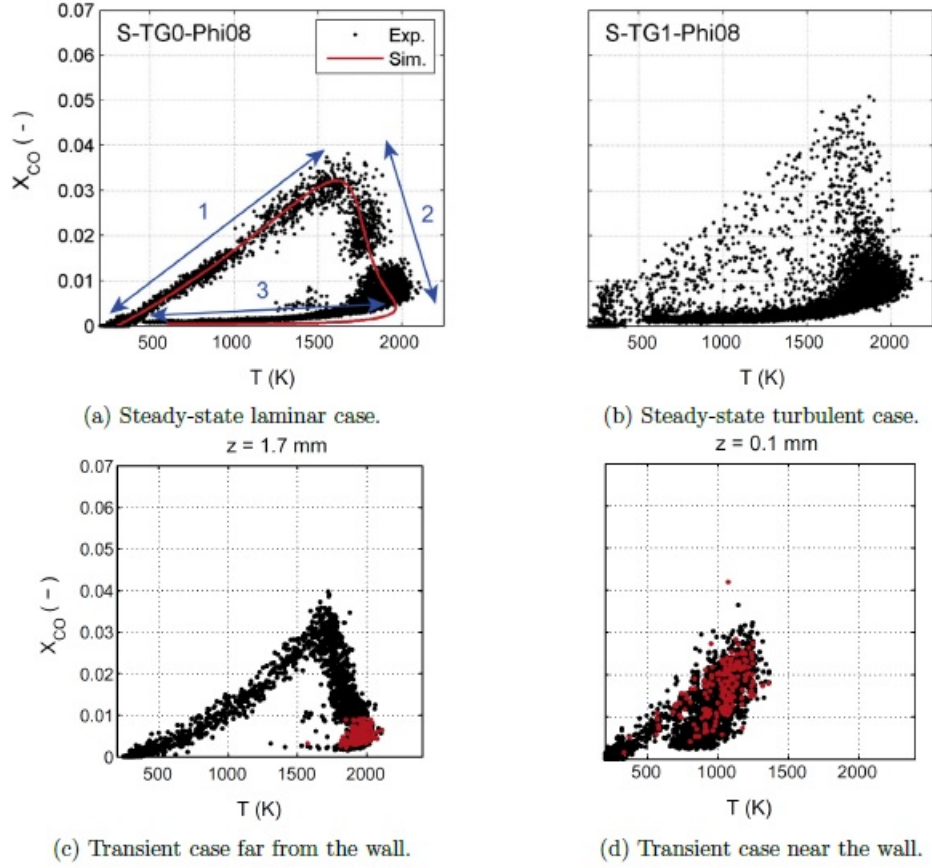


Figure 2.12: CO thermochemical states ($\phi=0.8$). Quenching instant is shown by the red dots. z denotes distance from the wall [25].

Near-wall CO emissions in side-wall quenching (SWQ) was explored in [27] (see Figure 2.13). The thermochemical states obtained from the experiment were compared to the computational results of a 1D freely-propagating flame (FPF). The results plotted in the wall-normal direction at the quenching point are shown in Figure 2.13. Very close to the wall ($y \leq 0.2 \text{ mm}$), Y_{CO} peaks at a much lower temperature compared to a FPF. Further away from the wall ($0.3 \leq y \leq 0.6 \text{ mm}$), the experimental results of the CO production branch match with the computational results of FPF, while the oxidation branch has a different behaviour compared with the FPF results. This indicates that the effect of the wall on the CO production branch is minimal in this zone while CO oxidation branch is still affected by the wall. For larger distances from the wall ($y \geq 0.6 \text{ mm}$), the production branch is not seen as these locations are in the post-flame zone.

To further understand the influence of wall heat transfer on CO formation and oxidation, a time-scale analysis was conducted [27, 28, 30]. The time-scale analysis

aims to understand the relative significance of the wall heat transfer, CO production and CO oxidation. The CO production and oxidation branches are likely to be affected by the wall heat transfer when the wall heat loss has a shorter time scale than those of CO production or oxidation. When unaffected by the wall heat loss, these branches are expected to be comparable to those in an FPF configuration. The time-scales of CO production (τ_{Pr}) and oxidation (τ_{Ox}), based on 10-90% criteria were calculated to be 0.25 ms and 5.5 ms [27]. Based on this criteria, τ_{Pr} is the time taken for X_{CO} to reach $X_{CO,max}$ from when X_{CO} is equal to the 10% of $X_{CO,max}$. After reaching $X_{CO,max}$, the time required to reduce X_{CO} by 90% of $(X_{CO,max} - X_{CO,eq})$ where $X_{CO,eq}$ is the equilibrium CO mole fraction, is defined as τ_{Ox} [30]. These chemical time scales were compared to the heat transfer time-scale (Figure 2.14) which is calculated [27, 28] as:

$$\tau_H = \frac{y^2}{\lambda} \rho C_p \quad (2.3.1)$$

where λ , ρ and C_p denote thermal conductivity, density and specific heat capacity of air (assumed for convenience). Equation 2.3.1 also assumes that the dominant mode of heat transfer near the wall is conduction.

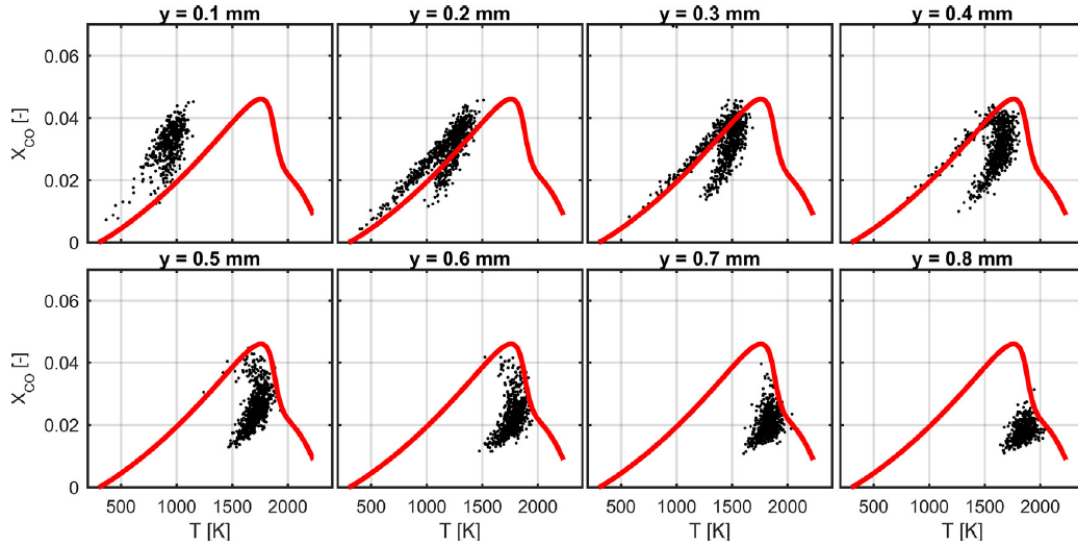


Figure 2.13: CO thermochemical states at several distances from the wall (y). Red lines show the results of 1D simulations of a freely propagating flame [27].

Figures 2.13 and 2.14 together show that the presence of a wall only affects chemical processes (CO production and oxidation) whose time scales are more than that of

the wall heat transfer (τ_H). Near the wall ($y \leq 0.2$ mm), the wall heat loss is faster than both CO production and CO oxidation, i.e. τ_H is less than τ_{Pr} and τ_{Ox} (Figure 2.14). Hence, both CO production and oxidation branches (Figure 2.13) differ from the FPF results in this range of y . Beyond this point, the CO production time scale is smaller than the heat transfer time scale (Figure 2.14). Hence, the production branch of CO is not influenced by the wall heat transfer and matches the corresponding FPF result (Figure 2.13). The CO oxidation branch is affected by the wall at all measured values of y due to the relatively high value of τ_{Ox} (relative to τ_H).

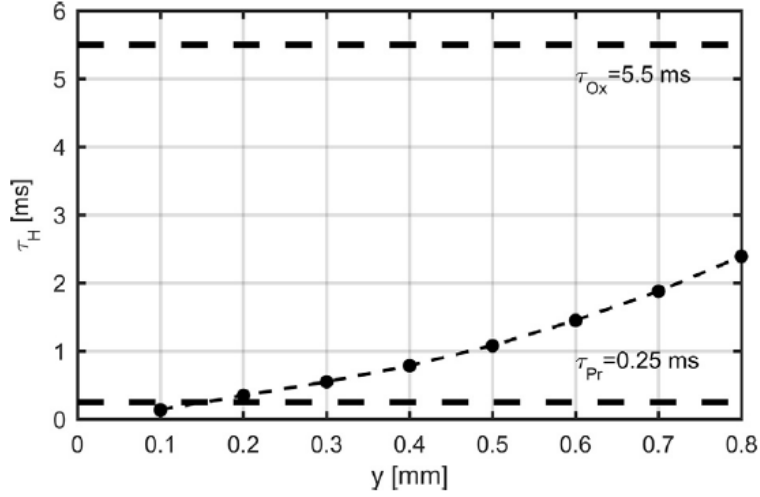


Figure 2.14: Comparison of time scale of heat transfer (τ_H) to the CO formation and oxidation time scales. y denotes the distance from the wall [27].

2.3.2 Computational studies

Recently, several computational studies exploring the near-wall CO in the context of FWI have been reported [31–34]. Two main topics addressed in these studies are (a) the transport mechanism of CO near the wall [31, 32] and (b) the ability of reduced chemical mechanisms to predict Y_{CO} [33, 34].

Species transport budget analysis [35] is a useful tool to understand the transport mechanism of species, described as follows:

$$\frac{\partial Y_k}{\partial t} = \left[-u_i \frac{\partial Y_k}{\partial x_i} \right] + \left[\frac{1}{\rho} \frac{\partial}{\partial x_i} \frac{\rho D_k}{W} \frac{\partial (Y_k W)}{\partial x_i} \right] + \left[\frac{\dot{\omega}_k}{\rho} \right] \quad (2.3.2)$$

where Y_k , D_k , and $\dot{\omega}_k$ denote mass fraction, diffusion coefficient, and rate of production of species k . The variables ρ , W , u , x and t represent density, average molar mass, flow velocities (in each direction identified by i), spatial coordinates and time, respectively.

This analysis quantifies the contribution of the transport phenomena namely, convection, diffusion and reaction, to the net change in species mass fraction. The three terms on the right hand side of Equation 2.3.2 represent convection, diffusion and reaction of species k , respectively while the left hand side shows the net change in mass fraction of k .

The species transport budget analysis has been used to explore different near-wall CO transport mechanisms [31, 32]. In a 2D DNS study of premixed, steady methane/air flames, Ganter et al. [31] compared the significance of diffusion and reaction processes in determining the near-wall CO . The convection term did not appear in the analysis as the authors adopted a Lagrangian approach. In the Lagrangian approach, the diffusion (d) and reaction (q) terms, as in Equation 2.3.2, were integrated along the trajectory of a particle that follows the flow. The integrated diffusion and reaction terms are denoted by D and Q , respectively. The contributions of d , q , D and Q are shown in Figure 2.15. Positive (negative) values of these terms result in an increase (decrease) of Y_{CO} , which is clear from Equation 2.3.2. Importantly, diffusion becomes more significant than reaction in the quenching zone. This is evident from the D and Q plots shown in Figure 2.15, and is further illustrated in Figure 2.16.

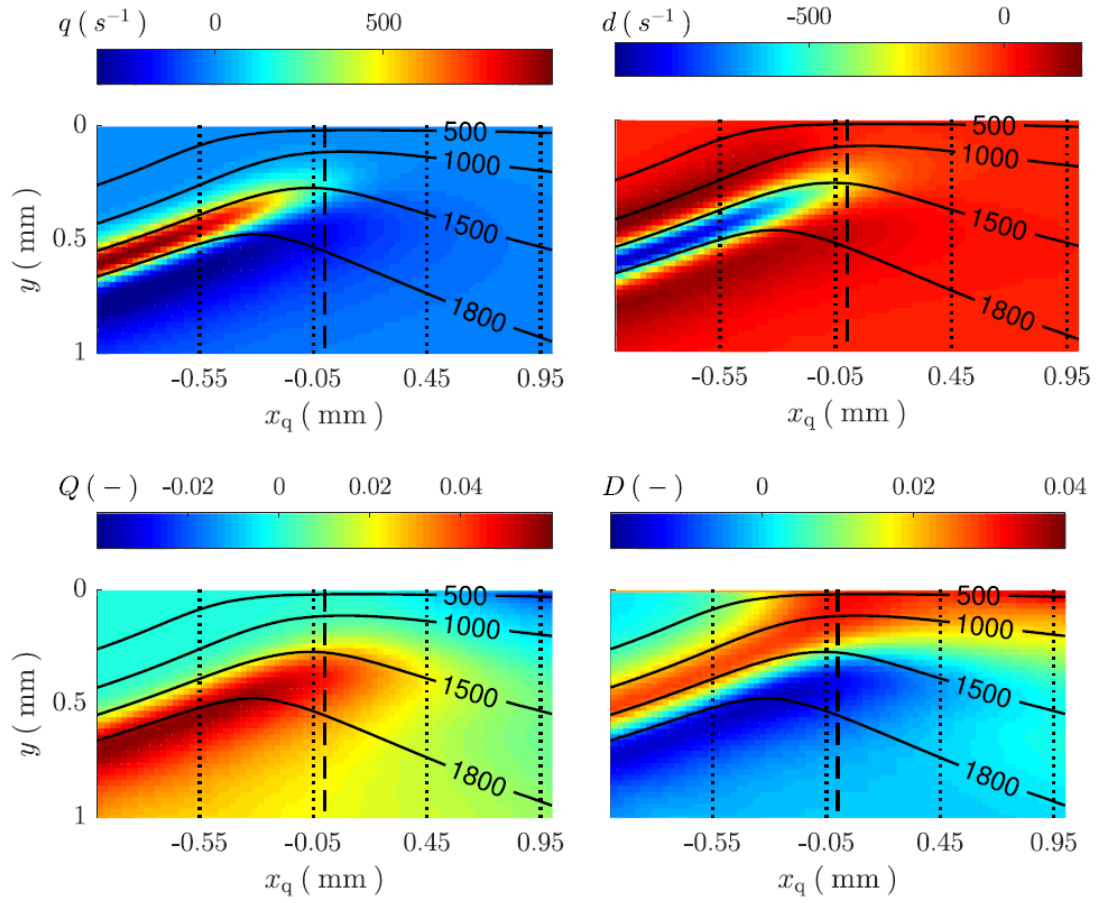


Figure 2.15: Reaction and diffusion terms (q and d) of CO and their integrated values (Q and D respectively) [31]. Temperature isolines (in K) are also shown. x_q is the streamwise distance relative to the flame tip position.

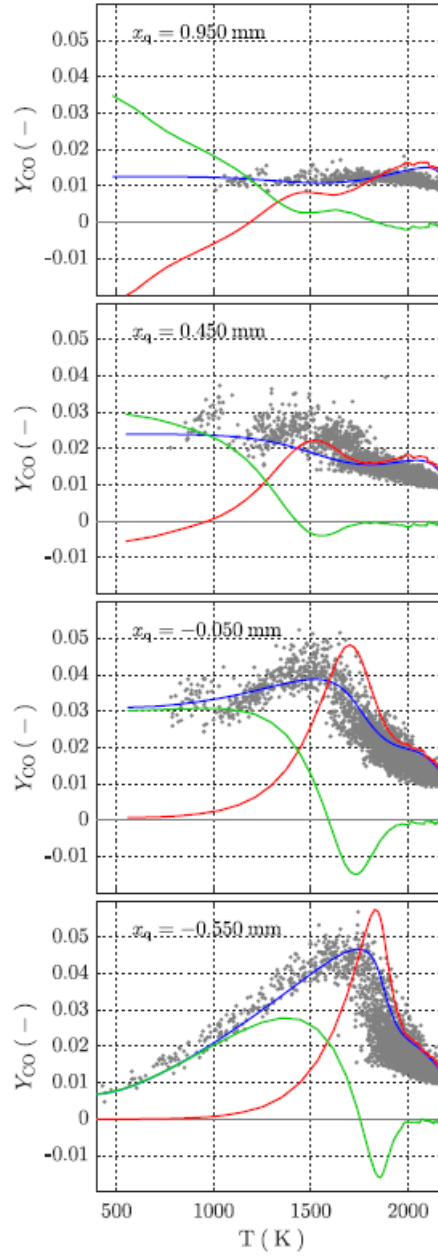


Figure 2.16: The variation of integrated source term (Q —), integrated diffusion term (D —), and mass fraction of CO (Y_{CO} —) with temperature at several streamwise locations (x_q) [31]. Experimental Y_{CO} (■) results [27] are also shown.

Figure 2.16 compares the roles of integrated diffusion (D) and source (Q) terms at several streamwise locations (x_q), along the wall-normal direction, before and after the flame tip. The CO thermochemical states obtained computationally [31] and experimentally (from [27]) are also shown. At $x_q = -0.55\text{mm}$, the flame is unaffected by the wall. As the quenching point, $x_q = 0$, is approached the near-wall CO diffusion starts to increase, indicating the diffusion of CO from the flame to the wall in the quenching zone. Some of this CO is later consumed downstream by

chemical reactions. This is clear from the negative source term near the wall for positive x_q values (see Figure 2.16).

Quantifying the roles of different CO transport mechanisms near a wall provides useful information for modelling [32]. This information may allow modellers to neglect certain transport mechanisms when appropriate. From the results of species transport budget analysis, Jiang et al. [32] observed that the CO mass fraction can be calculated as the integral of the diffusion term only, when the peak of spatial average of the absolute value of the diffusion term ($|D|_{mean}$) is more than 50% of that of the sum of convection and reaction terms ($|C + R|_{mean}$) under some conditions (see Figure 2.17).

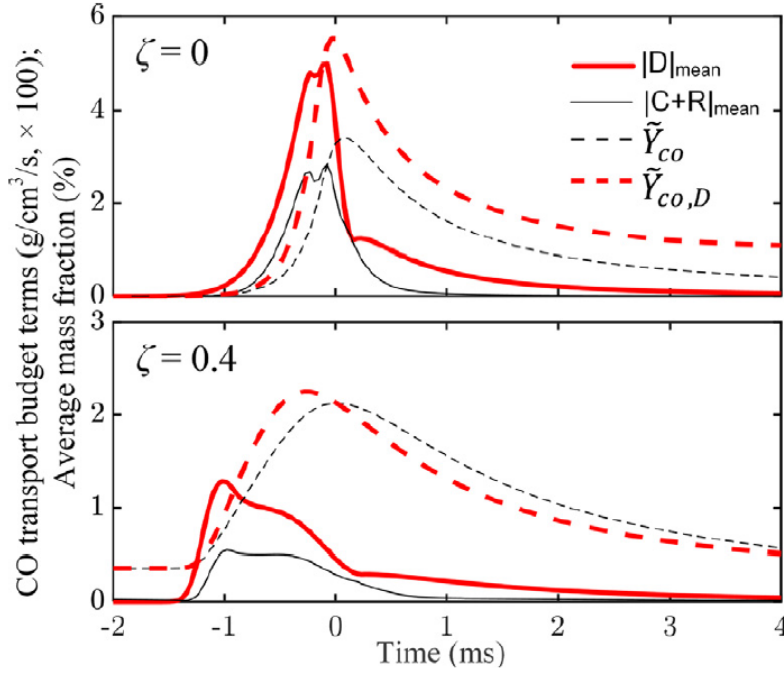


Figure 2.17: Actual CO mass fraction ($\tilde{Y}_{co}$) and that calculated ($\tilde{Y}_{co,D}$) by integrating diffusion (D) term, averaged in the quenching zone (0 to δ_Q). C and R are the convection and reaction terms. ζ is the dilution level, i.e. the ratio of mass flow rate of burned gases to the total mass flow rate.

Several studies have investigated the performance of reduced chemical mechanisms to capture the near-wall chemistry and particularly CO emission [33, 34]. Heinrich et al. [34] used the flamelet generated manifold method (FGM) which is a tabulated chemistry approach, in a SWQ burner. In this method, the results of a series of 1D simulations performed using GRI 3.0 were stored in a 3D table. The thermochemical states at any given point was represented by three variables: mass fraction

of CO_2 , mixture fraction and enthalpy. [34]. Using this reduction technique, the authors [34] found that the increase in the near-wall CO , which is observed close to the quenching instant, was not captured [34]. In a more exhaustive investigation of the cause of this error, Ganter et al. [33] identified the scalar dissipation rate in the enthalpy direction as the reason for the error. An extended tabulation technique, e.g. reaction-diffusion-manifold approach (REDIM) which considers the scalar dissipation rate, was found to predict the qualitative behaviour of the near-wall CO [33].

2.4 Effects of flame-cooling air interaction (FCAI) on CO emissions

One combustor liner cooling technique is effusion cooling, where the cooling air jets introduced into the combustor complement each other to form a sheet of cold air near the wall, without penetrating into the mainstream flow. The cooling air may then influence CO emissions through several effects, some of which are contradictory. First, the low temperature introduced by the coolant jet reduces the CO oxidation rate upon interaction with the coolant [36, 37]. Second, richer inlet mixture leads to generation of higher CO even if the overall equivalence ratio is low [38]. This can be because the air used for cooling reduces the air available for combustion in the primary zone. This leads to a rich mixture at the combustor inlet, generating higher CO . Third, the excess oxygen introduced by the cooling air can aid CO oxidation leading to a decrease in CO [39].

The above-mentioned effects are not independent of each other. An increase in the coolant flow can introduce more oxygen which should facilitate CO oxidation. However, the low temperature of the coolant reduces the rate of this CO oxidation due to reaction quenching. This is likely to reduce the rate of decrease of CO . In addition, the increase in the coolant flow makes the inlet mixture richer leading to higher CO . Due to the interrelated nature of these effects, this problem is not well understood.

Reduced levels of CO were observed in commercial combustor configurations when

2.4. EFFECTS OF FLAME-COOLING AIR INTERACTION (FCAI) ON CO EMISSIONS

effusion cooling was replaced by back-side combustor cooling [36, 37]. Figure 2.18 shows the CO emissions in an industrial combustor with and without effusion cooling. When the air used for effusion cooling was reduced from 20% (represents effusion cooling) to 0% (represents back-side cooling) of the available combustion air a significant reduction in CO was observed (see Figure 2.18). In other words, a higher CO was observed in the effusion cooled combustors. Although both the cooling methods reduce the combustor wall temperature, the coolant jet enters the combustor in effusion cooling and would create a region of low temperature. Authors noted that the reduction in CO oxidation rates (also called reaction quenching) due to such a low temperature region was the primary reason for the increase in CO emission [36, 37] in the effusion cooled combustor. This is in line with the observations of Correa [40] who found that the equilibrium CO levels are attained near a backside cooled (≈ 1100 K) combustor wall because the rate of transport of CO towards the combustor wall was slow compared to the time required to oxidise it [40]. However, the CO oxidation time scales were larger when trapped in the cold eddies (900 K) which are formed as a result of turbulent mixing of the dilution air jets with the hot gas [40].

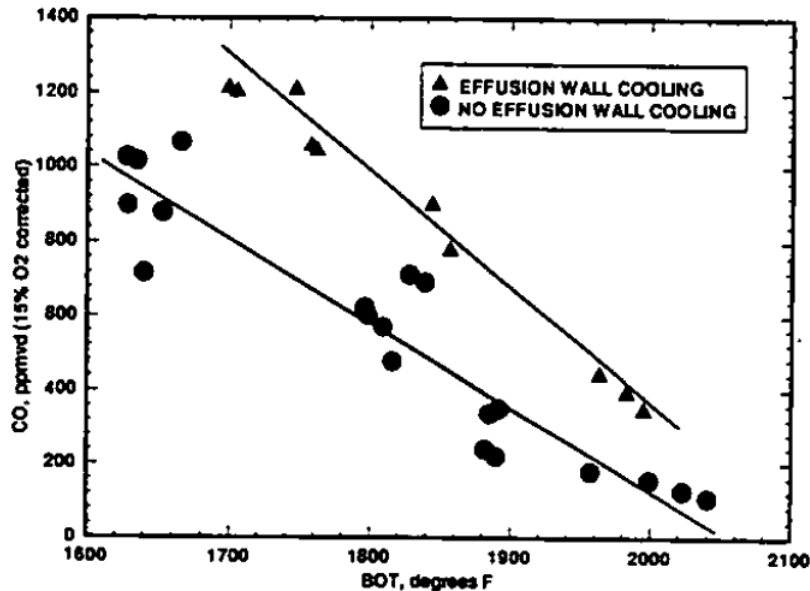


Figure 2.18: Effect of effusion cooling on CO emissions [36] for a range of burner outlet temperatures (BOT).

Andrews and Kim showed that richer mixtures at the inlet contribute to a higher

CO emission [38]. They studied a radial swirler combustor where 60% of the total combustor airflow entered the primary zone through a radial swirler while the remaining was fed as dilution air. They investigated the effect of overall equivalence ratio and swirler local equivalence ratio on *CO* emission. Figure 2.19 shows *CO* variation over a range of overall equivalence ratios for two different inlet temperatures (740 K and 600 K) with different cooling air proportions (0%, 16% and 42% of the total air flow). As the lower flammability limit is approached, regions of inefficient combustion and insufficient residence time lead to a higher *CO* emission. This is observed for equivalence ratios less than 0.4 and 0.47 for mixtures at 740 K and 600 K, respectively in the cases without effusion cooling. Beyond these limits, the *CO* concentration is observed to increase with an increase in the coolant flow. For instance, with an overall equivalence ratio of 0.45 with the 740 K mixture, the *CO* concentration varied from approximately 15 ppm to about 100 ppm as the cooling air proportion was changed from 0% to 42% of the total airflow (see Figure 2.19). However, Figure 2.20 shows that the effect of coolant flow rate on *CO* emission is different when studied in terms of the local equivalence ratio [38], as explained below.

The range of swirler local equivalence ratios shown in Figure 2.20 are similar to that of the overall equivalence ratio (shown in Figure 2.19), in the absence of cooling jets. In the cooled cases, one would expect a locally richer mixture at the inlet as a fraction of the air is used for cooling. Such an increase in the swirler equivalence ratio is seen in Figure 2.20. For instance, an inlet temperature of 600 K which had a maximum swirler equivalence ratio of about 0.6 when uncooled, developed regions of up to 0.8 equivalence ratio when effusion cooled with 42% coolant flow rate. A higher amount of *CO* is expected to be produced at such local fuel-rich regions. However, the *CO* emission reported in the cases with cooling air, particularly with 42% coolant flow, are less than the equilibrium *CO* values corresponding to the local equivalence ratios. The authors attributed this reduction in *CO* to the post swirler oxidation where *CO* interacts with the cooling air. The excess air introduced by the cooling air jet is likely to facilitate oxidation of the higher *CO* generated by the richer mixture at the inlet [38].

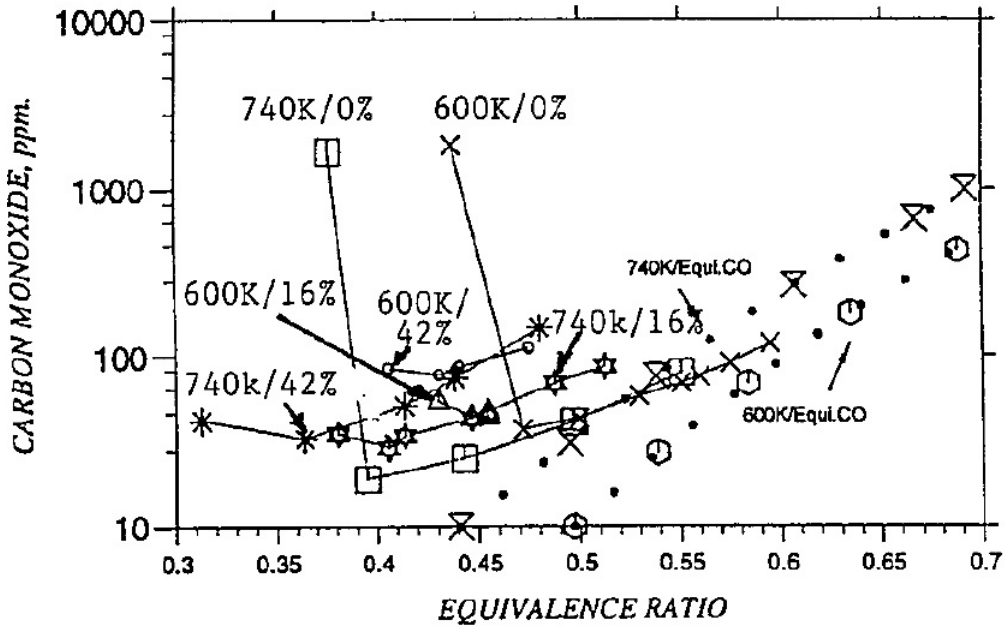


Figure 2.19: Variation of CO (in ppm) with overall equivalence ratio [38].

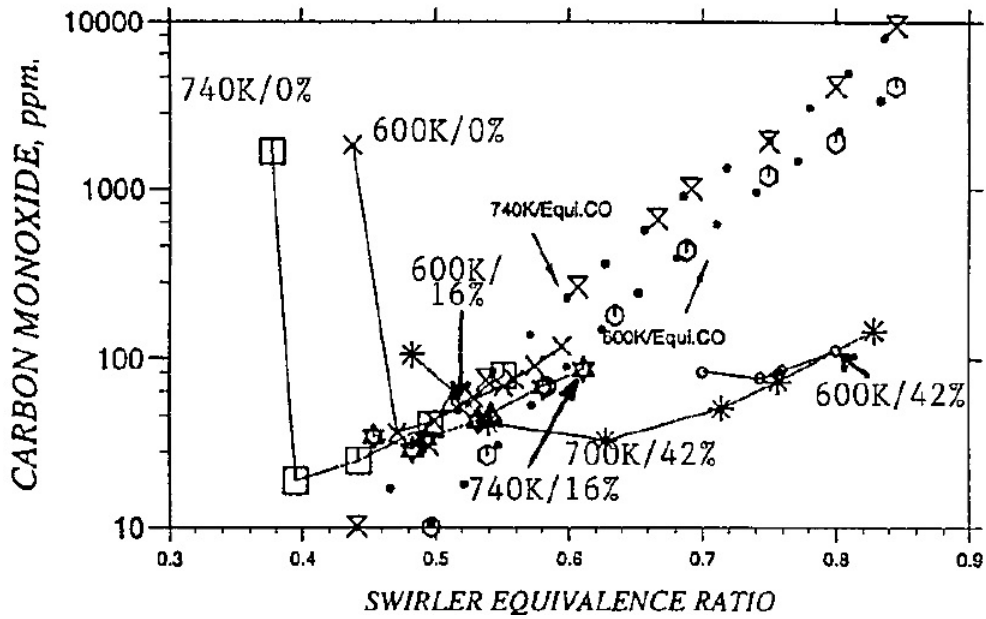


Figure 2.20: Variation of CO (in ppm) with swirler local equivalence ratio [38].

Rivera et al. [39] conducted experimental and numerical studies to understand the effect of coolant on a laminar premixed flame. Lower temperature and higher oxygenation due to the coolant stream were found to reduce the CO concentration. Figure 2.21 shows the temperature and CO profiles obtained using 1D fully resolved simulations in a case where the coolant is injected downstream of the flame. The

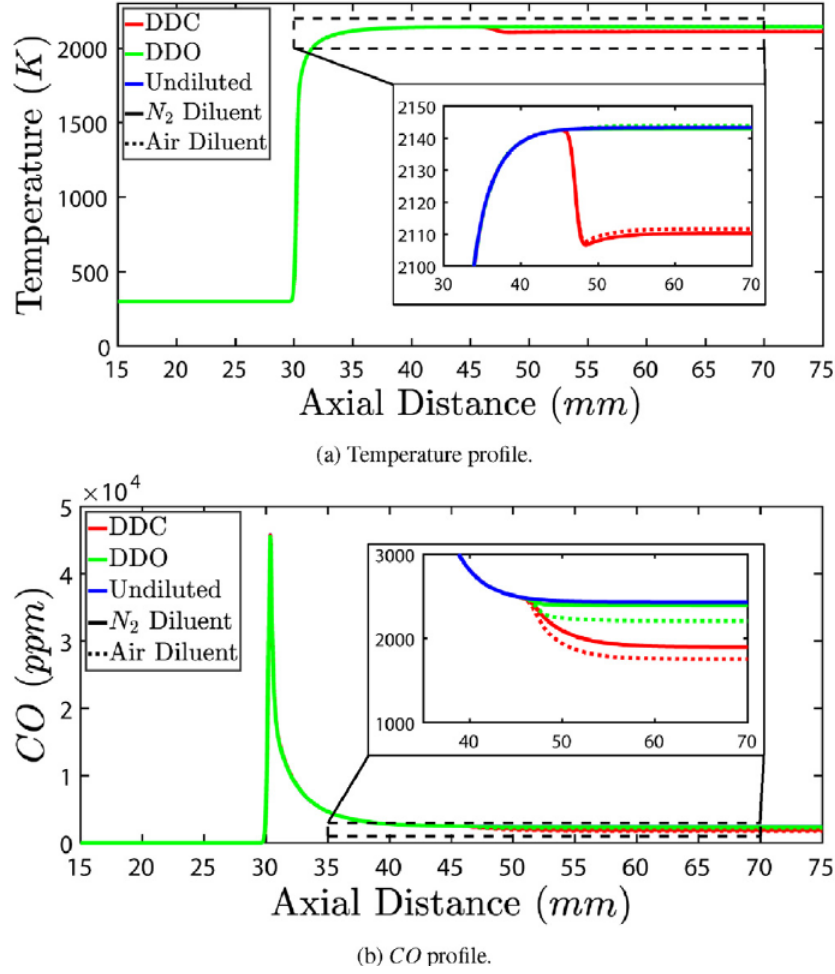


Figure 2.21: Temperature and CO profiles for DDC and DDO cases with air and N_2 . Undiluted case is also shown for comparison [39].

effects of dilution and cooling due to the coolant stream were decoupled by considering cases with (a) downstream dilution only (DDO) and (b) downstream dilution and cooling (DDC). For DDO cases, the cooling jet was injected at the local gas temperature, i.e. the cooling effect was not included. Also, two coolant types, air and N_2 , were considered in Figure 2.21 to understand the role of excess oxygen on temperature and CO profiles. Figure 2.21(a) shows a drop in temperature in DDC cases, with both air and N_2 . This is expected as the injection of the low temperature coolant decreases the enthalpy of the mixture. Also, associated with this decrease in temperature, both air-cooled and N_2 -cooled cases showed a lower CO emission. Air-cooled cases, which introduces excess oxygen compared to the N_2 -cooled cases, showed lower CO in both DDO and DDC cases, underlining the effect of excess oxygenation. Furthermore, a time-scale analysis conducted in this study using chemical reactor network (CRN) simulations revealed that an increase

in residence times, namely (a) mean dilution residence time of the cooling jet and (b) exhaust gas cooling residence time, led to more complete CO oxidation, except for when the coolant mass flow rate was very low.

Summarising, there are several hypotheses about the effect of cooling air on CO most of which are interrelated. Also, some of these hypotheses contradict each other. To improve the understanding of the influence of cooling air on CO , rigorous analyses of each of these hypotheses are required.

2.5 Turbulence-chemistry interaction near walls

Dreizler and Bohm summarised the advanced diagnostics methods and flame-wall interaction (FWI) related studies in [5]. Reviewing the existing studies, the authors confirmed that the experimental constraints in flame-wall interaction studies still exist, highlighting the importance of computational studies in flame-wall interaction. Various numerical studies investigated head-on quenching (HOQ) and side-wall quenching (SWQ) configurations, with and without detailed chemistry model. Flame-wall interaction becomes more complicated in turbulent conditions [5]. The wall heat loss is modified by the action of turbulent vortices [6] while the flame is strained by the vortices. Also, the impact of the combination of flame and wall on the turbulent flow is different from their individual effects [5]. For instance, Alshaalan and Rutland found the law-of-the-wall scaling to be invalid in the log layer in the presence of a flame, due to the introduction of more turbulent transport mechanisms than a cold flow near the wall [41].

Two-dimensional (2D) direct numerical simulation (DNS) of flame-wall interaction in the case of premixed turbulent methane/air flames was studied by Poinso et al. [8] using a single-step chemistry model. An initial laminar flame simulation (2D DNS) was conducted and the wall heat flux, flame power and Pe were plotted. It was noted that the flame power decreased drastically at a Pe of about 8, which was attributed to the influence of the wall (from this point to the wall is defined as the influence zone). The flame moved closer to the wall till $Pe = 3.4$ before being quenched. The non-dimensional wall heat flux reached the maximum value ($=0.36$) at this point. A scatter plot of the flame consumption speed, normalised by

the laminar flame speed, against Pe (refer Figure 2.22), revealed three branches of flame elements (also referred as “flamelets” in Figure 2.22) - one corresponding to head-on quenching (branch 1), another corresponding to side-wall quenching (branch 2) and a third branch which burnt faster as the flame elements approached the wall and quenched subsequently $Pe \approx 3.5$.

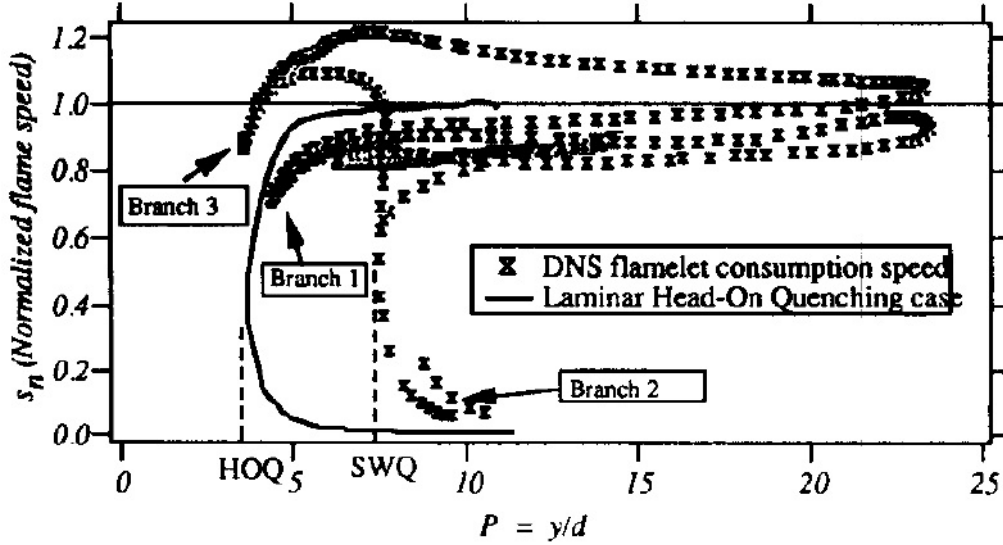


Figure 2.22: Flamelet consumption speed versus wall distance [8]

A more detailed analysis of these branches led the authors to hypothesise the typical events of flame-wall quenching (FWI) leading to quenching (Figure 2.23). Initially, the flame propagates normal to the wall (branch 1) until some elements reach a Pe of 3.4, similar to a head-on quenching case. At this stage, those elements close to the wall flatten and quench. Those elements which were not quenched, move away from the quenched zone propagating parallel to the wall. They stabilise at a distance corresponding to a Pe of 7, similar to a side-wall quenching case. A law-of-the-wall model was formulated and the conservation equation of flame surface density was modified by including the effects of the wall. The equation was integrated in two zones: the influence zone and the rest of the computational domain, to obtain a solution.

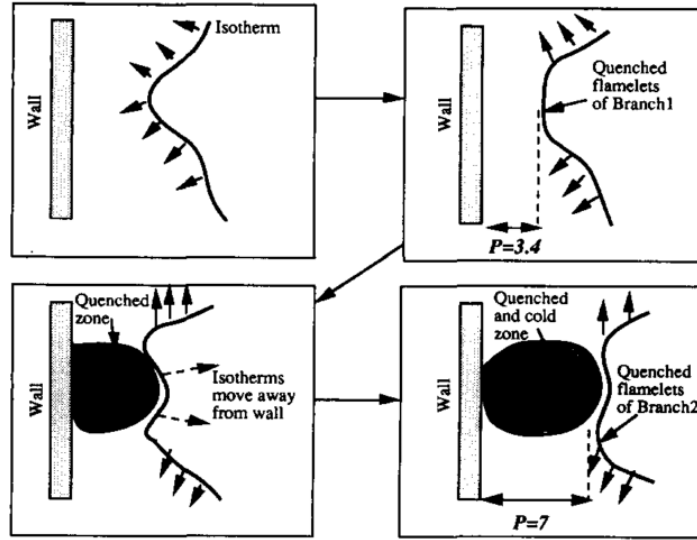


Figure 2.23: Observed flame behaviour before quenching [8]

Flame thickening effects near the wall have been reported by various studies in the literature [6, 41]. Three-dimensional DNSs of turbulent premixed H_2/O_2 flames in an anchored V-flame configuration was performed using a detailed chemistry model [6]. The contour of the time-averaged reaction progress variable (C) field is presented in Figure 2.24. The average flame thickness, bounded by $C = 0.05$ and 0.95 , increases as the boundary layer is approached [6]. The authors attributed two reasons to the flame thickening effect. First, the average flame thickness may increase due to the effect of unsteadiness and wrinkling. Second, a reduction in the turbulent length scale near the wall decreases the Damkohler number (Da) leading to a regime change from the ‘thin flamelet’ regime away from the wall to the ‘thickened wrinkled flame’ regime near the wall [6, 41].

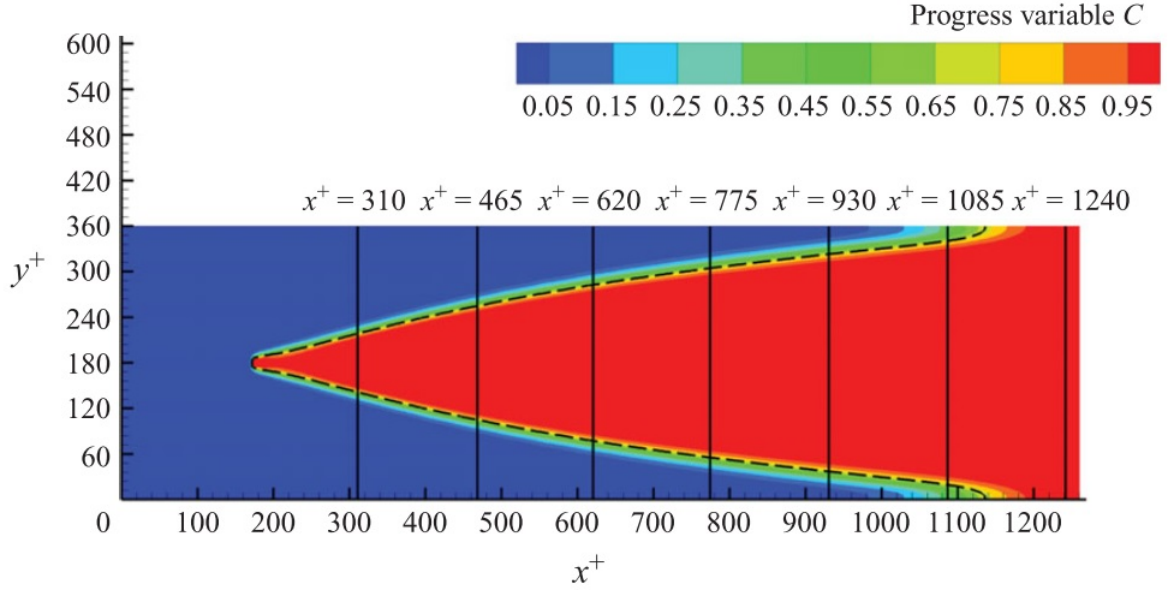


Figure 2.24: Reaction progress variable field [6]

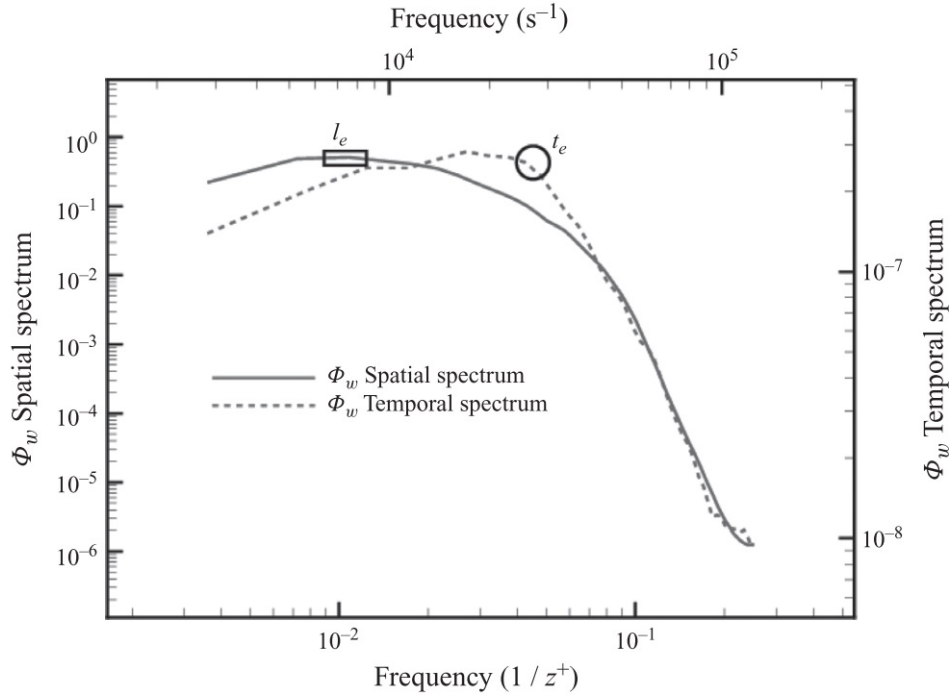


Figure 2.25: The fluctuating wall heat flux spectra (spatial and temporal) [6]

The spatial and temporal spectra (Figure 2.25) of the Fourier transforms of the fluctuating wall heat flux were plotted in a log-log scale (the temporal spectrum was calculated at the streamwise distance where the average wall heat flux was maximum). One important observation was that the time scale corresponding to the maximum wall heat flux in the frequency domain was comparable to that of the

near-wall vortices indicating the high impact of the near-wall vortices on the wall heat flux. In the temporal spectrum, the wall heat flux fluctuated majorly from 10 to 26 wall time units (9 to 27 kHz) while the time taken for the vortices to go past the flame-wall impingement region was 27 wall time units. An analysis of the vorticity and reaction rate contours of turbulent flames in 2D DNS [8] also showed the presence of near-wall vortex pairs, some of which pushed the flame towards the wall, while some others pushed it away from the wall. This is an important phenomenon which is also addressed in the more recent DNS studies reported in the literature [41–43]. Three dimensional DNSs of turbulent premixed flames were performed in a channel configuration using a single-step chemistry model in [42]. The turbulent flames were found to move closer to the wall than the laminar flames, thereby leading to a larger wall heat flux. In the case of turbulent flames, when compared with the corresponding laminar flames, the minimum Pe was less, while the maximum Pe were higher at most instants, as reported in [18]. This is because some vortices push a part of the flame closer to the wall at some places while other push the fresh reactants away from the wall at some places. Hence, the flame is closer to the wall than a laminar flame at some places, while it is away from the wall at some other places.

2.6 Summary and research questions

The phenomenon of flame-wall interaction is significant in practical combustion engine design. The presence of a wall can lead to incomplete combustion near the wall, thereby potentially contributing to emissions and fuel consumption. The existing trend in favour of high power density engines increases the importance of this phenomena.

The fundamental concepts related to FWI were summarised in this chapter. The effects of pressure, equivalence ratio, wall temperature, Lewis number (Le), surface coatings, radical recombination reactions and wall heat flux on FWI were reviewed. The key observations can be summarised as follows. A decrease in the flame thickness, which can result from increase in pressure or due to a change in equivalence ratio leads to a smaller quenching distance, thereby increasing the wall heat flux.

Another important observation from the literature is the role of the low activation energy reactions, i.e. the radical recombination reactions, which are important at the wall due to the relatively low wall temperature. These reactions, being exothermic, also increase the near-wall heat release rate and wall heat flux. Their contribution to wall heat flux can be reduced if the amount of available radicals for these reactions is reduced due to the surface adsorption characteristics of the wall.

Despite decades of research, there are unanswered questions on the topic of FWI relevant to engine design and simulation. *CO* emissions may be increased by FWI due to incomplete combustion near the wall. However, the controlling physics and chemistry interactions are only poorly understood. Recently, a few experimental and computational studies have reported on near-wall *CO*. One of the important results has been that a species transport budget analysis can be used to understand *CO* transport mechanisms near wall. This can provide useful information for near-wall *CO* modelling.

Introduction of cooling air jets in a gas turbine combustor also influences *CO* emissions. Several potential reasons such as reaction quenching and variations in the inlet equivalence ratio have been reported in the literature. However, the underlying physics of flame-cooling air interaction (FCAI) on *CO* need more rigorous investigation to make near-wall *CO* due to FCAI predictable. Near-wall turbulent vortices are another important phenomenon widely discussed in the literature. These vortices push the flame closer to the wall at some points and push them away from the wall at some other points, thereby influencing the quenching distance and the wall heat flux.

In this thesis, the near-wall *CO* emission characteristics and wall heat flux effects of laminar and turbulent premixed methane/air flames are investigated, with and without cooling jets. A preheated flame ($T_u = 800K$) is used to mimic the combustor inlet temperature condition of a gas turbine. The specific research questions are:

1. **How do the wall heat flux, emission characteristics and flame behaviour vary for a forced laminar premixed flame?**

Analysis of a laminar flame subject to velocity perturbations at the inlet, isolates certain characteristics of the flame and the impact of unsteadiness on the near-wall behaviour can be explored. In other words, a laminar flame subject to velocity perturbations, reproduces certain (though not all) traits of a turbulent flame, and hence is chosen for this study. This can serve as a first step towards complete understanding of the behaviour of a realistic turbulent flame.

2. How do cooling air jets influence the wall heat flux, emission characteristics and flame behaviour of forced laminar premixed flames?

Cooling air jets can trap the unburnt fuel near the wall, leading to either incomplete or delayed combustion of the mixture. As a result, the CO formed may not get enough time to oxidise. The relatively low temperature introduced by the coolant jets may also reduce the CO oxidation reaction rates. This quenching decreases the rate of consumption of CO . On the other hand, the cooling air jet provides excess oxygen to the flame tip thereby making the flame tip leaner. However, although a leaner flame produces lesser peak CO , the CO oxidation time scale is also higher in a leaner flame. A combination of such effects affect the near-wall CO emission, thereby making this a complex problem.

3. How do the cooling air jets and walls influence the wall heat flux, emission characteristics and flame behaviour of turbulent premixed flames?

Turbulent vortices near the wall push the flame close to the wall at some points, while pushing it away from the wall at some other points. The effect of these vortices when combined with recirculation effects associated with the cooling air jets may influence CO emission characteristics. Hence, consideration of turbulent flow conditions may be important in this study.

2.7 Publications

The appeared and submitted publications which resulted from the work related to this thesis are listed below:

Peer-reviewed papers

- Chapter 4 [Published]:

R. Palulli, M. Talei, and R. Gordon, Unsteady flame-wall interaction: impact on *CO* emission and wall heat flux, *Combustion and Flame*, 207, 2019.

Conference proceedings

- R. Palulli, B. Jiang, J. E. Rivera, M. Talei, and R. L. Gordon, Direct Numerical Simulation of Flame-Wall Interaction for a Forced Laminar Flame, in 20th *Australasian Fluid Mechanics Conference*, 2016.

Chapter 3

Numerical Methods

3.1 Introduction

Among various computational fluid dynamics (CFD) methods, i.e. the Reynolds-Averaged Navier-Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS), DNS is the most accurate method because the governing equations are solved by fully resolving all the flame and flow time and length scales. However, DNS is an expensive tool from the computational point of view. DNS studies are therefore limited to simplified configurations and/or covering a small range of physical parameters. In spite of these limitations, DNS provides useful insights into the physics of a problem and are very useful for developing models used in LES, RANS or low-order models. In this thesis, DNSs are used to understand the fundamental mechanisms involved in flame-wall interaction and flame-cooling air interaction.

In this chapter, an overview of the numerical methods relevant to the current study is presented. Section 3.2 introduces the DNS code used in this thesis while Section 3.3 discusses the governing equations solved in the code. The details of the computational domains and the boundary conditions imposed are reviewed in Sections 3.4 and 3.5, respectively. Section 3.6 shows a comparison of the reduced and detailed chemical mechanisms used in this thesis, in one-dimensional (1D) and two-dimensional (2D) configurations.

3.2 The DNS code: NTMIX-CHEMKIN

The simulations are performed using the DNS code for reacting flows, NTMIX-CHEMKIN [32, 44–48]. This FORTRAN code is a fully parallelised, high order accurate solver. An eighth-order finite difference scheme is applied to calculate the spatial derivatives, while a third-order Runge-Kutta method is used for time integration. A tenth-order explicit filter is also used to remove the spurious high frequency waves introduced by the high order finite difference scheme. Two chemical mechanisms were employed in this thesis. The 53-species, 325-reactions GRI 3.0 mechanism [49] was used for the 2D laminar cases, while a 16-species, 46-reactions mechanism reported by Smooke et al. [50], referred to as SK, is used for the computationally more expensive 3D turbulent cases.

3.3 Governing equations

3.3.1 Dimensional formulation

The governing differential equations [44] for multi-component reactive species are noted below. Equation 3.3.1 shows the conservation of mass while the conservation of momentum and energy are represented by Equations 3.3.2 and 3.3.3, respectively. The conservation of species is formulated by Equation 3.3.4.

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0, \quad (3.3.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}, \quad (3.3.2)$$

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial (\rho e_t + p) u_j}{\partial x_j} = \frac{\partial (u_j \tau_{ij})}{\partial x_i} - \frac{\partial q_j}{\partial x_j}, \text{ and} \quad (3.3.3)$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho Y_\alpha u_j}{\partial x_j} = -\frac{\partial \rho Y_\alpha V_{\alpha j}}{\partial x_j} + W_\alpha \dot{\omega}_\alpha, \quad (3.3.4)$$

where u_j refers to the j^{th} component of the fluid velocity. Y_α refers to the mass fraction of the species α . The total energy density per unit mass is denoted by e_t . The fluid mass density, the thermodynamic pressure, the viscous stress tensor and the heat flux tensor are respectively represented by ρ , p , $\boldsymbol{\tau}$ and $\mathbf{q}$. The rate of production and the molecular weight of species α are represented by $\dot{\omega}_\alpha$ and W_α , respectively. The diffusion velocity of species α , i.e. $V_{\alpha j}$, is calculated assuming it diffuses to a mixture average species equivalent, as explained in [48]. The variables x_j and t represent the j^{th} spatial coordinate and time, respectively.

The following relations, including the ideal gas equation, are needed for the closure of the governing equations.

$$p = \rho RT, \quad (3.3.5)$$

$$\tau_{ij} = \bar{\mu} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \sum_{k=1}^3 \frac{\partial u_k}{\partial x_k} \right), \quad (3.3.6)$$

$$e_t = \frac{1}{2} \sum_{k=1}^3 u_k^2 + \sum_{\alpha=1}^{N_s} h_\alpha Y_\alpha - \frac{p}{\rho}, \quad (3.3.7)$$

$$h_\alpha(T_1) = \Delta h_{f,\alpha}^0 + \int_{T_0}^{T_1} C_{p,\alpha}(T) dT, \text{ and} \quad (3.3.8)$$

$$q_j = -\bar{\lambda} \frac{\partial T}{\partial x_j} + \rho \sum_{\alpha=1}^{N_s} h_\alpha Y_\alpha V_{\alpha j} - \frac{p}{\rho} \sum_{\alpha=1}^{N_s} \frac{D_\alpha^T}{W_\alpha X_\alpha} \frac{\partial X_\alpha}{\partial x_j}, \quad (3.3.9)$$

where $\bar{\mu}$ and $\bar{\lambda}$ denote the mixture-averaged dynamic viscosity and the thermal conductivity, respectively. The enthalpy of species α is represented by h_α while its enthalpy of formation at standard temperature ($T_0 = 298.15$ K) is denoted by $\Delta h_{f,\alpha}^0$. The mole fraction of species α is denoted by X_α and the thermal diffusion coefficients by D_α^T . The variables T , δ_{ij} and R denote the temperature, the Kronecker delta and the specific gas constant, respectively. Species production and molecular transport terms are solved using the CHEMKIN and TRANSPORT packages.

3.3.2 Non-dimensionalisation

NTMIX-CHEMKIN solves dimensionless forms of the governing differential equations displayed in Section 3.3.1. Variables are non-dimensionalised using a set of dimensionally complementary reference values which are denoted by the subscript ‘ref’. The speed of sound, density and dynamic viscosity of the unburnt gas are the reference values for velocity (a_{ref}), density (ρ_{ref}) and viscosity (μ_{ref}), respectively. The reference temperature is defined as $T_{ref} = (\gamma_u - 1)T_u$ where γ_u is the ratio of specific heats of the unburnt gas and T_u is the unburnt gas temperature. The reference values for the 2D and 3D simulations are listed in Table 3.1. The acoustic Reynolds number Re_{ac} ($= a_{ref}\rho_{ref}L_{ref}/\mu_{ref}$) and the inlet Mach number Ma ($= U_{in}/a_{ref}$), where U_{in} is the peak convective velocity at the inlet, are provided as inputs to NTMIX-CHEMKIN to obtain the desired jet Reynolds number Re ($= U_{in}\rho_{ref}L_{ref}/\mu_{ref}$).

Table 3.1: Reference values.

Quantity	2D simulations	3D simulation
L_{ref} (cm)	0.28	0.31
a_{ref} (cm/s)	5.62×10^4	
ρ_{ref} (g/cm ³)	4.21×10^{-4}	
T_{ref} (in K)	249.8	

3.3.3 Stability limits

A time-advancing numerical solution is obtained by temporal discretisation, i.e. by expressing the governing differential equations in terms of algebraic finite-difference equations using Taylor series expansion [51]. As the higher order terms of the Taylor series expansion are truncated, the discretised equations carry a truncation error. A round-off error is also added as the obtained numerical solutions are rounded off to certain decimal points. These errors might grow in time if the time-step is too large, thereby leading to an unstable simulation. Several criteria are imposed while determining the time-step in order to avoid numerical instability.

The time-step is determined as follows in NTMIX-CHEMKIN. Limits of stability for the convective, diffusive and reactive parts are determined using the Courant-

Friedrichs-Lewy (*CFL*) number, the Fourier (*Fo*) number and a chemical number, respectively. The *CFL* and *Fo* numbers are defined as shown in Equations 3.3.10 and 3.3.11.

$$CFL = (u^+ + a^+) \frac{\Delta t^+}{\Delta X^+} \quad (3.3.10)$$

$$Fo = \frac{\bar{\mu}^+}{\rho^+} \frac{\Delta t^+}{\Delta X^{+2}} \frac{1}{Re_{ac}} \quad (3.3.11)$$

where u^+ is the streamwise flow velocity, a^+ is the local speed of sound and $\bar{\mu}^+$ is the mixture-averaged dynamic viscosity. The variables Δt^+ and ΔX^+ represent the time-step and the grid spacing in the streamwise direction. The superscript ‘+’ indicates non-dimensional values, non-dimensionalised by the corresponding reference values as briefed in Section 3.3.2. Although Equations 3.3.10 and 3.3.11 show only the calculation in the streamwise direction, a similar estimation is performed in all the relevant directions. For numerical stability, the *CFL* and *Fo* numbers are set to a maximum of 0.6 and 0.1, respectively.

An unrealistically large amount of species production/consumption can result from a large time-step and can therefore lead to numerical instability. To avoid such a scenario, an empirically chosen ‘chemical’ number is defined to limit the amount of species produced or consumed in one time-step.

The time-step is finally determined such that the above-mentioned limits on the *CFL*, *Fo* and chemical number are maintained at every point in the computational domain, ensuring a stable numerical solution.

3.4 Computational domains

3.4.1 2D laminar flow simulations

Premixed methane/air flames under laminar flow conditions are investigated in the two-dimensional domain shown in Figure 3.1. The inlet mixture is fed to the domain through the left boundary and exits the domain through the right boundary

where the 1D Navier-Stokes Characteristic Boundary Conditions (NSCBC) are applied [52]. The transverse direction is bounded by an isothermal, no-slip wall at the top and a symmetric boundary condition at the bottom edges. Imposing symmetric condition helps to reduce computational costs by simulating only half of the domain.

The coordinates in the streamwise and transverse directions, namely X^+ and Y^+ , have been non-dimensionalised by the reference length (L_{ref}), which is chosen to be ten times the laminar flame thickness. This was achieved by a jet Reynolds number of 400 and a Mach number of 0.021. The domain is 7 units (non-dimensional) long in the streamwise direction and 1.2 units wide in the transverse direction. The grid resolution in the streamwise direction is $15\mu m$ ($\Delta X^+ = 0.0054$). A stretched grid with a resolution of $5\mu m$ ($\Delta Y^+ = 0.0018$) at the wall and about $21\mu m$ ($\Delta Y^+ = 0.0075$) at the symmetry plane is used in the transverse direction. Details about the choice of the grid resolution are explained in Section 3.4.3. The flame is anchored at the inlet from $Y^+ = 0$ to 0.2 to simulate half a V-flame, as shown in Figure 3.1 (see Section 3.5.1 for details).

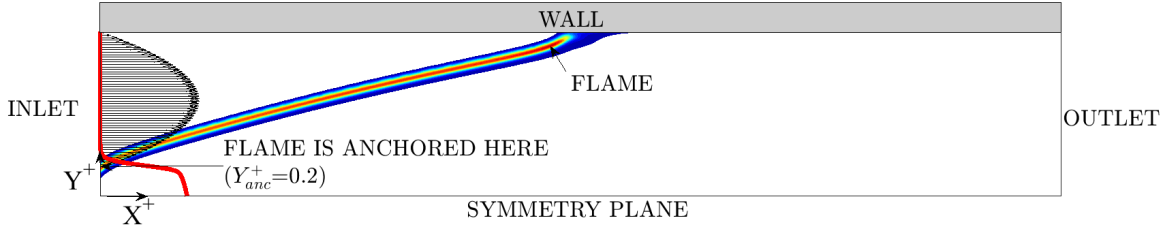


Figure 3.1: 2D computational domain. The profiles of streamwise velocity (black) and temperature (red) imposed at the inlet are also shown.

The computational domain shown in Figure 3.1 was modified to introduce a cooling hole at the top boundary, as shown in Figure 3.2. The modified boundary is therefore comprised of two parts: (a) a cooling hole and (b) a no-slip, isothermal wall. The boundary conditions at (a) are explained in Section 3.5.2.

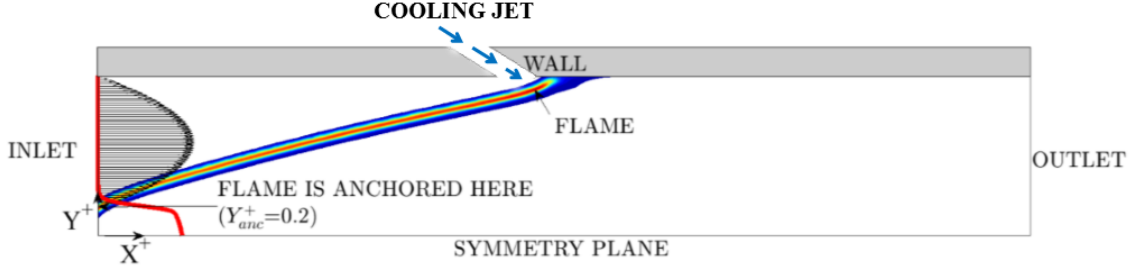


Figure 3.2: 2D computational domain with cooling hole.

3.4.2 3D turbulent flow simulation

Turbulent flow conditions are simulated in a three-dimensional domain ($L_x \times L_y \times L_z = 15L_{ref} \times 2L_{ref} \times 3L_{ref}$ with $N_x \times N_y \times N_z = 1675 \times 275 \times 335$ grid points) as shown in Figure 3.3, where x , y and z represent the streamwise, wall-normal and spanwise directions, respectively. The premixed stoichiometric methane/air mixture is fed to the domain through the inlet (left-side face). A hot sheet is imposed throughout the spanwise direction at $X^+ = 1$ from $Y^+ = 0.5$ to 1.5 , where the temperature and mass fractions of the burned gases are imposed. The flame is anchored at this hot sheet using the technique described in Section 3.5.4. The 1D NSCBC are imposed at the outflow (right-side face). Periodic boundary conditions are used in the spanwise direction. Isothermal, no-slip walls confine the flow in the transverse direction (top and bottom). At the top wall, cooling jets are injected through slots which extend along the spanwise direction at seven streamwise locations, i.e. $X^+ = 5, 6.5, 8, 9.5, 11, 12.5$ and 14 . Cooling slots have non-dimensional width of 0.2 and the spacing between two consecutive cooling slots is 1.5 . This spacing to width ratio of 7.5 is comparable to that reported in [53]. The blowing ratio (BR), i.e. the ratio of mass flux of the coolant to that of the inlet premixture, is unity.

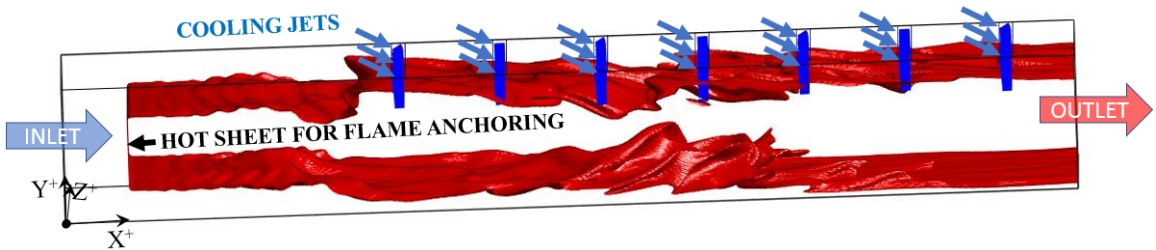


Figure 3.3: 3D computational domain.

The computational cost of the 3D DNS case was 720,000 CPU hours, running on 3840 Intel Xeon E5-2690V3 “Haswell” processors. This was equal to 188 physical hours.

3.4.3 Grid resolution

In general, finer grids are expected to give more accurate results. However, beyond a limit, finer grids do not improve the accuracy of the results significantly. When the results do not depend on the grid resolution, grid independence is said to be established.

3.4.3.1 Two-dimensional (2D) laminar simulations

Grid independence tests are performed to ensure that the flame is well resolved. As the 2D laminar simulations reported in this thesis focus on the near-wall behaviour of flames, particularly CO emissions and heat release rate, the near-wall heat release rate (HRR_{wall}) and the near-wall CO mass fraction ($Y_{CO,wall}$) have been chosen as the target parameters for the grid independence study. To ensure that the grid captures the required physics correctly, the following procedure is followed. The grid independence study is performed for the 2D case, presented in Section 4.3.3, which involved the maximum fluctuations in the flame position, i.e. for an inlet frequency of excitation corresponding to a unity Strouhal number. The instant when the flame is closest to the wall, i.e. the quenching instant (t_q), is considered for the analysis. The variable T_p shown in Figure 3.4 denotes the time period of excitation. The streamwise location (non-dimensional) where the flame is closest to the wall is denoted by X_q . Grid independence study is performed at (a) X_q , (b) two flame thicknesses upstream of X_q , i.e. $X^+ = X_q - 0.2$ and (c) two flame thicknesses downstream of X_q , i.e. $X^+ = X_q + 0.2$. The study is performed for the domain shown in Figure 3.1 and is also applicable for that shown in Figure 3.2.

Figure 3.4 shows HRR_{wall} (top row) and $Y_{CO,wall}$ (bottom) at the three streamwise locations mentioned above. The resolution in the streamwise direction ($15 \mu m$, i.e. $\Delta X^+ = 0.0054$) is chosen such that there are at least 15 grid points per flame thickness. Near-wall resolutions of $15 \mu m$, $10 \mu m$, $5 \mu m$ and $3 \mu m$ are compared. These resolutions correspond to $\Delta Y^+ = 0.0054$, 0.0036 , 0.0018 , and 0.0011 , respectively.

A stretched grid is used for the last two cases with the finest resolutions. As the grid becomes finer, the peak of HRR_{wall} increases. However, the difference in the peaks of HRR_{wall} captured with the $5\mu m$ and $3\mu m$ resolutions is small (about 5% at X_q). Near-wall CO mass fraction is also well captured with $5\mu m$, compared to the result with $3\mu m$ as the error in the peak Y_{CO} is within 5%. Therefore, a near-wall resolution of $5\mu m$ is considered to be sufficient to capture the physics of interest in the 2D computational domains used in this thesis.

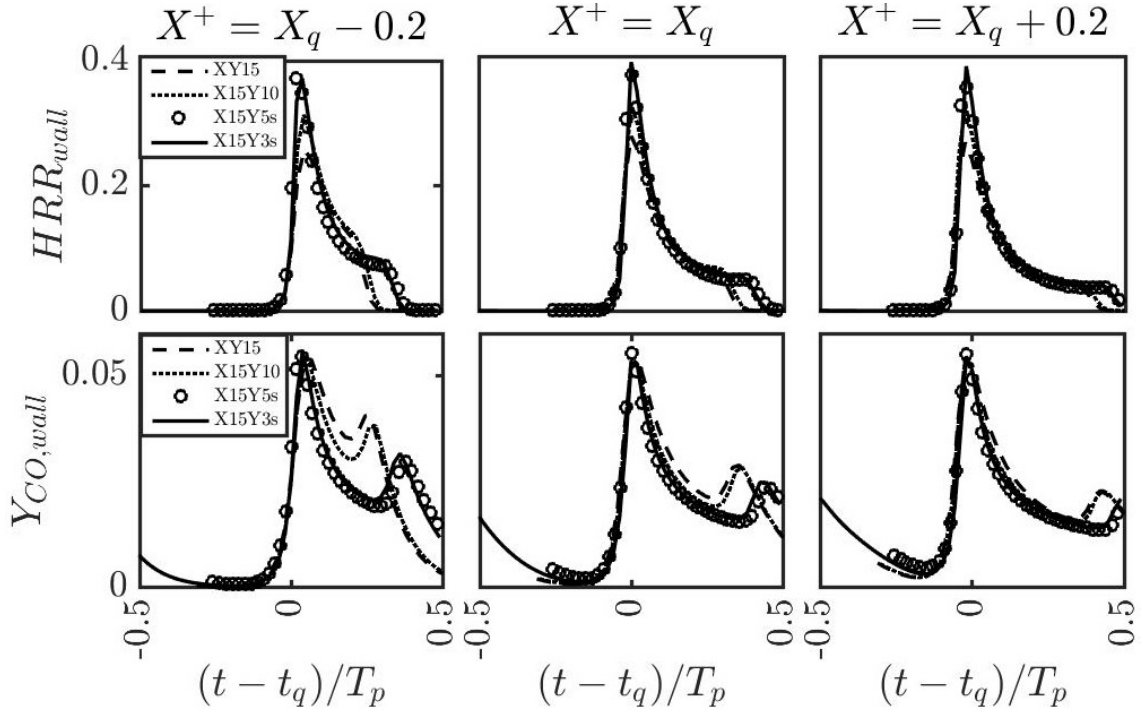


Figure 3.4: Grid independence study in the 2D laminar simulations.

3.4.3.2 Three-dimensional (3D) turbulent simulations

The grid resolution for the 3D turbulent simulations is chosen such that the following quantities are well resolved:

- Kolmogorov length scale
- Flame thickness
- Near-wall viscous sub-layer

To spatially resolve a non-reacting turbulent flow, one grid point per two Kolmogorov length scales (η) is needed, i.e. the spatial resolution should be less than 2η [54]. The

Kolmogorov length scale in this study is estimated as $62\mu m$, implying that a minimum spatial resolution of about $125\mu m$ (0.04 non-dimensional units) is necessary to resolve the turbulent flow characteristics.

To resolve the flame characteristics, 10 grid points are considered in the flame thickness in each direction. Note that a relevant 3D DNS study of a turbulent premixed flame reported in the literature has captured the flame and wall heat flux characteristics with only 6 grids within the laminar flame thickness [6]. The laminar flame thickness of the preheated premixed methane/air flame used in this study is about $280\mu m$. Therefore, to maintain 10 grid points within the flame thickness a minimum resolution of $28\mu m$ (0.009 non-dimensional units) is required.

To resolve the near-wall viscous sub-layer the following conditions have to be satisfied [6, 55]. First, at least two grid points are required within $yu_\tau/\nu = 1$, where y is the dimensional wall-normal coordinate, u_τ is the friction velocity and ν is the fluid kinematic viscosity. Second, at least 13 grid points are necessary within $yu_\tau/\nu = 10$. To satisfy the first condition, a near-wall resolution of $6.7\mu m$ ($\Delta Y^+ = 0.0022$) is used at the wall in the wall-normal direction. The grid is then stretched in the wall-normal direction. A parabolic function defines the grid resolution in the wall-normal direction such that the near-wall resolution is $6.7\mu m$ and the centreline resolution is about $38\mu m$ ($\Delta Y^+ = 0.0123$). There are about 20 grid points within $yu_\tau/\nu = 10$ thereby ensuring that the near-wall viscous sub-layer is resolved.

Table 3.2 summarises the above-mentioned criteria which are to be satisfied to resolve the flow, flame and near-wall viscous sub-layer characteristics. The minimum resolution requirements are as follows: $28\mu m$ in the streamwise and spanwise direction, a stretched grid with a $6.7\mu m$ resolution at the wall and about $38\mu m$ at the centreline. These resolutions are used in the 3D DNSs performed in this thesis.

Table 3.2: Grid resolution criteria.

Criteria	$\Delta X(\mu m)$	$\Delta Y(\mu m)$	$\Delta Z(\mu m)$
To resolve the Kolmogorov length scale	125	125	125
To resolve the flame	28	28	28
To resolve the near-wall viscous sub-layer	–	6.7 - 38	–
Minimum resolution required	28	6.7 - 38	28

3.5 Boundary conditions

3.5.1 Inlet boundary condition

The temperature and mass fractions of the incoming stoichiometric methane/air mixture are imposed at the inlet boundary. In the 2D laminar simulations, the inlet boundary conditions are used to anchor the flame, simulating a hot-plate-like boundary condition. This is done by imposing the temperature and the mass fractions of the burned gas from $Y^+ = 0$ to 0.2, along with a zero velocity condition. A parabolic velocity profile, with the maximum velocity corresponding to a Mach number of 0.021 (jet Reynolds number, $Re_{jet} = 400$), from $Y^+ = 0.2$ to the wall is applied. The velocity component in the transverse direction is set to zero. The inlet velocity profile is subject to temporal perturbations as shown in Equation 3.5.1.

$$u(1, y, t) = U_{in} \left(1 - \frac{(Y^+ - 0.7)^2}{0.25} \right) \left[1 + a \sin \left(\frac{2\pi t}{T_p} \right) \right] \quad (3.5.1)$$

The amplitude of the velocity perturbations imposed at the inflow was equal to 25% of the mean inflow velocity (i.e. amplitude of excitation, $a=0.25$) with the forcing frequency represented as a Strouhal number, $St = (fL_f)/U_{in}$, where f is the forcing frequency, L_f is the steady-state length of the flame and U_{in} is the peak convective velocity at the inlet. In Chapter 4, $St = 8.3, 5.5, 3.7, 1.9, 1$, and 0.5 are considered while $St = 8.3, 1$ and 0.5 cases are studied in Chapter 5.

The temperature and mass fraction profiles imposed at the inlet from $Y^+ = 0.2$ to the wall are taken from a 1D freely propagating flame with the same unburnt gas temperature (800 K) and pressure (1 atm) conditions as the 2D simulations. The velocity and temperature profiles are shown in Figures 3.1 and 3.2.

In the three-dimensional domain discussed in Section 3.4.2, the temperature (800 K) and mass fractions of the preheated, premixed, stoichiometric methane/air mixture are specified at the inlet. The mean streamwise velocity ($\bar{u}$) and fluctuating components of the streamwise (u'), wall-normal (v') and spanwise (w') velocities, corresponding to a jet Reynolds number of 3200 [6] based on the centreline velocity

and channel half-width [6] are used to generate the inlet turbulence, as discussed in Section 3.5.5.

3.5.2 Wall boundary condition

An isothermal boundary condition is imposed at the wall, where the wall temperature is the same as that of the fresh reactants ($T_u = T_{wall} = 800$ K). The velocity components are set to zero to ensure no-slip and no-penetration wall boundary conditions. The cooling holes/slots of the 2D and 3D cases, mentioned in Sections 3.4.1 and 3.4.2 require further modifications of the wall boundary condition. The resultant velocity of the coolant jet is calculated based on the chosen values of the blowing ratio (BR), i.e. the ratio of the mass flux of the coolant to that at the inlet. Several values of BR ($= 3, 5$ and 10) are considered in the 2D laminar study reported in Chapter 5 while a unity BR is considered in the 3D case presented in Chapter 6. The cooling jet velocity profiles imposed at the cooling hole/slots are parabolic. When air is used as coolant, the mass fractions Y_{O_2} and Y_{N_2} are set to 0.23 and 0.77, respectively. Similarly, the mass fraction of N_2 is set to unity when only N_2 is used as the coolant.

3.5.3 Outflow boundary condition

The 1D Navier-Stokes Characteristic Boundary Conditions (NSCBC) [52] are used to impose non-reflecting outflow boundary conditions. In this method, the governing differential equations are modified in terms of the amplitudes of characteristic waves using characteristic wave analysis [52]. Local one-dimensional inviscid (LODI) relations applied at the boundaries are used to infer the variations in amplitudes of these characteristic waves.

To impose a non-reflecting outflow boundary condition, the amplitude of characteristic waves entering the domain at the outlet, called L_1 , has to be specified. A perfect non-reflecting boundary condition could be set by imposing $L_1 = 0$. However, this results in an ill-posed problem, where the pressure inside the domain can drift indefinitely. To solve this issue, the pressure at the outlet boundary is relaxed towards the static pressure at infinity (p_∞). This is done by imposing the amplitude

of the incoming wave to $L_1 = K(p - p_\infty)$, where K is a relaxation constant, such that the static pressure at the outlet (p) gradually relaxes to p_∞ [52]. If the outlet pressure is not close to p_∞ , reflected waves enter the domain to maintain a mean static pressure close to p_∞ at the outlet.

3.5.4 Flame anchoring in 3D simulations

In the three-dimensional domain (Figure 3.3), the flame is anchored using a rounded-rectangle hot sheet. This hot sheet region extends throughout the spanwise direction. Temperature and species mass fractions corresponding to the burned products are applied to the points which are within the anchor region, following [6]. The flame is anchored at a streamwise location $X^+ = X_{anc}^+ = 1$, from $Y^+ = Y_{anc_1}^+ (= 0.5)$ to $Y_{anc_2}^+ (= 1.5)$. The width of this region is denoted by the variable ‘ r_{anc} ’ (see Figure 3.5(c)). The exponential function ($e^{f(X^+, Y^+)}$) based on $f(X^+, Y^+)$ (see Equation 3.5.2) is used to smoothly blend the anchor region profiles into the solution. This function ($e^{f(X^+, Y^+)}$) gradually changes from 0 far away from the anchor region to 1 inside the anchor region, as shown in Figure 3.5. The temperature (T) and mass fractions (Y_k) at each point in the domain is calculated using Equations 3.5.3 and 3.5.4. Here, the variables T_{anc} and $Y_{k,anc}$ represent the target values of temperature and mass fraction in the anchor region which are the same as the burned gas temperature and mass fractions. The temperature and species mass fractions before applying this procedure are denoted by T' and Y'_k , respectively. Note, the temperature and mass fractions far away from the anchor region will be unaffected as $e^{f(X^+, Y^+)}$ is zero in these regions.

$$f(X^+, Y^+) = -\left(\left|\frac{X^+ - X_{anc}^+}{3 \times r_{anc}}\right|^4 + \left|\frac{Y^+ - 0.5 \times (Y_{anc_1}^+ + Y_{anc_2}^+)}{0.5 \times [r_{anc} + (Y_{anc_2}^+ - Y_{anc_1}^+)]}\right|^{18}\right). \quad (3.5.2)$$

$$T = T' + (T_{anc} - T') \times e^{f(X^+, Y^+)}, \quad (3.5.3)$$

$$Y_k = Y'_k + (Y_{k,anc} - Y'_k) \times e^{f(X^+, Y^+)}, \quad (3.5.4)$$

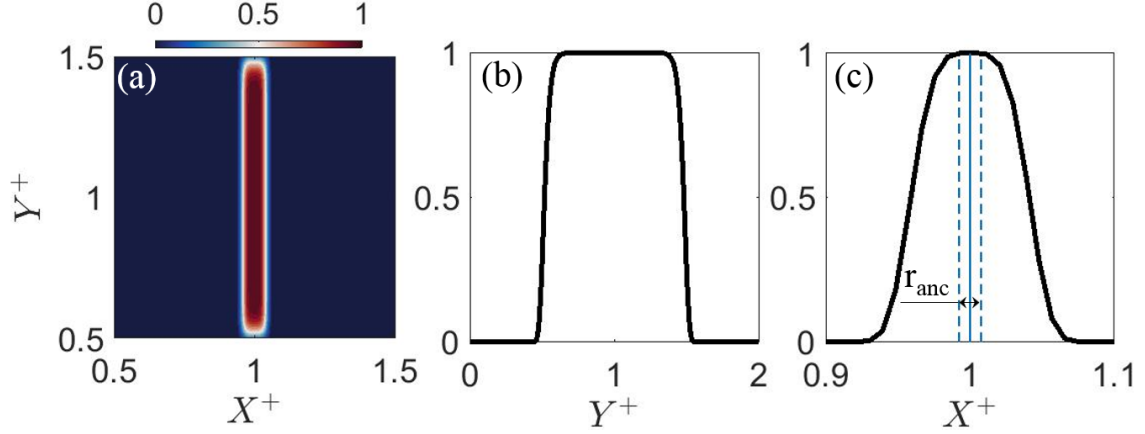


Figure 3.5: Subfigure (a) shows the 2D field of the exponential function $e^{f(X^+, Y^+)}$ illustrating the rounded rectangle shaped anchor region. Only the section of the domain around the anchor region is shown here. Subfigures (b) and (c) show the variation of $e^{f(X^+, Y^+)}$ along the streamwise and wall-normal directions.

3.5.5 Turbulence generation

Turbulent flow conditions are imposed at the inlet of the three-dimensional domain discussed in Section 3.4.2. First, fluctuating components of velocities corresponding to an isotropic turbulent field are computed based on the Passot-Pouquet energy spectrum [56] using the method proposed in [57]. These components are then rescaled to match the streamwise (u), wall-normal (v) and spanwise (w) fluctuation amplitudes of [6], corresponding to a channel flow with a jet Reynolds number of 3200. These rescaled fluctuating velocities are then added to the mean streamwise profile to obtain the inlet turbulent flow condition. The velocity components are imposed at the inlet using Taylor's hypothesis [58, 59]. The convection velocity is chosen to be 70% of the centreline mean velocity following the recommendation in [59, 60]. More realistic turbulent inflow conditions can be generated using auxiliary temporally evolving DNS. However, such simulations increase the computational cost and therefore were not attempted in this study. Furthermore, it is worth noting that synthetic turbulence generation methods have been used in several recent DNS studies [24, 48] investigating topics such as flame-wall interaction [24] and thermoacoustics [48].

3.6 Chemical mechanisms

In an ideal scenario, it is preferable to use the most detailed chemical mechanism in the simulations to ensure that the most accurate results can be obtained. However, the choice of the chemical mechanism is often constrained by the computational cost. Addition of each species in the chemical mechanism adds another species conservation equation (Equation 3.3.4) to be solved, thereby increasing the computational cost. For this reason, a computationally expensive 3D simulation may have to use reduced chemistry, while a 1D or 2D simulation can usually afford more detailed chemical mechanisms. However, in a reduced chemical mechanism, it is necessary to ensure that the parameters of interest are captured with reasonable accuracy.

The 2D simulations (Chapters 4 and 5) reported in this thesis use GRI 3.0 which is a chemical mechanism with 53 species and 325 reactions [49]. Due to the computational constraints, a reduced 16-species 46-reactions [50] chemical mechanism (denoted as SK) is used in the 3D turbulent flow simulations. To assess the performance of the reduced mechanism, this mechanism is compared with GRI 3.0 in 1D head-on quenching (HOQ) and 2D laminar FWI configurations.

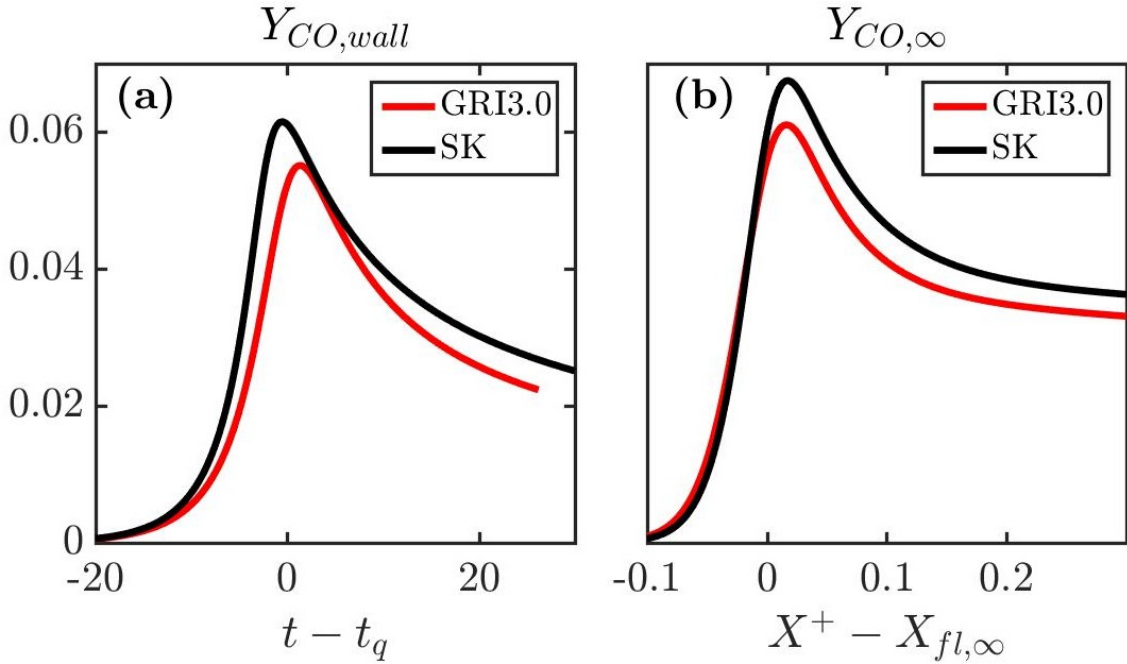


Figure 3.6: (a) Temporal variation of Y_{CO} at the wall ($Y_{CO,wall}$) and (b) the spatial variation of Y_{CO} at the far-field instant ($Y_{CO,\infty}$) obtained using GRI 3.0 and SK chemical mechanisms. The quenching instant is denoted by t_q in (a) while the flame position, defined as the X^+ location of peak HRR, is denoted by $X_{fl,\infty}$ in (b).

The SK chemical mechanism is compared against the 53-species GRI 3.0 mechanism in a 1D HOQ configuration in Figure 3.6 using the same unburnt gas temperature (800 K) and pressure (1 atm) as those in the 2D and 3D cases. Figure 3.6(a) shows the temporal variation of Y_{CO} at the wall while the spatial variation of Y_{CO} at an instant when the flame is far away from the wall, referred hereafter as the far-field instant, is presented in Figure 3.6(b). The qualitative trends of the CO mass fraction captured by the SK mechanism, matched with those obtained with the GRI 3.0 mechanism at the wall and at the far-field instant. Quantitatively, the peak Y_{CO} obtained using these two mechanisms differed by about 10% from the results presented here.

Figures 3.7 and 3.8 show the CO mass fraction results from 2D DNSs of forced ($St = 1$) laminar flames using the GRI 3.0 and the SK mechanisms. The computational domain discussed in Section 3.4.1 is used. The presented Y_{CO} results are time-averaged over one period of excitation and are denoted as $\overline{Y_{CO}}$. The qualitative trend of $\overline{Y_{CO}}$ captured by the two mechanisms are similar (see Figure 3.7) while a quantitative comparison is shown in Figure 3.8.

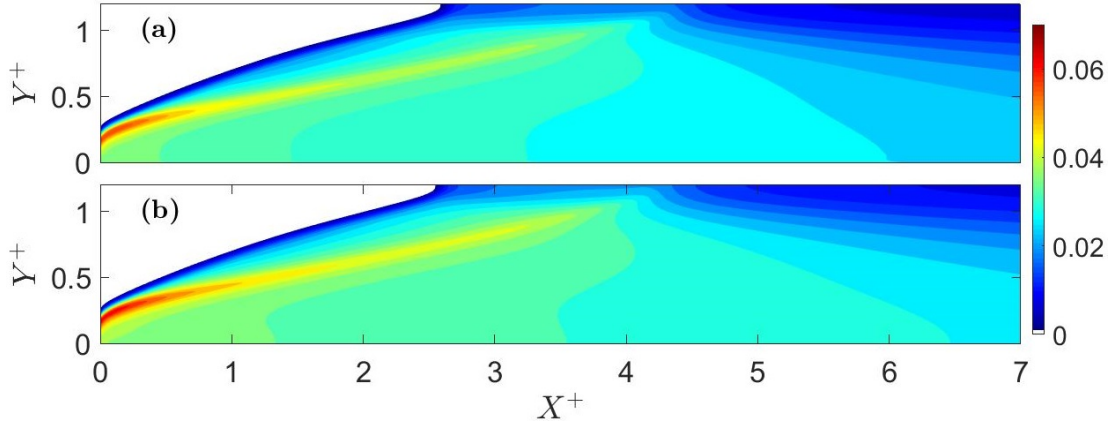


Figure 3.7: Time-averaged contours of Y_{CO} ($\overline{Y_{CO}}$) calculated from 2D DNS of forced ($St = 1$) laminar flames using the (a) GRI 3.0 and (b) SK chemical mechanisms.

Figure 3.8 compares the variation of $\overline{Y_{CO}}$ along the wall-normal direction at several streamwise locations (X^+) with the two mechanisms under consideration. The variable $\overline{Y_{CO}}$ at the wall captured by these two mechanisms differ between 20% to 25% at the streamwise locations presented in Figure 3.8. Overall, the comparison shows that the SK mechanism captures the CO and HRR trends even though an error of

a few tens of percent on Y_{CO} can be expected. The SK mechanism was therefore used in the 3D simulation, leading to a significant reduction of the computational cost.

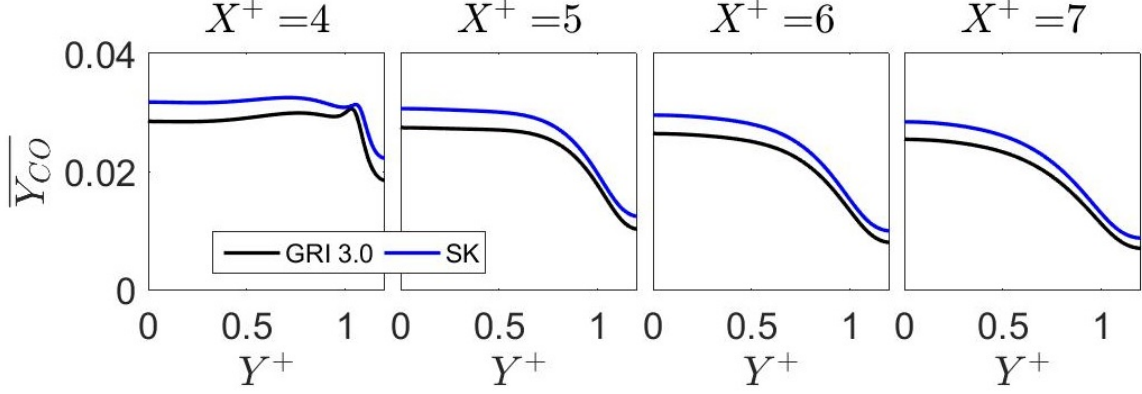


Figure 3.8: Comparison of $\overline{Y_{CO}}$ obtained from 2D DNS using GRI 3.0 and SK chemical mechanisms at several streamwise locations, plotted against the wall-normal direction.

3.7 Summary

This chapter discussed the numerical methods, boundary conditions and the chemical mechanisms used in this thesis to study flame-wall interaction and flame-cooling air interaction. First, the fundamentals of the DNS code and the governing equations were presented. Then, the computational domains and the boundary conditions were discussed. A grid independence study was performed to determine the required grid resolution in the 2D and 3D simulations. Finally, the performance of the reduced chemical mechanism used in the 3D turbulent simulations was examined by comparing the results with the more detailed GRI 3.0 chemical mechanism. The results obtained using these mechanisms were compared in a 1D head-on quenching and a 2D forced laminar flame configurations.

Chapter 4

Laminar flame-wall interaction (FWI)

4.1 Introduction

The objective of this chapter is to investigate the interaction of a preheated, laminar, stoichiometric methane/air flame with a relatively cold wall. The impact of this flame-wall interaction on flame dynamics, wall heat flux and *CO* emissions is discussed. The effect of low-temperature chemistry on the near-wall heat release rate is studied. The relative significance of the *CO* transport phenomena is analysed to understand the near-wall *CO* transport.

This chapter is structured as follows. Section 4.2 discusses the simulation parameters. Sections 4.3.1 and 4.3.2 present studies on 1D HOQ and 2D steady configurations, respectively. The flame dynamics, *HRR* and wall heat flux characteristics of forced flames are explained in Section 4.3.3 using three representative cases. The effect of radical recombination reactions on the near-wall heat release rate is detailed in Section 4.3.4 and the near-wall *CO* emissions are explored in Sections 4.3.5 and 4.3.6. While Section 4.3.5 intends to provide an understanding of the variations of the near-wall *CO*, the transport mechanisms controlling the same are studied in Section 4.3.6.

4.2 Simulation parameters

A stoichiometric ($\phi = 1$) mixture of methane and air at a preheated temperature of 800 K (T_u) and the pressure (p) of 1 atm is considered. This preheated temperature is relevant to the conditions of modern gas turbines. A 53-species, 325-reactions GRI 3.0 chemical mechanism is used. The Mach number at the inlet is set to 0.021 resulting in a jet Reynolds number (Re_{jet}) of 400. The transverse velocity at the inlet was set to zero whereas the streamwise velocity was imposed at the inlet using the analytical solution of a laminar ducted flow. The details of the domain (see Section 3.4.1), inlet velocity perturbation (see Section 3.5.1) and the grid resolution (see Section 3.4.3) have been discussed earlier. The Strouhal number, $St = (f \times L_f) / U_{in}$ is the non-dimensional form of frequency of excitation, where f is the forcing frequency, L_f is the steady-state length of the flame and U_{in} is the peak convective velocity at the inlet. The non-dimensional time periods of velocity excitation imposed at the inlet, namely $T_p=20, 30, 45, 90, 180$ and 360 correspond to the Strouhal numbers of 8.3, 5.5, 3.7, 1.9, 1 and 0.5. The simulations were run for at least two jet flow through times to obtain a stationary flow and the data produced for a given cycle after that was used for analysis. The simulation parameters including the thermal flame thickness (δ_{th}) and the flame speed (s_L) are shown in Table 4.1. The speed of sound (a_{ref}) is the reference velocity while the distance of the flame, represented by the peak HRR , from the wall is denoted by y_{wall} .

Table 4.1: Simulation parameters and non-dimensional numbers

Simulation parameters:		
$T_u = T_{wall} = 800K$	$U_{in}/a_{ref} = 0.021$	$\delta_{th} / L_{ref} = 0.1$
$p = 1 \text{ atm}$	$Re_{jet} = 400$	$s_L/a_{ref} = 0.00432$
$L_x^+ \times L_y^+ = 7 \times 1.2$	$N_x \times N_y = 1296 \times 243$	$a = 0.25$
$\phi = 1$	$Y_{anc}^+ = 0.2$	$St = 8.3, 5.5, 3.7, 1.9, 1, 0.5$
Non-dimensional parameters:		
Peclet number (Pe) = y_{wall} / δ_L		
Wall heat flux (ϕ_{wall}) = $\Phi_{wall} / (\rho_u Y_f s_L \Delta H)$		
Reynolds number (Re_{jet}) = $(L_{ref} U_{in} \rho_{ref}) / \mu_{ref}$		
Strouhal number (St) = $(f L_f) / U_{in}$		
Subscripts:	u : unburnt gas	anc : anchor point
	in : inlet	ref : reference condition
Superscripts:	+: Non-dimensional value	

4.3 Results and discussion

4.3.1 1D HOQ simulations

To provide baseline data for comparison, a 1D head-on quenching (HOQ) simulation was initially performed under the same conditions as the 2D simulations ($T_u=T_{wall}=800 \text{ K}$, $p = 1 \text{ atm}$). At $X^+ = 0$, isothermal ($T_{wall} = 800K$), inert wall boundary condition was imposed while non-reflecting boundary condition was imposed at $X^+ = 2$ using Navier-Stokes Characteristic Boundary Condition (NSCBC). The grid was stretched such that the resolution at the wall was $2 \mu m$ ($\Delta X^+ = 0.0007$) and that at $X^+ = 2$ was $6 \mu m$ ($\Delta X^+ = 0.0021$). With this resolution, the peak HRR and Y_{CO} at the wall were well-captured; the maximum difference was less than 1% when compared to the results with $1 \mu m$ resolution at the wall. Figure 4.1 (a) shows the heat release rate and CO mass fraction (Y_{CO}) profiles at various instants as the flame approaches the wall. The variables $t1$, $t2$, $t3$ and $t4$ are representative of times where the flame is far away from the wall ($t1$), affected by the wall ($t2$), in the process of quenching ($t3$), and extinguished ($t4$), respectively.

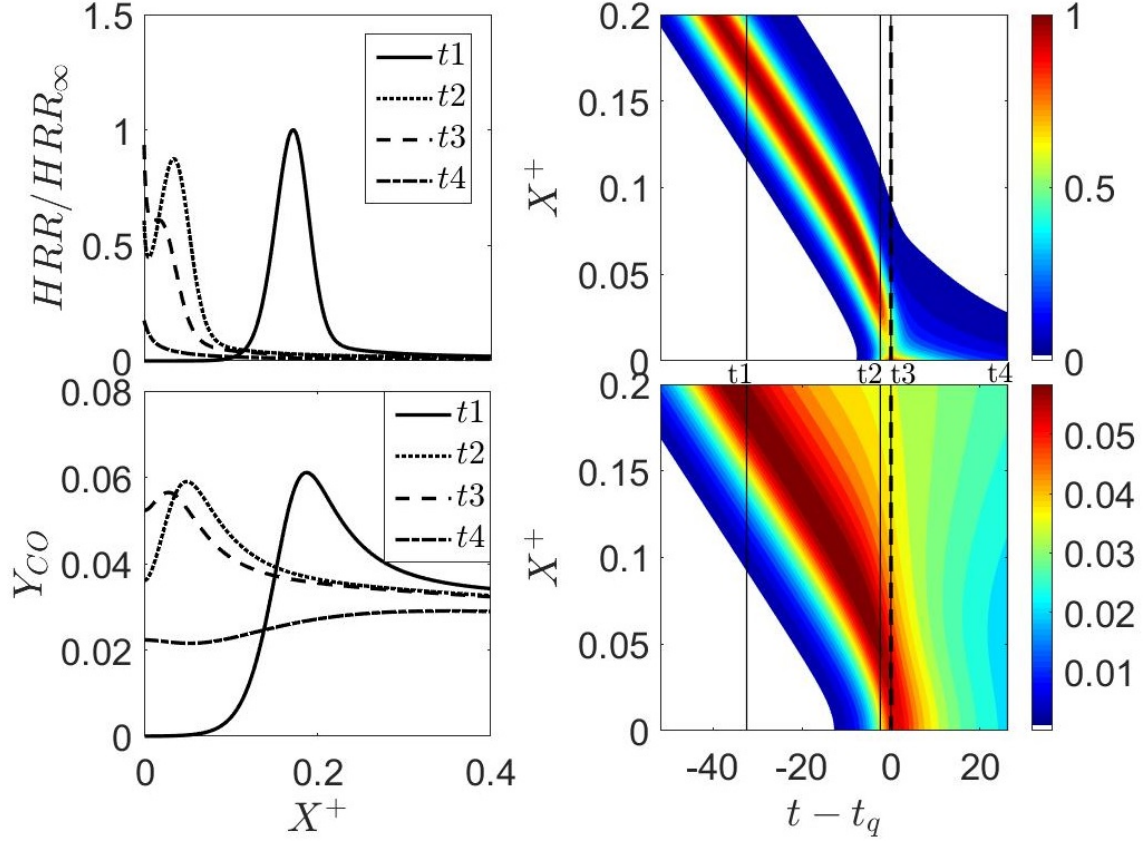


Figure 4.1: (a) Time evolution of heat release rate (top) and CO mass fraction (bottom) during 1D HOQ simulation. (b) $X^+ - t$ contours of heat release rate (top) and CO mass fraction (bottom). HRR is normalised by the maximum HRR when the flame is far away from the wall (HRR_∞).

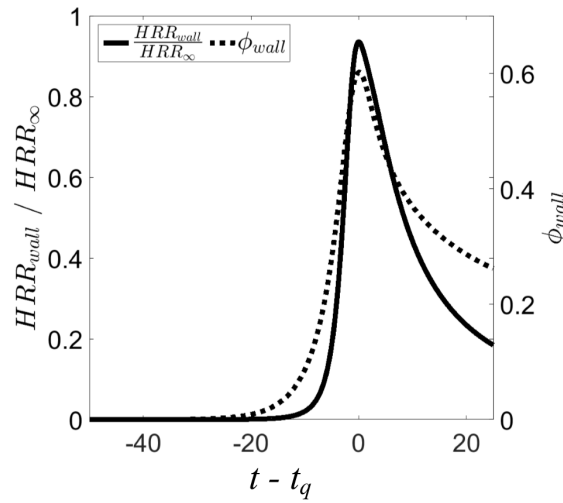


Figure 4.2: Variation of wall heat flux and HRR (normalised by HRR_∞ , i.e. the maximum HRR when the flame is far away from the wall) at the wall with time.

The points of local peak HRR are used to define flame position at a given time.

The time instant when the flame is closest to the wall is defined as the quenching time (t_q). During quenching, high values of HRR are observed at the wall, as seen in previous studies of HOQ [6] and will be explained more in Section 4.3.4. Also, it is seen from Figure 4.1 (a) that the quenching of the flame coincides with the initial increase of CO emissions at the wall and then it reduces to the equilibrium value which is consistent with previous observations [31]. The $X^+ - t$ contours of heat release rate (normalised as explained above) and CO mass fraction, shown in Figure 4.1 (b), illustrate flame deceleration as well as accumulation of CO at the wall as the flame approaches the wall.

Figure 4.2 shows the temporal variation of HRR at the wall and the wall heat flux. The wall heat flux (Φ_{wall}) is non-dimensionalised using flame power ($=\rho_u Y_f s_L \Delta H$) [8] where ρ_u and Y_f denote the unburnt gas density and fuel mass fraction, respectively. The heat of reaction and the unstretched laminar flame speed are denoted by ΔH and s_L , respectively. The non-dimensional wall heat flux is denoted by ϕ_{wall} . As can be seen, the peak HRR at the wall coincides with the peak heat flux. Importantly, the peak heat flux and HRR are still relatively large even after the quenching instant.

4.3.2 2D Steady flame

The results of a 2D steady flame quenching at the wall are presented here. The contours of CO mass fraction and heat release rate are shown in Figure 4.3. High values of Y_{CO} close to the peak value are found near the flame tip at the wall. Furthermore it can be seen that the HRR at the wall close to the flame tip is not insignificant. To further elucidate this, the HRR at the wall normalised by the peak HRR of 1D freely propagating flame is plotted in Figure 4.4. The maximum HRR at the wall is found to be about half of that of a freely propagating flame. The HRR remains non-zero over a range of X^+ in the post-flame zone; the width of HRR profile at 10% peak is about $6\delta_{th}$. The variation in wall heat flux is also plotted in Figure 4.4. Similar to the observation in 1D HOQ the HRR at the wall shows a similar trend to the wall heat flux as a function of the streamwise location.

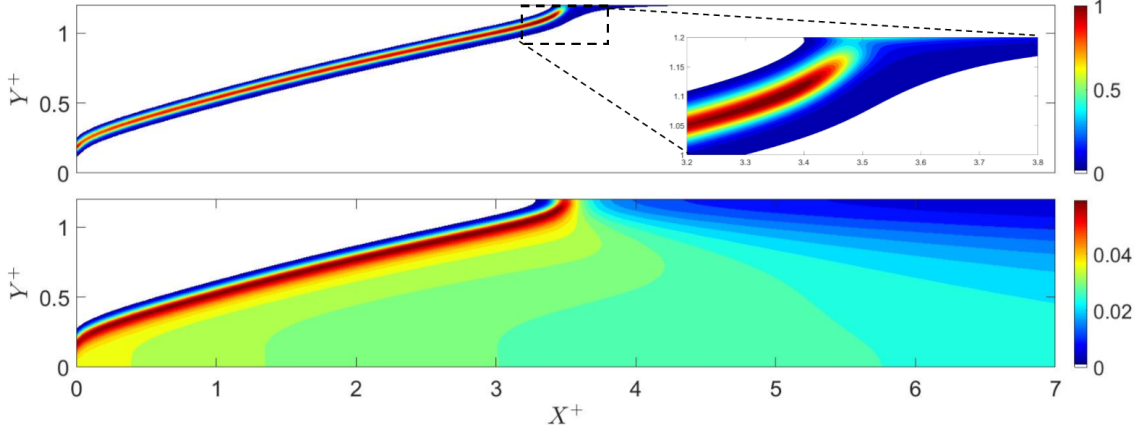


Figure 4.3: Contours of heat release rate (top) and CO mass fraction (bottom) for the steady flame. A zoomed image of near-wall HRR is also shown.

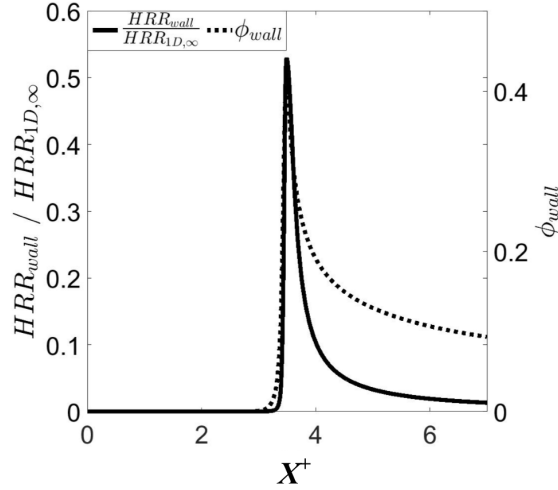


Figure 4.4: Wall heat flux (ϕ_{wall}) and HRR at the wall for the steady flame (normalised by the peak HRR of 1D flame unaffected by the wall).

4.3.3 Forced flame dynamics and wall heat flux

The flame response to the incoming velocity fluctuations at the inflow is studied in this section. Figure 4.5 shows the contour plots of the heat release rate at three representative Strouhal numbers ($St=8.3$, 1 and 0.5) at several instants during a forcing cycle. The changes in the flame position during a cycle is represented in Figure 4.6. The flame position at a given streamwise location (X^+) is determined as the point of maximum HRR along the wall-normal (Y^+) direction. The flame is defined only at the X^+ locations where maximum HRR along the wall-normal direction is at least 10% of the maximum HRR in the whole domain. At a given

instant, the flame tip is considered as the point where the minimum Pe , defined as Pe_{min} is achieved. The Peclet number (Pe) is the distance of the flame's peak HRR from the wall (y_{wall}) normalised by the reference diffusive flame thickness (δ_L).

At the highest forcing frequency examined ($St = 8.3$), the flame shows a similar behaviour to the steady flame shown in Figure 4.3. This is also shown by the relatively constant Pe_{min} observed at $St = 8.3$ in Figure 4.6. The convective wavelength, defined as U_{in}/f , is smaller than the flame length (about $1/9^{th}$) at this St . As a result, the flame does not respond strongly to the incoming fluctuations [61, 62]. As the frequency of excitation decreases, the convective wavelength increases and the flame responds more strongly. At $St = 1$, the flame propagates towards the wall perpendicularly from $t=0$ to $t=T_p/5$. This behaviour is similar to that of a 1D head-on quenching flame at the quenching instant. The Pe_{min} reaches the minimum value of 1.7 at $t=0.23T_p$. After that, the flame moves upstream along the wall (see $t=2T_p/5$). The Pe_{min} remains constant during this time. However, the flame tip, which was normal to the wall, changes orientation during this phase of the cycle. The downstream motion of the flame coincides with an increase in Pe_{min} reaching its peak ($Pe_{min} = 9.3$) at about $t=3T_p/5$. The flame motion during this part of the cycle is similar to a SWQ flame. It can also be seen that the flame orientation becomes almost normal to the wall. The main observation from the flame behaviour at $St = 1$ is that FWI involves both HOQ and SWQ at different stages. This case also experiences a significant change of Pe_{min} compared with other cases. For the lowest frequency of excitation, i.e. $St=0.5$, the flame extends and retracts in a quasi-steady manner with a reduced amount of distortion. This is because the convective wavelength is now larger than the flame length (about twice). The flame moves downstream between $t=T_p/5$ and $3T_p/5$. During this time, the value of Pe_{min} varies from 1.7 to 4.9. A small change in the flame orientation is also observed as the flame becomes less normal to the wall. An upstream motion of the flame, during which the flame tip gets closer to the wall, then follows.

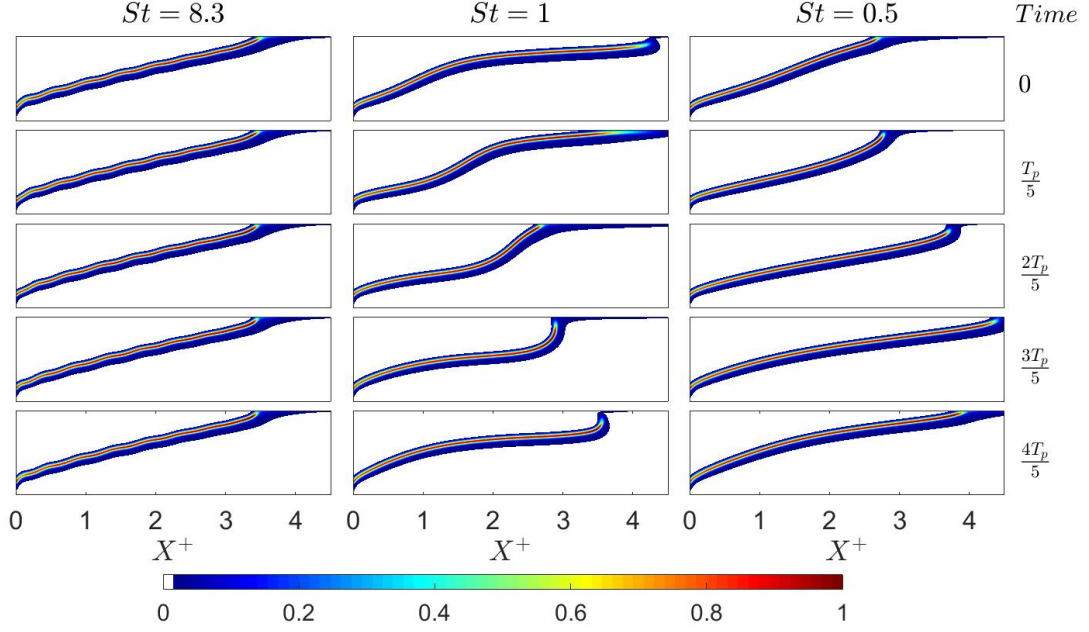


Figure 4.5: Heat release rate (normalised by the peak HRR of 1D flame unaffected by the wall) contours at several instants with the same time interval during one cycle for $St=8.3$, 1 and 0.5, respectively.

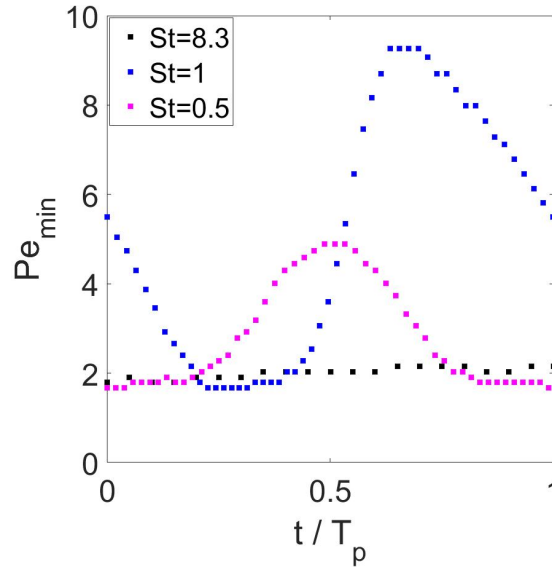


Figure 4.6: Variation of Pe_{min} in one time period of excitation for $St=8.3$, 1 and 0.5.

The $X^+ - t/T_p$ diagram of HRR at the wall is shown for each of these cases in Figure 4.7 (top row). The contours of wall heat flux are also plotted in Figure 4.7 (bottom row). The HRR and wall heat flux are observed to have similar qualitative trends. The maximum HRR and wall heat flux are observed between $t = 0.2T_p$ and $0.4T_p$.

This period coincides with the minimum Pe instants shown in Figure 4.6. Also, during this period, large values of HRR and wall heat flux in the post-flame zone are observed. This highlights the significant role of the flame wall distance on the HRR and wall heat flux.

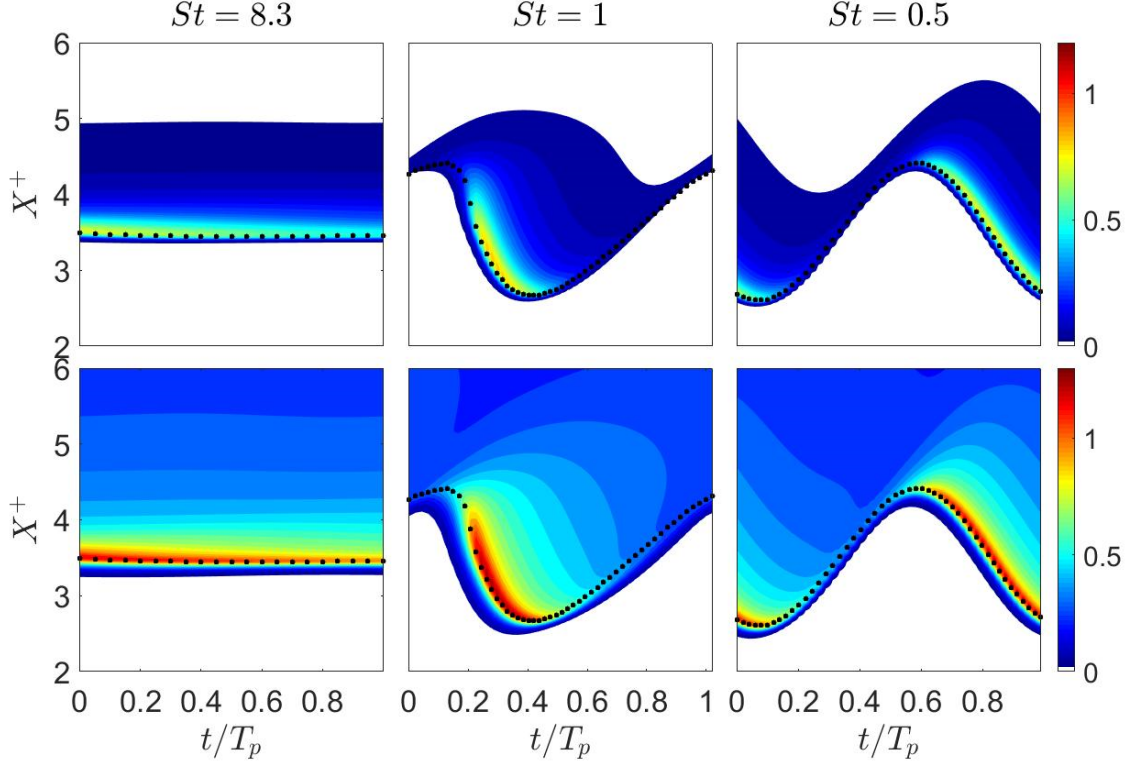


Figure 4.7: $X^+ - t$ contours of HRR at the wall normalised by the peak HRR of 1D flame unaffected by the wall (top row) and wall heat flux normalised by the maximum wall heat flux in the steady case (bottom row) for $St=8.3, 1, 0.5$. The X^+ of Pe_{min} at every time instant is represented by the black dots.

To examine this effect in more detail, Figure 4.8 shows variation of the wall heat flux as a function of Pe_{local} , defined as the wall-normal distance of the flame from the wall at a given streamwise position. A correlation for the maximum wall heat flux ($\phi_{wall,max}$) was proposed by Poinso et al. [8], expressed as,

$$\phi_{wall,max} = \left[\frac{T_{ad} - T_{wall}}{T_{ad} - T_u} \right] Pe_{min} \quad (4.3.1)$$

where T_{ad} is the adiabatic flame temperature. This is also shown in Figure 4.8 as a reference. Of note is that the wall heat flux (ϕ_{wall}) shown in Figure 4.8 (for $St=1$), normalised by the maximum wall heat flux in a steady flame (ϕ_s) can have

values greater than 1. This is because Pe_{min} can achieve smaller values compared with the steady flame. At low values of Pe_{local} (less than about 2.5), which refers to the HOQ-like behaviour of the flame, the obtained results match with the above-mentioned correlation. However, a large degree of variation is observed for higher Pe_{local} , suggesting that heat flux can not be estimated as a function of local Pe only for transient FWI. Note, wall heat flux is found to be approximately constant for a range of high Pe_{local} values. This behaviour corresponds to the SWQ-like instants where the flame tip is almost perpendicular to the wall, as observed at $t = 3T_p/5$ and $4T_p/5$ in Figure 4.5.

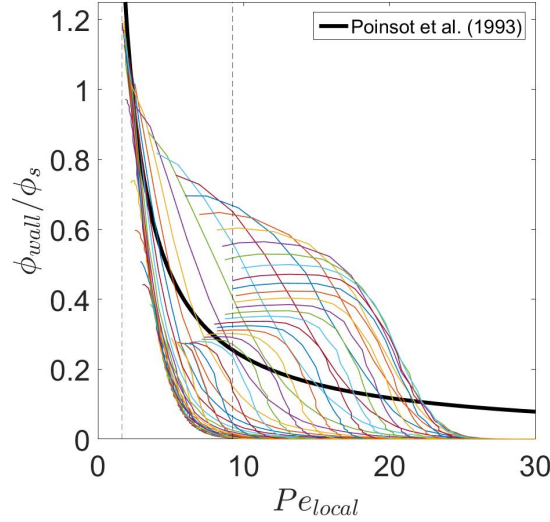


Figure 4.8: Variation of non-dimensional wall heat flux (ϕ_{wall} , normalised by the peak wall heat flux in a steady case, ϕ_s) with the local flame position (Pe_{local}) at different instants during a cycle ($St=1$). Results are compared with the correlation proposed by Poinso et al. [8] (black line). Minimum ($=1.7$) and maximum ($=9.3$) values of Pe_{min} are shown by vertical lines.

The time-averaged mean and root mean square (RMS) values of the wall heat flux (ϕ_{mean} and ϕ_{rms}) for representative cases ($St = 8.3, 1, 0.5$) are now plotted against the streamwise distance (X^+) in Figure 4.9. The wall heat flux in the steady case is also plotted for comparison. The wall heat fluxes are normalised by the maximum wall heat flux observed in the steady case. It is observed that ϕ_{mean} is similar to the steady results for $St=8.3$ in which case ϕ_{rms} is low. This is consistent with what was shown in Figure 4.5 as the flame behaves like a steady flame. The mean and RMS values of the wall heat flux show similar behaviour for $St=1$ and $St=0.5$ although

the flame response at these Strouhal numbers show different features such as a much larger range of Pe_{min} observed in the $St=1$ case.

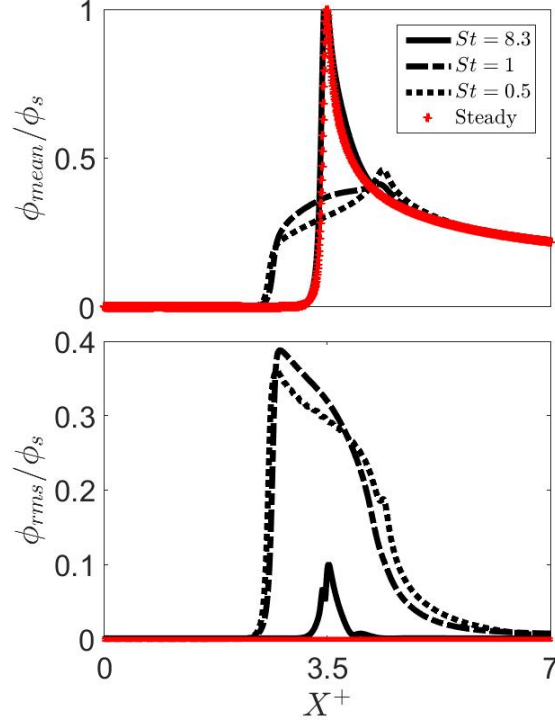


Figure 4.9: The variation of mean (top) and RMS (bottom) of the wall heat flux (normalised by ϕ_s) along the streamwise distance for $St=8.3$, 1, 0.5.

Figure 4.10 shows the amplitude of quantities associated with the wall heat flux at the forcing frequency, obtained with Fast Fourier Transform (FFT). The variables $\phi_{@maxmean}$ and $\phi_{@maxrms}$ refer to the temporal variation of the wall heat flux at the streamwise distances where ϕ_{mean} and ϕ_{rms} , respectively, attain maximum values. The variable ϕ_{total} refers to the wall heat flux (normalised by ϕ_s) integrated over the total length in the streamwise direction. As expected, low level of fluctuations in the wall heat flux is observed at the highest Strouhal number. At low frequencies of excitation, where the flame features a SWQ behaviour, considerable fluctuations are observed. The integrated wall heat flux peaks at $St=1$. This is the forcing frequency when the flame displays a combination of HOQ and SWQ. The trend observed for ϕ_{total} agrees with the wall heat flux analysis in a turbulent flame, reported in the literature [6]. The single-point and the total wall heat flux analyses show different trends of wall heat flux variation, indicating that the former approach may not always be sufficient to describe the variation of wall heat transfer.

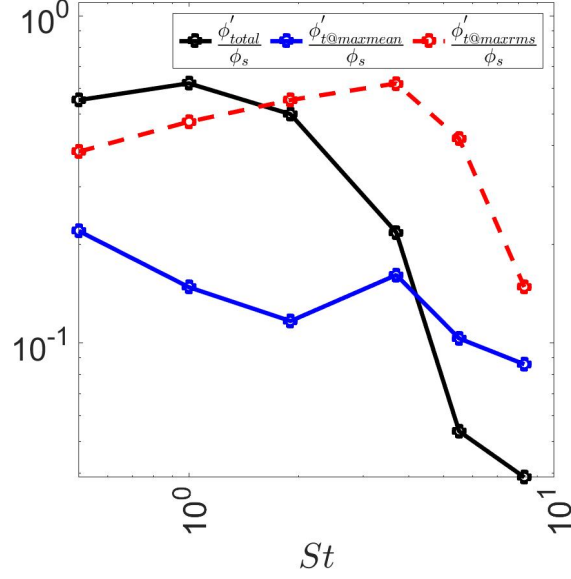


Figure 4.10: Amplitude of the wall heat fluxes (normalised by ϕ_s) fluctuation as a function of St .

4.3.4 Effect of radical recombination reactions near wall

Our earlier findings showed high values of HRR at the wall during FWI. This suggests that radical recombination reactions are important near the wall, as seen previously [6, 21]. Hence, the contribution of these reactions to the overall HRR is examined here. They are defined as zero-activation energy, exothermic reactions [6]. The analysis is done for the intermediate frequency ($St=1$) where the maximum variation in Pe_{min} was observed.

To identify the reactions which are important near the wall, the HRR due to each reaction and the overall HRR at the wall were integrated along the streamwise direction (X^+) to get $HRR_{rn,wall}$ and HRR_{wall} , respectively. The contribution of $HRR_{rn,wall}$ to HRR_{wall} due to each individual reaction was obtained at the quenching instant. The reactions whose HRR contribution are at least 0.1% of the total HRR at the wall are shown in Table 4.2 in the descending order of their contribution.

All reactions which contribute to at least 1% of the total HRR at the wall involve reactive radicals such as H , O or OH . Only two of these reactions (reactions 52 and 99) contain carbon atoms. The conversion of CO to CO_2 by reacting with OH

radicals (reaction 99) is an important fuel-oxidation reaction at high temperatures [63]. However, the contribution of this reaction is less than that of several radical-recombination reactions (as seen from Table 4.2) at the cold wall. Reaction 52, which is the recombination of methyl radicals back to methane, is expected to be more important at low temperatures [63]. According to the definition for radical recombination reactions [6], only the zero-activation energy reactions are highlighted in Table 4.2. Overall, these reactions account for about 50% of the total HRR at the wall.

The sum of the HRR due to the identified radical recombination reactions (HRR_{rad}) is compared with the overall HRR in Figures 4.11 and 4.12. Figure 4.11 shows the contours of total HRR (top) and HRR due to radical recombination near the wall at t_q . The complete domain is not shown here. The values of HRR are normalised by the peak HRR in a freely propagating 1D flame. The contour plots show a high HRR zone at the wall between $X^+=3$ and $X^+=3.5$ in which, radical recombination reactions show relatively high values up to 50% of the peak HRR in the 1D flame.

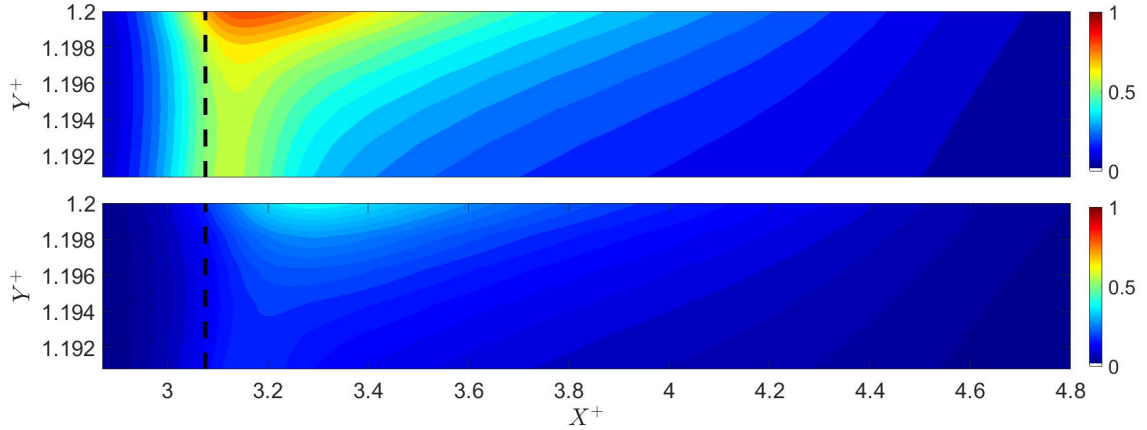


Figure 4.11: Contours of total heat release rate, HRR (top) and the heat release rate due to radical recombination reactions HRR_{rad} (bottom) for $St=1$ at the quenching instant (t_q). HRR and HRR_{rad} are normalised by the peak HRR in a freely propagating 1D flame. The X^+ location of the flame tip at t_q is indicated by the vertical black line.

Figure 4.12 provides further insight into the contribution of radical recombination reactions since it shows the HRR and HRR_{rad} at several Y^+ close to the wall. The peak HRR_{rad} contributes to about half of the overall HRR at the wall. The

Table 4.2: List of the major reactions (in *GRI3.0* chemical mechanism) which contribute to the *HRR* at the wall at the quenching time (t_q) sorted in the descending order of their contribution (shown in column 2) towards total HRR_{wall} . E_a is the activation energy in cal/gmol.

Reaction no.	$HRR_{rn,wall}$ (%)	Reaction	E_a
35	22.44	$H + O_2 + H_2O \rightleftharpoons HO_2 + H_2O$	0.00
46	13.8	$H + HO_2 \rightleftharpoons 2OH$	635.00
43	9.22	$H + OH + M \rightleftharpoons H_2O + M$	0.00
45	8.51	$H + HO_2 \rightleftharpoons O_2 + H_2$	1068.00
52	8.4	$H + CH_3(+M) \rightleftharpoons CH_4(+M)$	536.00
36	8.37	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	0.00
38	4.16	$H + O_2 \rightleftharpoons O + OH$	17041.00
99	3.68	$OH + CO \rightleftharpoons H + CO_2$	70.00
87	3.17	$OH + HO_2 \rightleftharpoons O_2 + H_2O$	-500.00
84	2.11	$OH + H_2 \rightleftharpoons H + H_2O$	3430.00
33	1.86	$H + O_2 + M \rightleftharpoons HO_2 + M$	0.00
4	1.39	$O + HO_2 \rightleftharpoons OH + O_2$	0.00
41	1.28	$2H + H_2O \rightleftharpoons H_2 + H_2O$	0.00
168	0.95	$HCO + O_2 \rightleftharpoons HO_2 + CO$	400.00
44	0.94	$H + HO_2 \rightleftharpoons O + H_2O$	671.00
55	0.74	$H + HCO \rightleftharpoons H_2 + CO$	0.00
95	0.72	$OH + CH_3(+M) \rightleftharpoons CH_3OH(+M)$	1330.00
86	0.67	$2OH \rightleftharpoons O + H_2O$	-2110.00
10	0.55	$O + CH_3 \rightleftharpoons H + CH_2O$	0.00
158	0.54	$2CH_3(+M) \rightleftharpoons C_2H_6(+M)$	654.00
98	0.53	$OH + CH_4 \rightleftharpoons CH_3 + H_2O$	3120.00
85	0.5	$2OH(+M) \rightleftharpoons H_2O_2(+M)$	0.00
39	0.48	$2H + M \rightleftharpoons H_2 + M$	0.00
101	0.47	$OH + CH_2O \rightleftharpoons HCO + H_2O$	-447.00
34	0.41	$H + 2O_2 \rightleftharpoons HO_2 + O_2$	0.00
284	0.37	$O + CH_3 \rightleftharpoons H + H_2 + CO$	0.00
119	0.28	$HO_2 + CH_3 \rightleftharpoons OH + CH_3O$	0.00
100	0.22	$OH + HCO \rightleftharpoons H_2O + CO$	0.00
290	0.18	$CH_2 + O_2 \rightleftharpoons 2H + CO_2$	1500.00
147	0.18	$CH_2(S) + H_2O(+M) \rightleftharpoons CH_3OH(+M)$	1145.00
145	0.16	$CH_2(S) + O_2 \rightleftharpoons CO + H_2O$	0.00
125	0.15	$CH + O_2 \rightleftharpoons O + HCO$	0.00
58	0.15	$H + CH_2O \rightleftharpoons HCO + H_2$	2742.00
76	0.15	$H + C_2H_5(+M) \rightleftharpoons C_2H_6(+M)$	1580.00
144	0.14	$CH_2(S) + O_2 \rightleftharpoons H + OH + CO$	0.00
48	0.12	$H + H_2O_2 \rightleftharpoons OH + H_2O$	3600.00
2	0.12	$O + H + M \rightleftharpoons OH + M$	0.00
65	0.12	$H + CH_3O \rightleftharpoons H_2 + CH_2O$	0.00
12	0.12	$O + CO(+M) \rightleftharpoons CO_2(+M)$	2385.00
135	0.11	$CH_2 + O_2 \rightleftharpoons OH + H + CO$	1500.00

contribution of HRR_{rad} is also considerable slightly away from the wall where radical recombination reactions contribute to about one-third of the overall HRR at the peak at a wall-normal distance of about 10% of the thermal flame thickness from the wall.

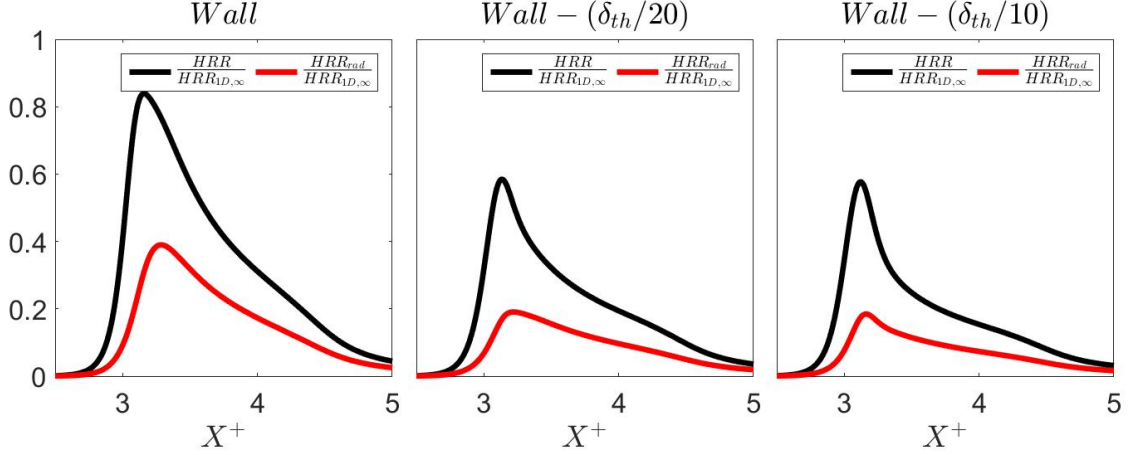


Figure 4.12: Total HRR and the HRR due to radical recombination reactions (HRR_{rad}) at and near ($\delta_{th}/20$ and $\delta_{th}/10$ away from the wall, respectively) the wall (both the HRR terms are normalised by the peak HRR in a freely propagating 1D flame) for $St=1$.

4.3.5 Analysis of near-wall CO

The influence of wall on CO emission was presented in Figure 4.1 and was briefly discussed in Section 4.3.1. A detailed investigation of near-wall CO mass fraction for the forced flame is performed in this section. The flame subjected to the intermediate frequency of excitation ($St=1$), showing the maximum variation of Pe_{min} , was chosen for the analysis.

Figure 4.13 shows the contours of CO mass fraction and temperature at several instants (same as those in Figure 4.5) in a forcing cycle. The first two instants, i.e. $t = 0$ and $T_p/5$, show the wall-normal propagation of the flame. During this motion of the flame, a substantial amount of CO is found between the flame and the wall. It is also shown that the downstream motion of the flame ($t=4T_p/5$ and $5T_p/5$) leaves some CO behind the flame close to the wall. This CO , which is in the low temperature region, is not oxidised until the flame starts to move upstream again. The temperature dependence of Y_{CO} at these instants is quantitatively represented

in Figure 4.14.

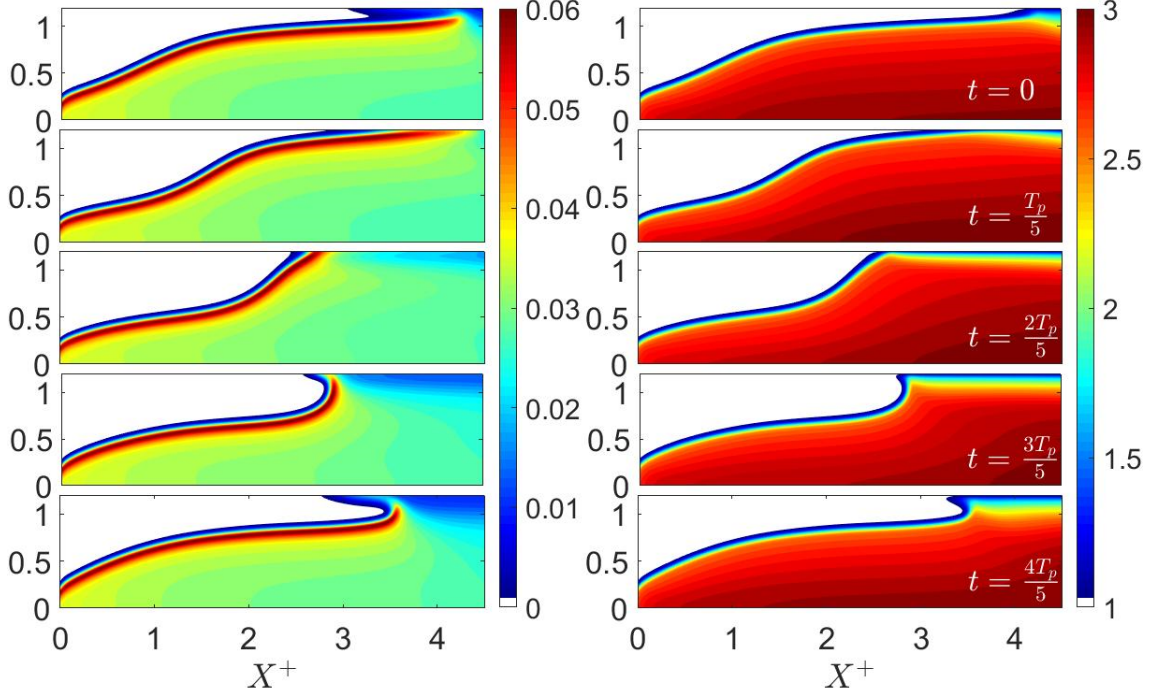


Figure 4.13: Contour plots of CO mass fraction (left) and temperature normalised by the fresh gas temperature (right) for $St=1$ at several instants during one cycle.

Figure 4.14 shows the scatter plots of CO mass fraction in a near-wall window against temperature for the time instants shown in Figures 4.5 and 4.13. The selected window is $10\delta_{th}$ wide on the either side of the flame tip along X^+ and $2\delta_{th}$ from the wall along Y^+ direction. The $Y_{CO} - T$ plots in a 1D HOQ simulation at the quenching instant and 1D freely propagating flame (FPF) configurations are also plotted as reference. The 1D HOQ configuration shows the behaviour of a quenched flame while that of a flame unaffected by the wall is shown by 1D FPF. The scatter plots are colour coded based on the distance from the wall. At $t=0$, which is the start of the HOQ process, the 1D FPF solution seems to provide an upper bound for a large range of temperatures. However, the near-wall CO is non-zero demonstrating that FWI is contributing to near-wall CO . As the flame gets closer to the wall ($t = T_p/5$), the near-wall CO increases and now the combination of the 1D HOQ and 1D FPF solutions set the limit to Y_{CO} . Large fluctuations of Y_{CO} at a given temperature is observed at different instants and the distance from the wall does not seem to be responsible for these fluctuations. The level of fluctuations in the vicinity of the wall (where temperature is close to 800 K) decreases for $t=0$ and $4T/5$. These

are the instants which show SWQ-like behaviour. However, the instants relevant to the HOQ-like interaction show a higher level of fluctuations. This might not be surprising given that at these instants, the HOQ is not a 1D phenomenon and occurs at an angle which can cause these large fluctuations. Overall, this shows the complex nature of transient FWI which prevents us from describing the near-wall CO simply by using distance from the wall and temperature.

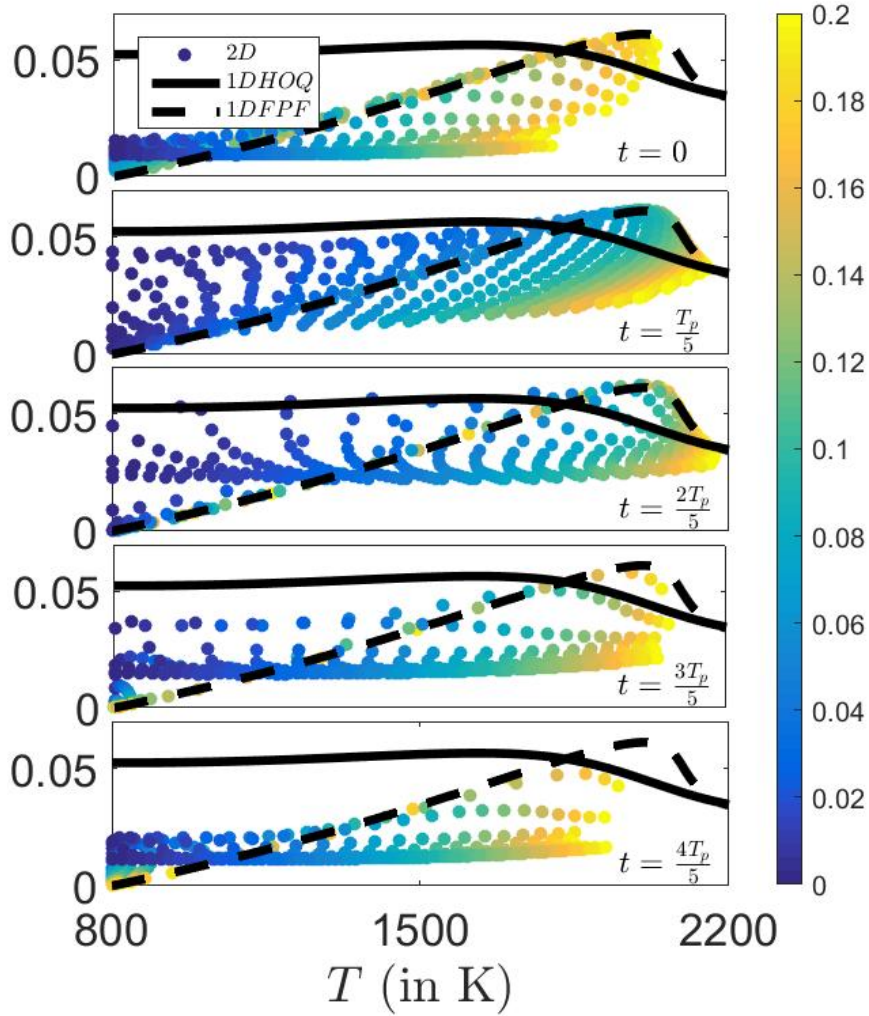


Figure 4.14: Scatter plots of CO mass fraction against temperature (in K) at several time instants in a forcing cycle for $St=1$ in a window with a width of $10\delta_{th}$ on either side of the flame tip and a height of $2\delta_{th}$ from the wall. $Y_{CO} - T$ plots of 1D HOQ and 1D FPF are also shown for reference. The points are coloured by the distance from the wall.

4.3.6 Species transport budget analysis of near-wall CO

A better understanding of the near-wall CO behaviour requires a more comprehensive analysis of the transport phenomena. Equation 3.3.4 can be used to conduct a species transport budget on the unsteady flame. We consider the $St=1$ case for this analysis.

$$\frac{\partial Y_\alpha}{\partial t} = \left[-u_j \frac{\partial Y_\alpha}{\partial x_j} \right] + \left[-\frac{1}{\rho} \frac{\partial(\rho V_{\alpha j} Y_\alpha)}{\partial x_j} \right] + \left[\frac{\dot{W}_\alpha \dot{\omega}_\alpha}{\rho} \right] \quad (4.3.2)$$

The terms on the right hand side of Equation 4.3.2 represent the contribution of mass convection (C), molecular diffusion (D) and reaction rate (R), respectively to the transport of a given species. This framework, known as CDR analysis, is commonly used to provide insight into the transport of a species of interest [35] which is CO in our study.

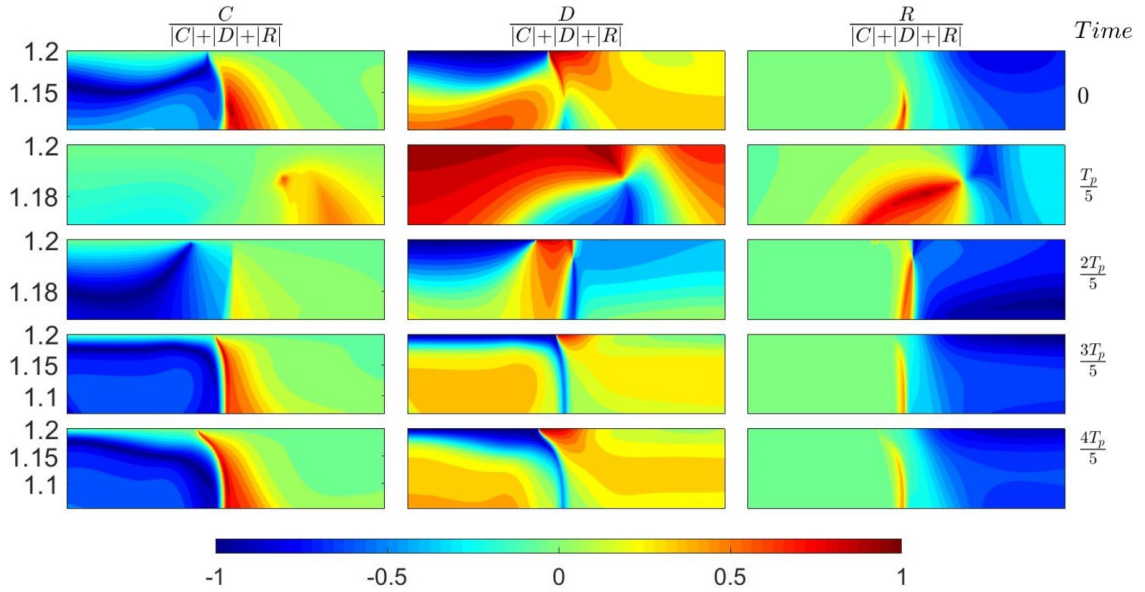


Figure 4.15: Convection (C), diffusion (D) and reaction (R) terms of the species conservation equation at several time instants. C , D and R are plotted in a window which is ten flame thicknesses wide on either side of the flame tip in streamwise direction. The Y^+ dimension of the window varies from the instantaneous flame tip to the wall. C , D and R terms are normalised by the sum of the absolute values of C , D and R .

The convection, diffusion and reaction terms in Equation 4.3.2 for CO , normalised

by the sum of the absolute values of these terms, are shown in Figure 4.15 at several instants (same as those used in Figures 4.5, 4.13 and 4.14). The contours are plotted in a changing window position with a width of $20 \delta_{th}$ centered at the flame tip in the streamwise direction. The height of the window varies from the flame tip to the wall. During the HOQ process, i.e. $t=0$ to $T_p/5$, the diffusion of CO is important near the wall. This is clear from Figure 4.15 which shows an almost unity value for the normalised diffusion. During the upstream and downstream movements of the flame, the convection term also becomes important. However, the reaction term is insignificant compared with the other terms close to the flame tip near the wall. This observation can be useful for modelling as it suggests that the rate of change of Y_{CO} close to the wall at the flame tip might be predictable by only considering convection and diffusion.

4.4 Conclusions

This chapter investigated the flame behaviour near walls by studying the interaction of unsteady laminar premixed flames with a constant temperature wall. Two-dimensional direct numerical simulations of a forced flame were carried out for a range of excitation frequencies. The flame behaviour was analysed in detail at three representative Strouhal numbers defined based on the steady-state length of the flame and peak convective velocity at the inlet ($St=8.3, 1$ and 0.5). While the flame did not respond strongly at high forcing frequencies, it showed a side-wall quenching like interaction at low frequencies. At an intermediate forcing frequency ($St=1$), the flame showed a combination of head-on quenching and side-wall quenching. In addition, the analysis of the total integrated wall heat flux showed a similar trend to that in turbulent flames.

A systematic study of the contribution of reactions towards HRR at the wall indicated that low activation energy, exothermic reactions are significant near the wall. These reactions, collectively known as the radical recombination reactions contributed to about 50% of the total HRR at the wall for $St=1$. This confirms the importance of low temperature chemistry in understanding the HRR behaviour at the wall and the wall heat flux. The analysis of CO mass fraction close to the wall

for $St=1$ showed that a head-on quenching like interaction coincides with a high concentration of CO near the wall. This indicates that the geometry of interaction can have a significant effect on the produced CO . The temperature dependence of Y_{CO} showed that a combination of one-dimensional freely propagating and head-on quenching solutions for Y_{CO} provide an upper bound for the near-wall Y_{CO} . The so-called Convection-Diffusion-Reaction (CDR) analysis was performed to investigate the CO transport mechanism in detail. The significance of various transport phenomena near the wall varied within a forcing cycle. During the HOQ-like behaviour of the flame, diffusion was found to be more important than convection and reaction. As the flame moved upstream along the wall, the streamwise convection was found to be significant. The downstream movement of the flame (like SWQ), showed that both convection and diffusion were important. CO diffused from the flame and wall to the region between them. During the downstream motion of the flame, all three transport phenomena were important. However, the reaction terms were significant in the post-flame region only. Overall, the CDR analysis shows that the near-wall CO transport in the vicinity of the flame tip is dominated by convection and diffusion which can have important implications for modelling.

Chapter 5

Laminar flame-cooling air interaction (FCAI)

5.1 Introduction

The objective of this chapter is to study flame-cooling air interaction (FCAI) using 2D DNSs of a preheated, laminar, premixed methane/air flame interacting with a jet of coolant. Several cases are considered by varying different parameters such as the cooling jet mass flow rate, cooling hole position and dilution type. Furthermore, similar to the approach taken in Chapter 4, the flame is acoustically forced for a range of frequencies to introduce a range of flow time scales. After analysing the flame features, their impact on the wall heat flux and *CO* emissions are examined. Finally, the implications of our findings for modelling *CO* emission due to flame-cooling air interaction (FCAI) are elaborated.

This chapter is structured as follows. The simulation cases considered in this chapter are discussed in Section 5.2. Section 5.3.1 presents the results of 1D freely-propagating flames over a range of equivalence ratios. The effects of FCAI on flame behaviour, wall heat flux and *CO* characteristics are discussed later in the Sections 5.3.2 to 5.3.4. Analysis of *CO* thermochemical states near the cooled wall is presented in Section 5.3.6.

5.2 Simulation matrix and post-processing framework

A summary of the different cases considered in this chapter is presented in Table 5.1. The BR , St , streamwise location of the cooling hole (X_{cool}) and the coolant type used in each simulation are shown in this table. The blowing ratio, BR , is defined as the ratio of the mass flux of the coolant to that of the inlet mixture. Case 5 is chosen as the baseline case here.

Table 5.1: The simulation matrix.

Case	BR	St	X_{cool}	Coolant
1	3	8.3	3	Air
2	5	8.3	3	Air
3	10	8.3	3	Air
4	3	1	3	Air
5	5	1	3	Air
6	10	1	3	Air
7	3	0.5	3	Air
8	5	0.5	3	Air
9	10	0.5	3	Air
10	5	1	2	Air
11	5	1	4	Air
12	5	1	3	N_2

5.2.1 Post-processing parameters

5.2.1.1 Modified mixture fraction

To quantify the effects of dilution, a modified mixture fraction, ξ , was used, which is a conserved scalar to quantify the extent to which the inlet premixture and the coolant are mixed. The mixture fraction defined by Bilger [64] is modified such that the value in the pure inlet stream is unity while that in the coolant stream is zero.

$$\xi = \frac{2Y_C/W_C + Y_H/2W_H + (Y_{O,cool} - Y_O)/W_O}{2Y_{C,inlet}/W_C + Y_{H,inlet}/2W_H + (Y_{O,cool} - Y_{O,inlet})/W_O}, \quad (5.2.1)$$

where Y_C , Y_H and Y_O refer to the element mass fractions of carbon (C), hydrogen

(H) and oxygen (O), respectively while their atomic masses are denoted by W_C , W_H and W_O . The subscripts ‘inlet’ and ‘cool’ indicate the inlet stoichiometric mixture and the coolant stream, respectively.

Based on the conventional definition of mixture fraction (ξ^{con}) defined by Bilger [64], the equivalence ratio (ϕ) can be defined as:

$$\phi = \frac{\xi^{con}(1 - \xi_{st}^{con})}{\xi_{st}^{con}(1 - \xi^{con})}, \quad (5.2.2)$$

where ξ_{st}^{con} is the stoichiometric value of ξ^{con} .

The definition of ξ presented in Equation 5.2.1 is related to ξ^{con} and ξ_{st}^{con} as follows: $\xi = \xi^{con}/\xi_{st}^{con}$. Thus, Equation 5.2.2 can be written as:

$$\phi = \xi \frac{(1 - \xi_{st}^{con})}{(1 - \xi \xi_{st}^{con})} \quad (5.2.3)$$

When a stream of pure methane mixes with a stream of pure air to form a stoichiometric mixture, the value of ξ_{st}^{con} is 0.054. For $\xi_{st}^{con} \ll 1$, Equation 5.2.3 results in:

$$\phi \approx \xi \quad (5.2.4)$$

5.2.1.2 Progress variable

A progress variable based on Y_{CO_2} is defined locally. Here, the variables $Y_{CO_{2,u}}$ and $Y_{CO_{2,b}}$ refer to the unburnt and burnt mass fractions of CO_2 at an equivalence ratio corresponding to ξ .

$$c_{CO_2} = \left(\frac{Y_{CO_2} - Y_{CO_{2,u}}}{Y_{CO_{2,b}} - Y_{CO_{2,u}}} \right) \quad (5.2.5)$$

The reason for choosing CO_2 to define the progress variable will be discussed in Section 5.3.1.

5.2.1.3 Enthalpy deficiency

To quantify the effect of wall heat loss, enthalpy deficiency was calculated as follows:

$$h_{def,norm} = \frac{h_{ad} - h}{h_{ad} - h_{prod}}, \quad (5.2.6)$$

where h is the local mixture enthalpy at a given point and h_{ad} is the adiabatic enthalpy of the mixture at that point. The mixture enthalpy (h) is calculated as $\sum h_i Y_i$ where h_i and Y_i are the enthalpy and mass fraction of species i , respectively. The variable h_{ad} is obtained from adiabatic 1D freely-propagating flame simulations performed in CHEMKIN PRO [65] for the equivalence ratio corresponding to the local ξ . The mixture enthalpy is obtained from such a simulation for a progress variable corresponding to the local c_{co_2} and is identified as h_{ad} , as shown in Figure 5.1. For very low equivalence ratios outside the flammability limits, a 0-D closed homogeneous reactor model in CHEMKIN PRO is used to obtain the adiabatic enthalpy. The variable h_{prod} is the mixture enthalpy of the burned products, for an equivalence ratio corresponding to the local ξ , at the wall temperature. Note, a higher value of the normalised enthalpy deficiency indicates a higher heat loss to the wall.

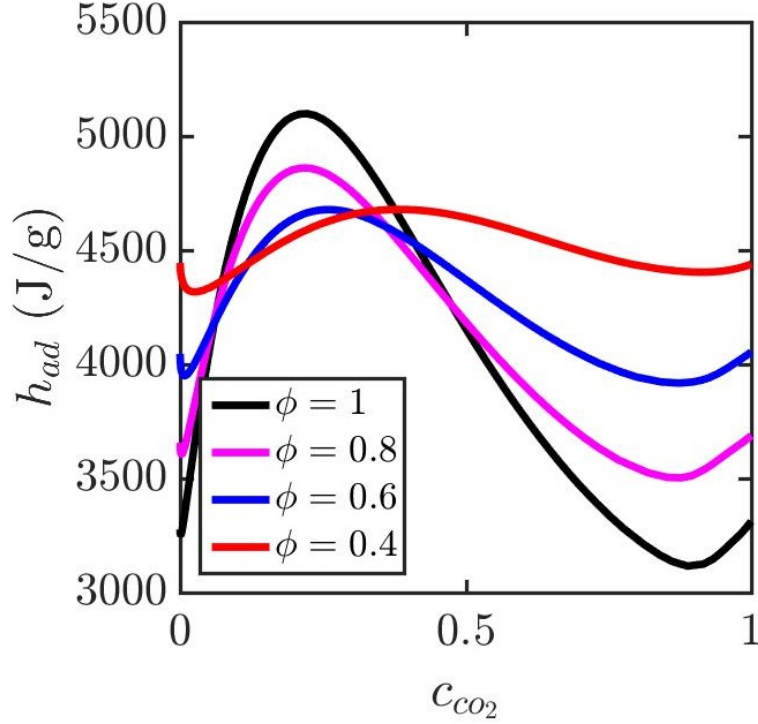


Figure 5.1: Variation of adiabatic enthalpy (h_{ad}) with c_{CO_2} obtained from 1D freely propagating flame simulations. Only four equivalence ratios are shown here.

5.2.1.4 Flame length

The flame length X_{fl} is defined as the maximum X^+ at which the time-averaged HRR is 5% of the maximum time-averaged HRR . The variable ΔX_{fl} , is then defined as:

$$\Delta X_{fl} = X_{fl}(\text{each case}) - X_{fl}(\text{baseline case}), \quad (5.2.7)$$

showing the difference between each case and the baseline case.

5.2.1.5 Variation of CO mass fraction relative to the baseline case

To compare the CO mass fraction (Y_{CO}) obtained in each case with the baseline case, away from the wall ($Y^+ < 1$) and in the near-wall region ($Y^+ \geq 1$), at a streamwise location near the domain exit ($X^+ = 6$), the following variables are defined,

$$\Delta CO_{far}(\%) = \frac{\overline{Y}_{CO, far}(\text{each case}) - \overline{Y}_{CO, far}(\text{baseline case})}{\overline{Y}_{CO, far}(\text{baseline case})} \Big|_{X^+=6, Y^+ < 1} \times 100, \quad (5.2.8)$$

$$\Delta CO_{wall}(\%) = \frac{\overline{Y}_{CO, wall}(\text{each case}) - \overline{Y}_{CO, wall}(\text{baseline case})}{\overline{Y}_{CO, wall}(\text{baseline case})} \Big|_{X^+=6, Y^+ \geq 1} \times 100, \quad (5.2.9)$$

The variable ΔCO_{far} represents the percentage difference of time-averaged Y_{CO} between each case and the baseline case far from the wall ($Y^+ < 1$) and close to the outflow boundary ($X^+ = 6$). The variable ΔCO_{wall} shows this difference close to the wall ($Y^+ \geq 1$) at the same streamwise location.

5.2.1.6 Cooling jet trajectory

To show the differences in the coolant jet trajectory for different cases, relative to the baseline case, at a streamwise location close to the exit of the domain, a variable $\Delta Y_{cool|X6}$ is defined. This variable is used to investigate how a change in the coolant trajectory affects CO emissions near and away from the wall.

$$\Delta Y_{cool|X6} = Y_{cool|X6}(\text{each case}) - Y_{cool|X6}(\text{baseline case}). \quad (5.2.10)$$

The variable $Y_{cool|X6}$ is defined as the Y^+ at $X^+ = 6$ of the streamline that starts from the centre of the cooling hole. A positive value of $\Delta Y_{cool|X6}$ indicates that this streamline at $X^+ = 6$ for the considered case is closer to the wall compared to the baseline case.

5.3 Results and discussion

5.3.1 1D freely-propagating flames (FPF)

The interaction of the cooling air jet with the flame changes the local stoichiometry and dilution and so is likely to influence the near-wall CO . To independently evaluate the impact of stoichiometry changes, 1D unstrained freely propagating flames (FPFs) were simulated with GRI 3.0 chemical mechanism using the CHEMKIN package [65]. A range of equivalence ratios with the same premixture temperature of 800 K as the 2D cases were considered. Only four equivalence ratios, i.e. $\phi = 0.4, 0.6, 0.8$ and 1, are illustrated in Figure 5.2. The variation of CO mass fraction (Y_{CO}) with distance and temperature are shown in Figures 5.2 (a) and (b), respectively. As the mixture becomes leaner, the peak Y_{CO} and its associated temperature both reduce, as expected. Furthermore, the time scales of CO production and oxidation, calculated based on a 10 % - 90 % criterion [27, 28], increase for leaner mixtures, as shown in Table 5.2. In other words, although a smaller amount of CO is produced in a lean mixture, it takes longer for this amount to be oxidised. Figure 5.2(c) also shows the thermochemical states of CH_4 , O_2 , CO_2 , H_2O , CO and a combination of CO and CO_2 . Out of the species shown in Figure 5.2(c), the mass fraction of CO_2 shows a significant variation with temperature even after complete consumption of the fuel, hence it was used to define a progress variable in Equation 5.2.5.

Figure 5.3 shows the variation of Y_{CO} , Y_{CH_4} , Y_{CO_2} and dY_{CO_2}/dT in the 1D FPF configuration for several equivalence ratios, normalised by their maximum values for that ϕ . The peak location of dY_{CO_2}/dT in the temperature space coincides with $Y_{CH_4} \approx 0$. A threshold value is defined based on this peak location referred to as c' . This threshold will be later used as a marker for the post combustion zone where production of CO_2 with respect to temperature starts to slow down.

Table 5.2: Time-scales (in milliseconds) of CO production (t_{pr}) and oxidation (t_{ox}).

ϕ	t_{pr} (ms)	t_{ox} (ms)
1	0.1	0.45
0.8	0.12	0.51
0.6	0.22	0.61
0.4	0.96	1.28

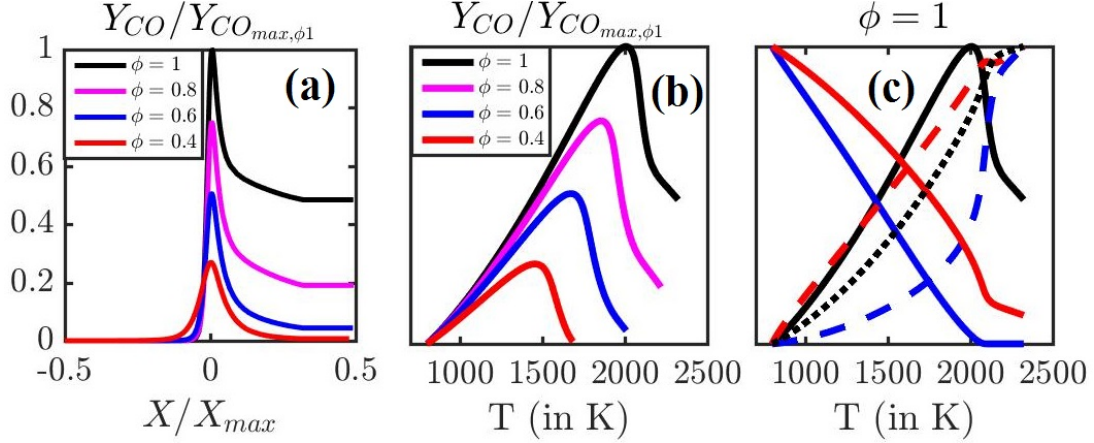


Figure 5.2: Variation of CO mass fraction (Y_{CO}), normalised by the maximum Y_{CO} of the stoichiometric case, against distance (a) and temperature (b) in a 1D freely-propagating flame configuration for several equivalence ratios (ϕ). The temperature dependence of the reactants (CH_4 and O_2), products (CO_2 and H_2O), CO and ($CO + CO_2$), normalised by their maximum values, under stoichiometric conditions is shown in (c). Legend for subfigure (c): $\blacksquare$ $Y_{CO}/Y_{CO,max}$, $\blacksquare$ $Y_{CH_4}/Y_{CH_4,max}$, $\blacksquare$ $Y_{CO_2}/Y_{CO_2,max}$, $\blacksquare$ $Y_{O_2}/Y_{O_2,max}$, $\blacksquare$ $Y_{H_2O}/Y_{H_2O,max}$, $\cdots$ $(Y_{CO}+Y_{CO_2})/(Y_{CO}+Y_{CO_2})_{max}$.

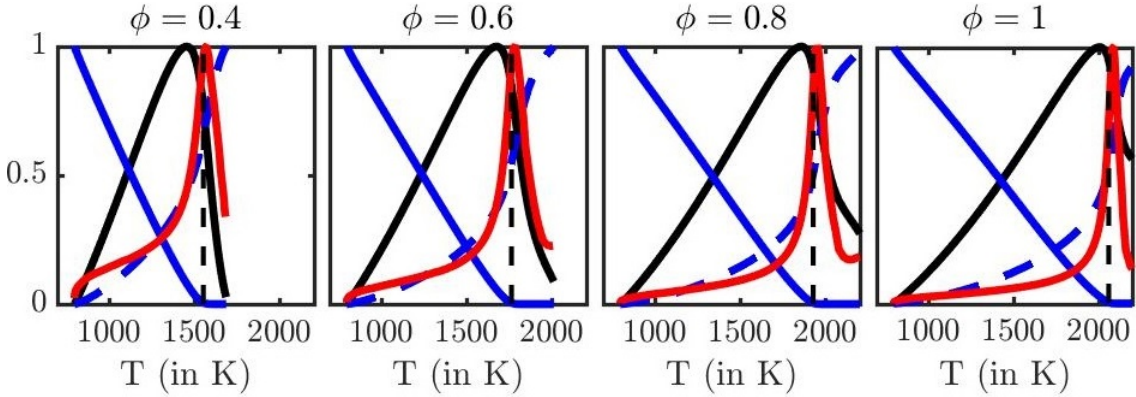


Figure 5.3: The temperature dependence of Y_{CO} , Y_{CH_4} , Y_{CO_2} and dY_{CO_2}/dT in a 1D freely-propagating flame configuration for several equivalence ratios (ϕ), normalised by their maximum values for that ϕ . The vertical dashed lines mark the temperature at which dY_{CO_2}/dT is maximum. Legend: $\blacksquare$ $Y_{CO}/Y_{CO,max}$, $\blacksquare$ $Y_{CH_4}/Y_{CH_4,max}$, $\blacksquare$ $Y_{CO_2}/Y_{CO_2,max}$, $\blacksquare$ $(dY_{CO_2}/dT)/(dY_{CO_2}/dT)_{max}$.

5.3.2 Flame dynamics

Figure 5.4 shows the contour plot of the mixture fraction for Case 5 at five equally spaced instants during one forcing period. The flame boundary, defined as the isoline of the HRR at 5% of the maximum HRR in the time period of excitation (T_p), is shown with a solid line. As can be seen, the cooling air leads to formation of a long

flame sheet in the vicinity of the wall. This very lean flame sheet becomes longer during the upstream motion of the flame up to $t = T_p/5$, then quickly burns out at the final stages of the upstream motion ($t = 2T_p/5$). This sheet starts to form again during the downstream motion ($t = 3T_p/5 - 4T_p/5$) as the flame passes the cooling hole. The time-averaged HRR and ξ , shown in Figure 5.5, also illustrate the lengthening of the flame and reduction in the local stoichiometry near the wall.

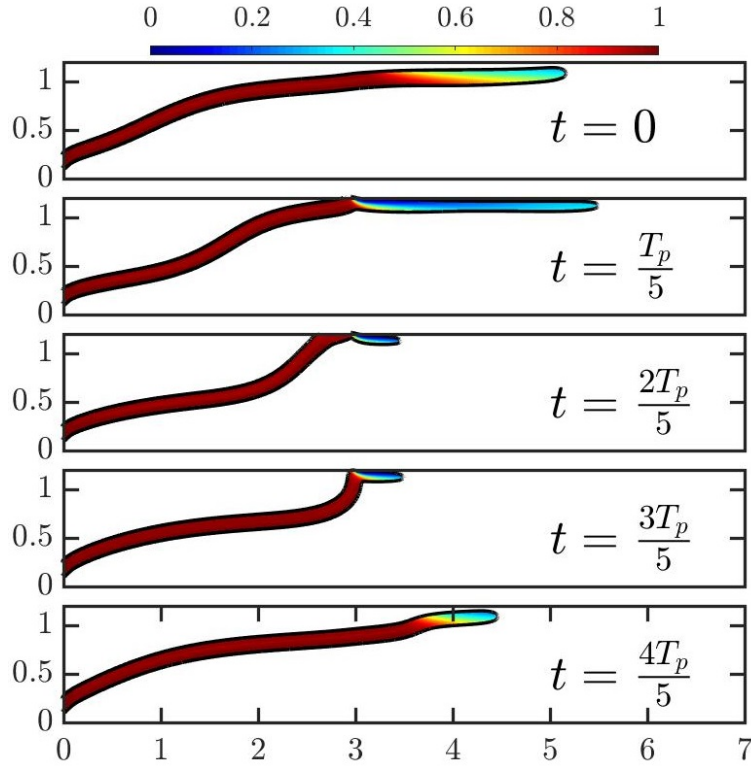


Figure 5.4: The variation of modified mixture fraction, ξ within the flame, defined by the isolines of heat release rate (HRR) at 5% of peak HRR , for Case 5 (see Table 5.1) at several instants within a forcing cycle.

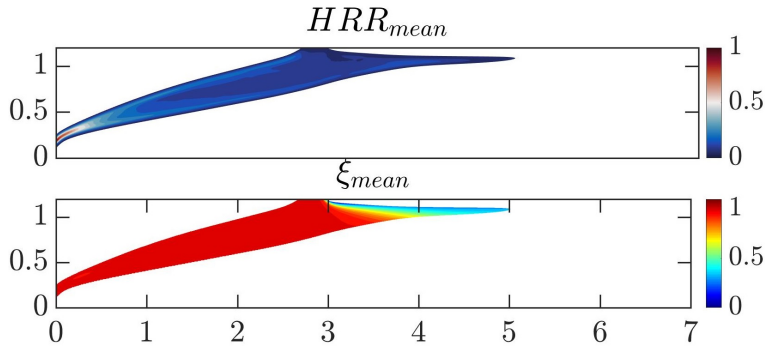


Figure 5.5: Contours of time-averaged HRR (top) and time-averaged modified mixture fraction (ξ_{mean}) within the flame region (bottom) for Case 5. HRR is normalised by the peak HRR of a 1D flame unaffected by the wall.

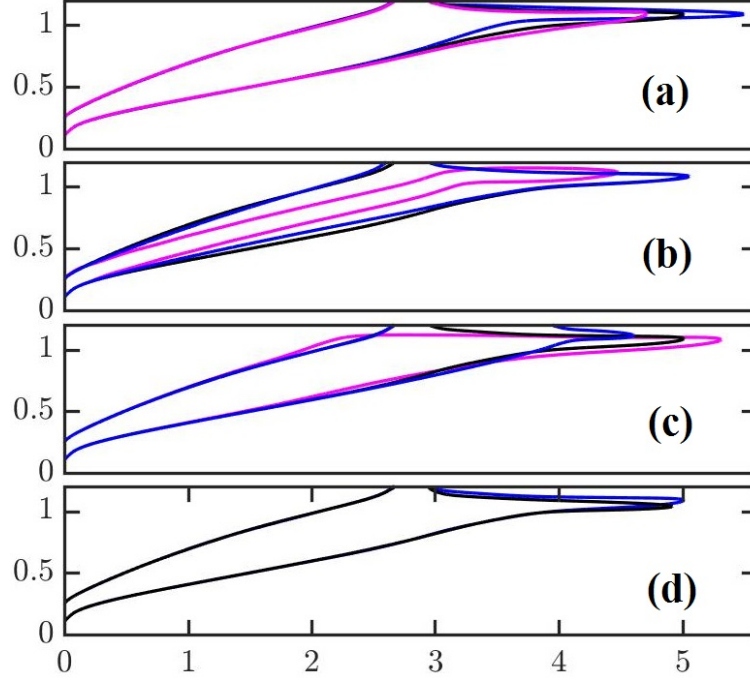


Figure 5.6: Isolines of HRR , at 5% of the maximum HRR , for a range of BR , St , X_{cool} and coolant (air/ N_2). Subfigures (a), (b), (c) and (d) show the effect of BR , St , X_{cool} , and coolant type, respectively. Legends: (a) — $BR = 3$, — $BR = 5$, — $BR = 10$; (b) — $St = 8.3$, — $St = 1$, — $St = 0.5$; (c) — $X_{cool} = 2$, — $X_{cool} = 3$, — $X_{cool} = 4$; (d) — N_2 , — Air.

The effects of BR , St , X_{cool} and the coolant fluid (air/ N_2) on the overall flame shape are illustrated in Figure 5.6. The flame boundaries using the time-averaged HRR are also shown. Increasing the BR from 3 to 10 increases the flame length (also shown in Table 5.3), while changes in the cooling hole position, X_{cool} from 2 to 4, decreases the flame length. This shows that positioning the cooling hole in upstream locations has a similar effect to increasing of the blowing ratio, both making the lean flame sheet longer. The impact of St is only observable when St was changed from 8.3 to 1 and a minimal impact by the coolant type is observed.

Table 5.3: Values of the parameters defined in Equations 5.2.7, 5.2.8, 5.2.9 and 5.2.10 for the cases shown in Figure 5.11. The values of ΔCO_{far} and ΔCO_{wall} shown here are averaged in Y^+ .

Case	BR	St	X_{cool}	Coolant	ΔX_{fl}	$\Delta Y_{cool X6}$	$\Delta CO_{far}(\%)$	$\Delta CO_{wall}(\%)$
2	5	8.3	3	Air	-0.53	0.001	1.9	-14.8
4	3	1	3	Air	-0.3	-0.001	-2.7	-55
5	5	1	3	Air	0	0	0	0
6	10	1	3	Air	0.49	0.038	27.5	25.1
8	5	0.5	3	Air	0.04	-0.001	-0.57	5
10	5	1	2	Air	0.3	-0.023	-10	27.8
11	5	1	4	Air	-0.4	0.03	21.3	-29.9
12	5	1	3	N_2	-0.09	0.006	59.7	115.8

5.3.3 Wall heat flux

The effects of BR , St and X_{cool} on the wall heat flux in the wall-cooled region are shown in Figure 5.7 (a)-(c), respectively. Only the values after the cooling hole are presented. The coolant type (air/ N_2) has negligible impact on the wall heat flux and hence is not shown here. The uncooled case, which represents $BR = 0$, is shown in Figure 5.7 (a) as reference. The time-averaged mean and root mean square (RMS) of the wall heat flux, denoted by ϕ_{mean} and ϕ_{rms} , respectively, are normalised by the peak wall heat flux in the uncooled, steady state case (ϕ_s). A significant reduction of the mean and RMS values compared with the uncooled case is observed in the vicinity of the cooling hole, as expected. Also, not surprisingly, the injection of more air reduces the mean and RMS values. An increase in BR from 3 to 10 decreased the peak ϕ_{mean} by about 30%. Decreasing the forcing frequency lowers the peak ϕ_{mean} up to a certain St due to a larger motion of the flame in the streamwise direction. For the same reason, higher fluctuations of the heat flux are observed for lower forcing frequencies.

Furthermore, as the cooling hole is shifted from $X^+ = 2$ to 4, a reduction in peak ϕ_{mean} of about 30% was observed in the post-cooling hole region. This is because for $X_{cool} = 4$, the wall downstream of the cooling hole is less affected by the flame movement. The value of $(X_{fl} - X_{cool})$ decreases from 3.3 to 0.6 as X_{cool} moves from 2 to 4.

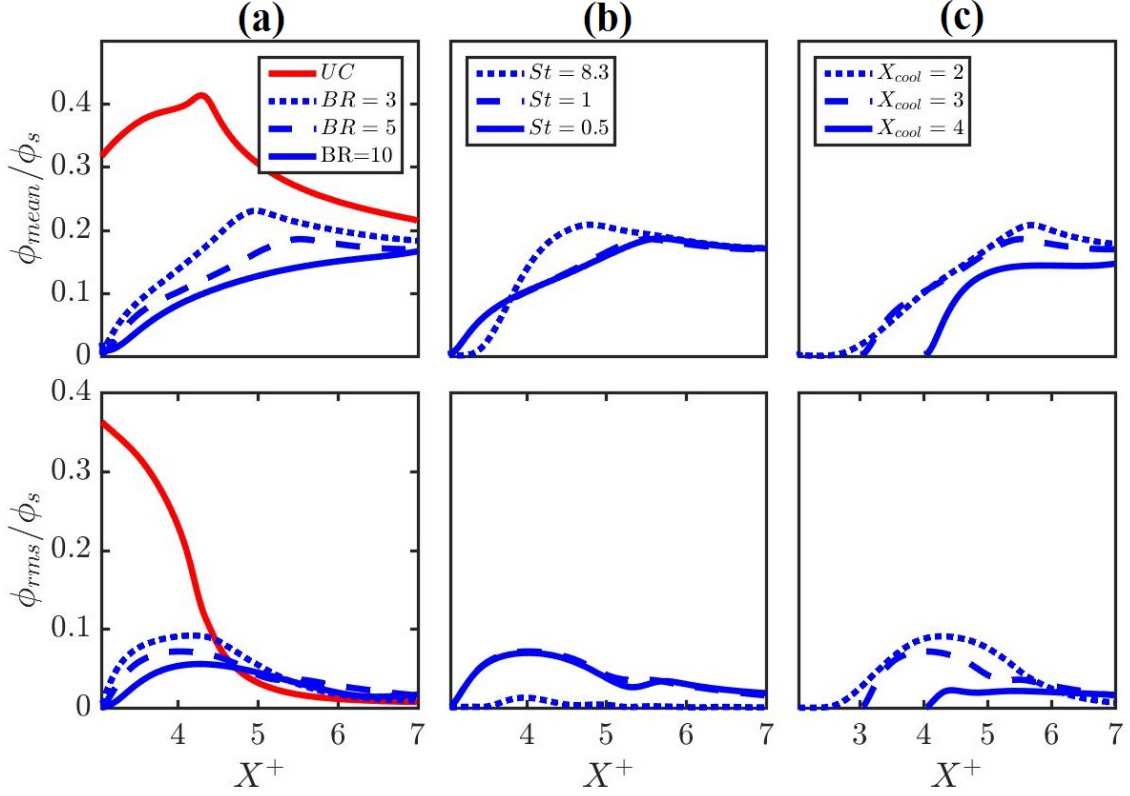


Figure 5.7: Mean (top) and RMS (bottom) wall heat flux, normalised by ϕ_s , for a range of (a) BR (b) St and (c) X_{cool} . The uncooled case is denoted by UC in this plot.

The effects of FCAI on the wall heat flux is further analysed for the baseline case in Figure 5.8. The normalised wall heat flux, i.e. ϕ_{wall}/ϕ_s , is shown as a function of the local Peclet number (Pe_{local}), defined as the distance of the isoline of the reduced temperature, $\theta = (T - T_{u|\phi 1})/(T_{b|\phi 1} - T_{u|\phi 1}) = 0.6$, to the wall at every $X^+ > X_{cool}$, normalised by the diffusive flame thickness (δ_L). The chosen value of θ corresponds to the peak HRR of an unstrained laminar flame at the same conditions as the 2D cases. The wall heat flux is expected to be high when Pe_{local} is low for an uncooled case (see Equation 4.3.1). However, Figure 5.8 shows that small values of Pe_{local} correspond to a lower wall heat flux for the FCAI case. To examine this further, the points in the FCAI case are colour coded by X^+ . This shows that while Poinot's correlation (Equation 4.3.1) breaks down near the cooling hole, it has a good performance for $X^+ > 5$. Of note is that X_{fl} for the baseline case is also 5.

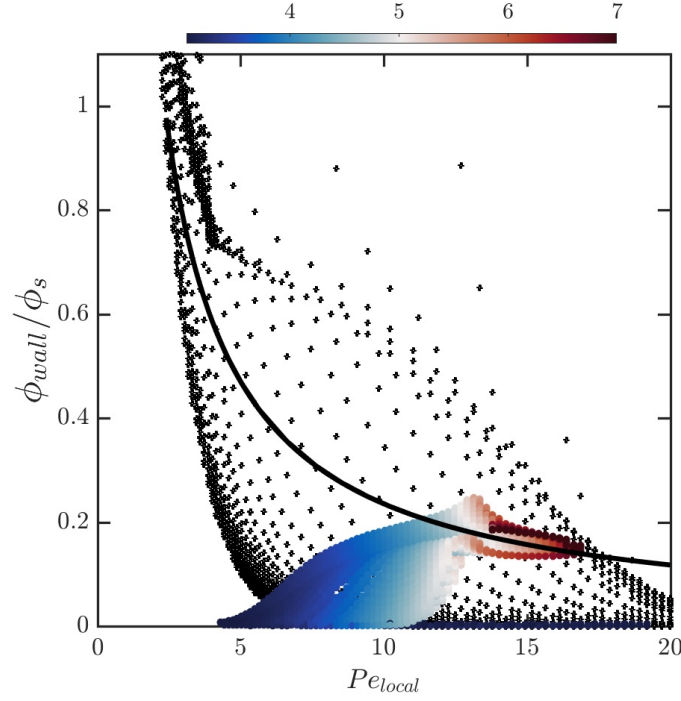


Figure 5.8: The variation of wall heat flux, normalised by ϕ_s , with the local flame position denoted by Pe_{local} . The region before the cooling hole is denoted by black circles while that after the cooling hole are coloured by X^+ . The black line represents Poinsot's correlation mentioned in Equation 4.3.1.

5.3.4 Near-wall and exhaust CO emissions

Figure 5.9 shows the contours of CO mass fraction at five equally spaced instants for Case 5. It can be seen that the cooling air has a large impact on reducing the post-combustion CO . Another observation is formation of a pocket of CO downstream of the flame in the vicinity of the wall. This pocket is detached from the lean flame sheet, and as it convects further downstream, it also moves towards the wall while the CO concentration within the pocket reduces. Such a lean pocket features a relatively large CO oxidation time scale and therefore, can be transported to the outlet before being oxidised. This phenomenon will be investigated later in this chapter.

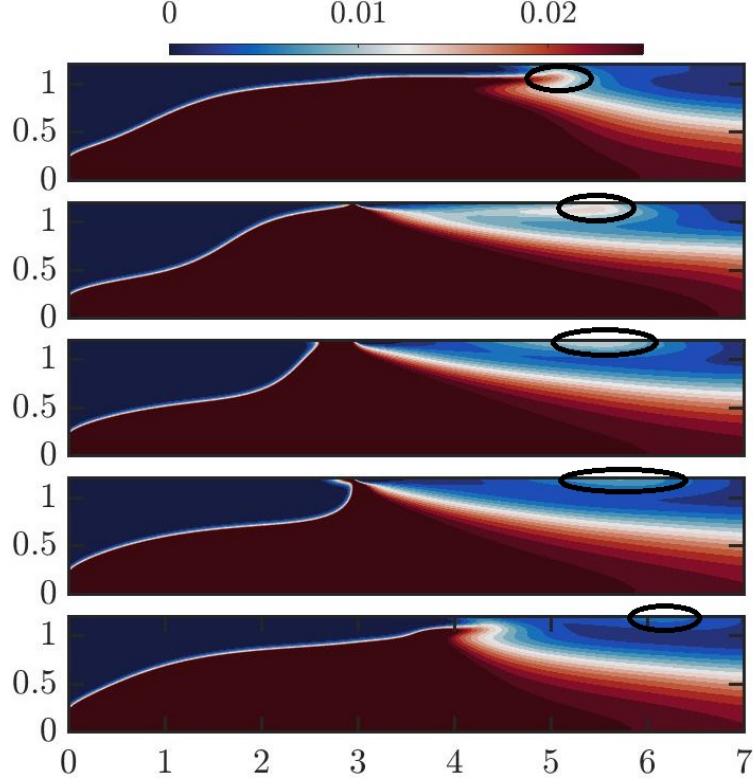


Figure 5.9: Contour plots of CO mass fraction for Case 5 at several instants (same as in Figure 5.4) in an excitation cycle. The black circles highlight a pocket of CO being transported towards the wall.

The effects of BR , St , X_{cool} and coolant type on the time-averaged CO in the whole domain and at $X^+ = 6$ are shown in Figures 5.10 and 5.11, respectively. Here, the terms near-wall and far-field regions are defined as $Y^+ \geq 1$ and $Y^+ < 1$ regions, respectively. The values of ΔX_{fl} , $\Delta Y_{cool|X6}$, ΔCO_{far} and ΔCO_{wall} for all cases shown in Figures 5.10 are also listed in Table 5.3. A combination of factors are observed to influence the CO emission, including the flame tip dilution, the coolant flow trajectory, and the transport of the CO pocket.

The mean CO in the far-field and most parts of the near field is the highest when $BR = 10$ at $X^+ = 6$. As can be seen in Figure 5.10, the cooling jet has an almost flat trajectory, locating closer to the wall for $BR = 10$, compared with other cases. This is also evident from the results presented in Table 5.3. Therefore, for this case, the flame tip is mostly affected by the coolant and the influence of the coolant on CO oxidation in the far field is limited. Note that the flatter coolant trajectory observed at $BR = 10$ can be due to the Coandă effect, the flow tends to stay closer to the surface for higher jet flow rates due to formation of a low pressure zone in that

region [66]. The Strouhal number appears to have a negligible impact on CO . As the cooling hole position is moved further downstream, an increase in the far-field Y_{CO} is observed while an opposite trend is observed for the near-wall CO . This is because when the cooling hole is further downstream, the cooling air has less influence on the far-field CO indicated by a high value of $\Delta Y_{cool|X6}$ (see Table 5.3) but leads to further decrease in the near-wall CO . For the cooling holes at upstream locations, the cooling jet has a larger zone of influence, producing less CO in the far field. On the other hand, a longer flame is present in the vicinity of the wall and the near-wall CO will be higher for this case. Using nitrogen as the coolant leads to a higher CO compared with when air is used. This is consistent with the observation by Rivera et al. [39] where providing the additional oxygen results in further oxidation of CO .

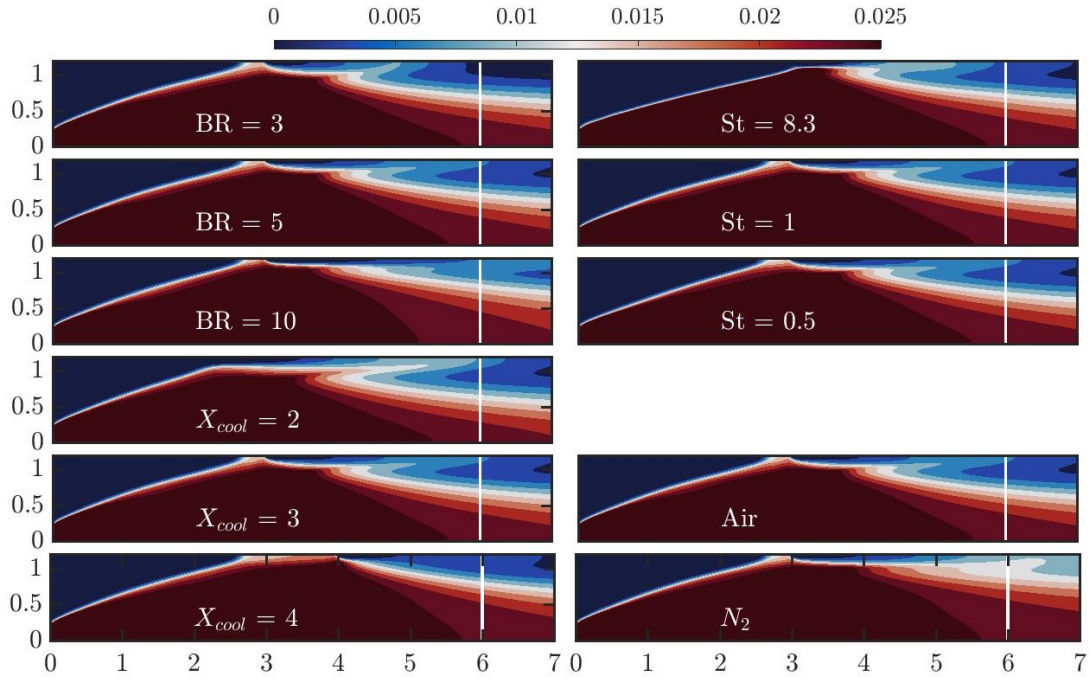


Figure 5.10: Contours of time-averaged CO mass fraction for different blowing ratios (BR), Strouhal numbers (St), cooling hole positions (X_{cool}) and coolant fluid (air/ N_2). The white line marks the $X^+ = 6$ location.

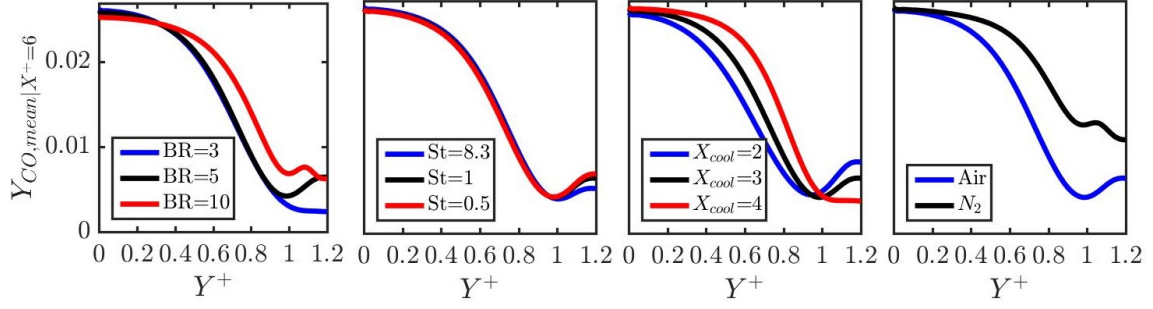


Figure 5.11: The effect of BR , St , X_{cool} and the coolant type (air/ N_2) on time-averaged CO mass fraction at a streamwise location near the exhaust ($X^+ = 6$).

The effects of BR , St , X_{cool} and the coolant type on CO at the exit of the domain, averaged in the wall-normal direction and in time, denoted as $Y_{CO,mean,exit}$, are presented in Table 5.4 for the cases shown in Figure 5.11. A similar qualitative behaviour as that in the far-field region shown in Figure 5.11 is observed here. For instance, Table 5.4 confirms that the exhaust CO decreases due to excess oxygenation as the N_2 -cooled case produces higher exit CO than the air-cooled case. Also, both an increase in BR and the downstream movement of the cooling hole increases the exhaust CO while the effect of St is negligible.

Table 5.4: Mean Y_{CO} at the exit of the domain, averaged in the wall-normal direction and in time ($Y_{CO,mean,exit}$).

Case	BR	St	X_{cool}	Coolant	$Y_{CO,mean,exit}$
2	5	8.3	3	Air	0.0106
4	3	1	3	Air	0.0103
5	5	1	3	Air	0.0105
6	10	1	3	Air	0.013
8	5	0.5	3	Air	0.0105
10	5	1	2	Air	0.0097
11	5	1	4	Air	0.0116
12	5	1	3	N_2	0.0163

The results for CO and wall heat flux lead to some interesting conclusions for the optimum values of BR and the cooling hole location. An increase in the blowing ratio can decrease the mean wall heat flux, but can also increase the exhaust CO , as seen in the $BR = 10$ case. For the cooling hole position, the most upstream location provides a better performance both in terms of the wall heat flux and exhaust CO .

These conclusions certainly need further examination in a more realistic configuration but they still provide suggestions for the expected trends of the wall heat flux and CO emission when BR and the cooling hole position are changed.

5.3.5 CO transport budget analysis

The species transport budget analysis, i.e. CDR analysis (Equation 4.3.2), for CO was carried out to investigate the transport of the pocket of CO towards the wall, observed in Figure 5.9 for the baseline case. Figure 5.12 shows the normalised convection (C), diffusion (D) and reaction (R) terms of the species transport budget analysis in the near-wall, post-cooling hole region at several instants, same as those in Figure 5.4. A positive (negative) value of C , D or R indicates an increase (decrease) in CO mass fraction due to convection, diffusion or reaction, respectively. Selected isolines of CO mass fraction are shown in Figure 5.12 such that the pocket of CO observed earlier can be visualised. Contours of C and D in the streamwise (C_x and D_x) and wall-normal (C_y and D_y) directions are shown in Figures 5.13 and 5.14, respectively.

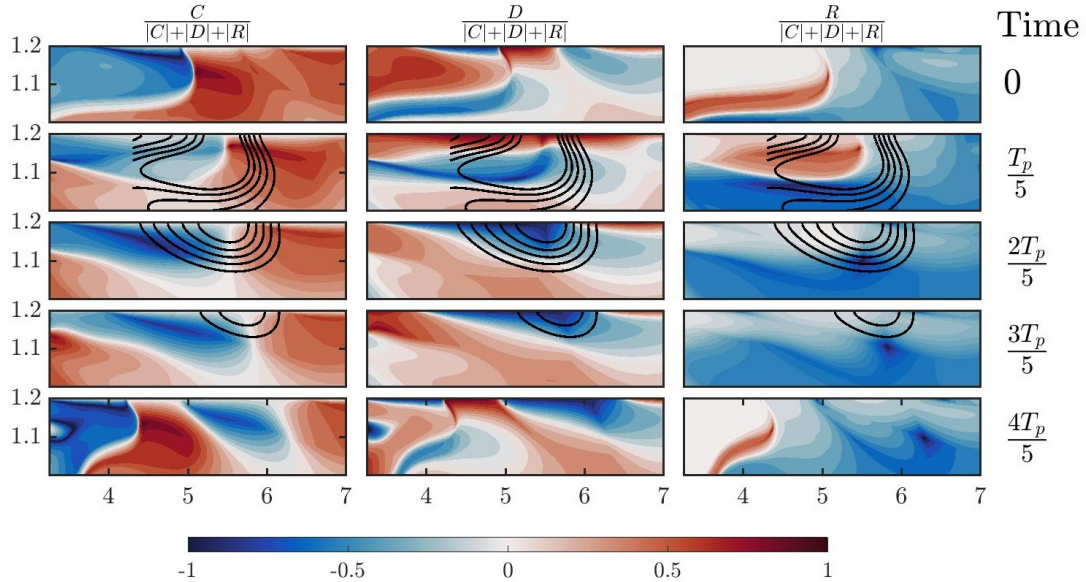


Figure 5.12: Contours of CO transport phenomena, namely, convection (C), diffusion (D) and reaction (R), normalised by the sum of absolute values of C , D , and R are shown for the baseline case at five equally spaced instants. The window considered is $X^+ \geq 3$ and $Y^+ \geq 1$. The contour lines of CO mass fraction are shown (black lines) to locate the CO pocket diffusing towards the wall. Aspect ratio is not preserved in this figure as the contours are stretched in Y^+ direction for better readability.

In general, convection is dominant in the streamwise direction and diffusion is dominant in the wall-normal direction. At the locations where the CO pocket is observed, the diffusion term is dominant at $t = T_p/5$, indicating the diffusion of CO pocket towards the wall. In the following instants, the diffusion term becomes negative at the location of the pocket, showing that CO is now diffusing away from the wall. This coincides with the reduction in concentration of the CO pocket, as observed in Figure 5.9. In general, the dominant mechanism of transport for the CO pocket is diffusion.

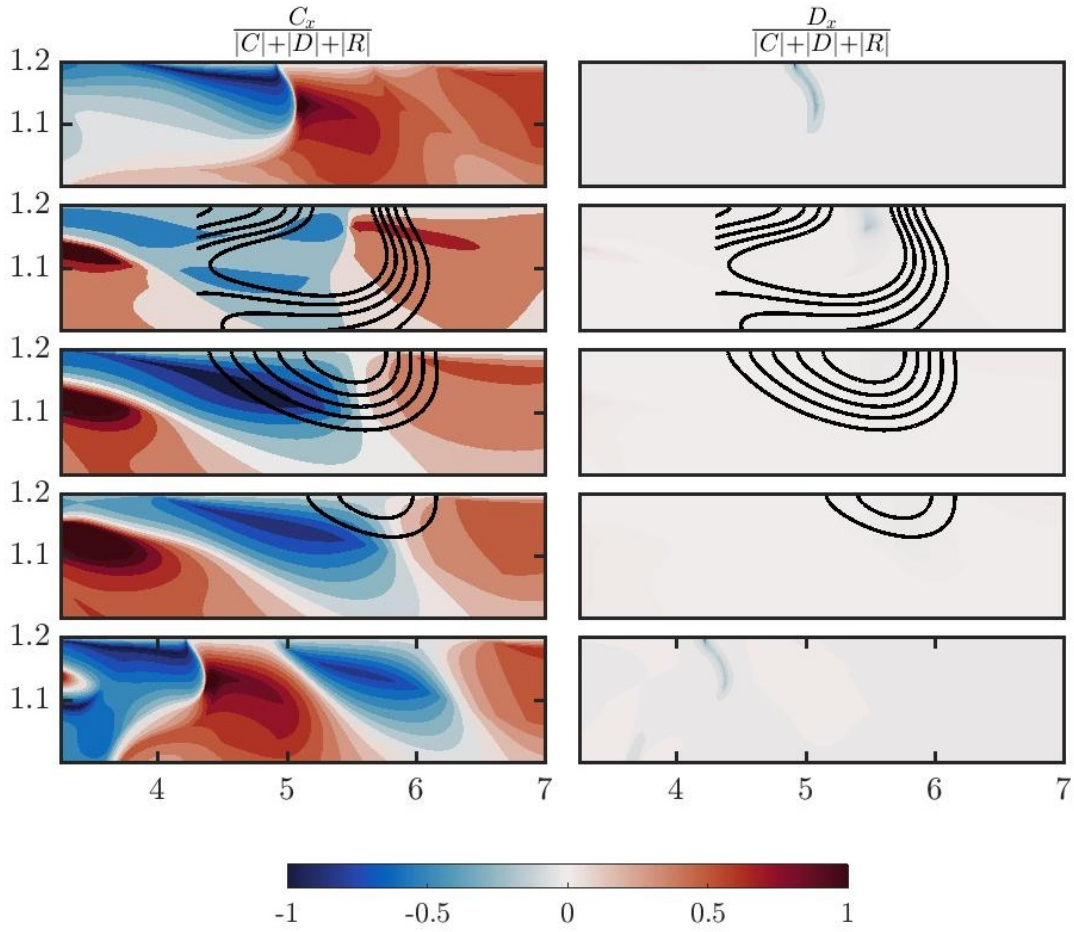


Figure 5.13: Streamwise components of convection (C) and diffusion (D), normalised by the sum of absolute values of C , D , and R are shown for the baseline case at five equally spaced instants. The window considered is $X^+ \geq 3$ and $Y^+ \geq 1$. The contour lines of CO mass fraction are shown (black lines) to locate the CO pocket diffusing towards the wall. Aspect ratio is not preserved in this figure as the contours are stretched in Y^+ direction for better readability.

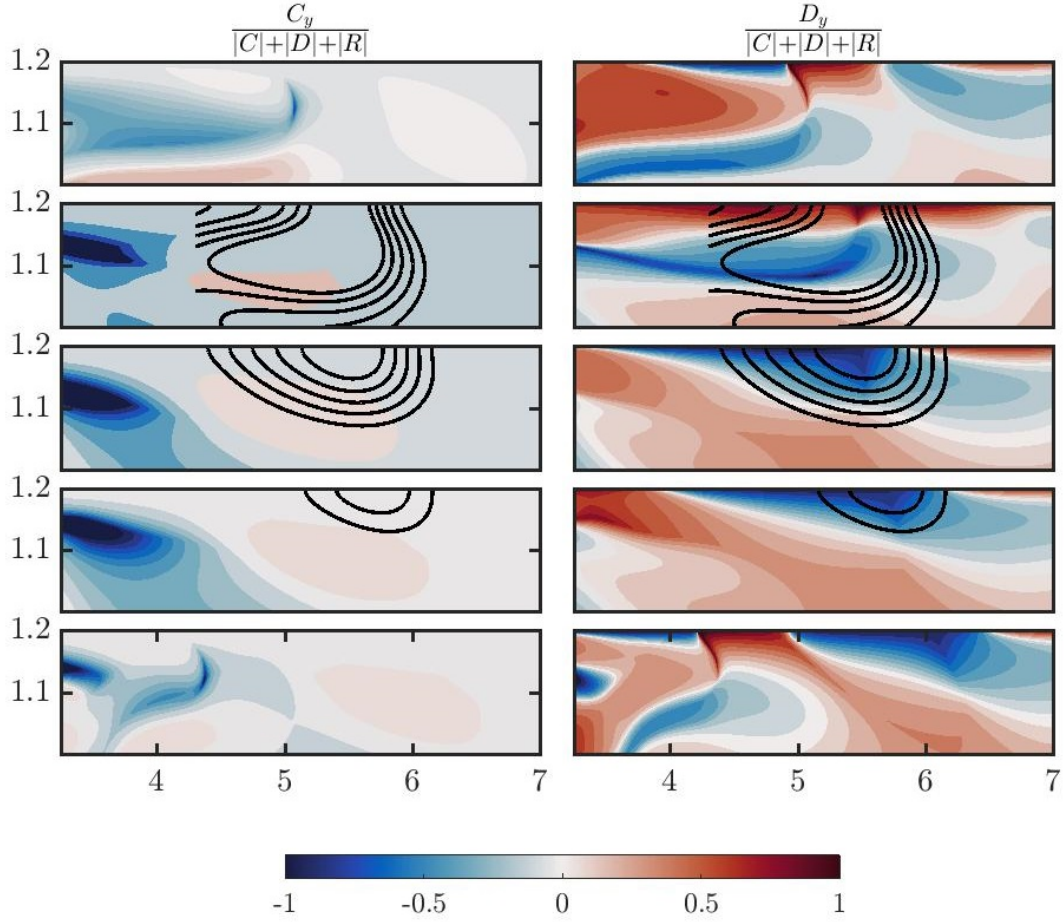


Figure 5.14: Wall-normal components of convection (C) and diffusion (D), normalised by the sum of absolute values of C , D , and R are shown for the baseline case at five equally spaced instants. The window considered is $X^+ \geq 3$ and $Y^+ \geq 1$. The contour lines of CO mass fraction are shown (black lines) to locate the CO pocket diffusing towards the wall. Aspect ratio is not preserved in this figure as the contours are stretched in Y^+ direction for better readability.

5.3.6 CO thermochemical states

Further analysis of the near-wall CO mass fraction in the wall-cooled region from $X^+ \geq 3$, $Y^+ \geq 1$ is shown in Figure 5.15. Scatter plots of Y_{CO} versus temperature at all instants in a forcing cycle are shown for the baseline case. To examine the role of dilution with excess oxygen, the scatter plots are coloured based on ξ . The Y_{CO} - T plots of 1D FPFs with the same chemical mechanism as that used in the DNS (GRI 3.0, see Section 3.6) for equivalence ratios $\phi = 0.24$ to 1 are also shown. It can be seen that on average, the 1D FPFs can capture the temperature dependence of Y_{CO} in the near-wall, post-cooling hole region. The Y_{CO} - T scatter plots are coloured by $R/|R|$ in Figure 5.16 to identify the CO production and CO

oxidation branches. A positive reaction rate indicates the production of CO while a negative value of reaction rate indicates CO oxidation. To further analyse the above-mentioned temperature dependence of Y_{CO} , representative bands of ξ are shown in Figure 5.17. The scatter plot of the case with no cooling hole is also shown here in the background. Once again, it can be seen that FCAI cases can be potentially modelled with FPF solutions. A horizontal branch of Y_{CO} is present for $\xi = 0.4 - 0.45$ which can not be captured with the FPF solution. Also, a small discrepancy is observed in the production branch of CO of this range of ξ . For small values of ξ , CO is outside the region of corresponding FPFs in the production branch. The reason for this discrepancy will be investigated with chemical reaction network modelling later in this section.

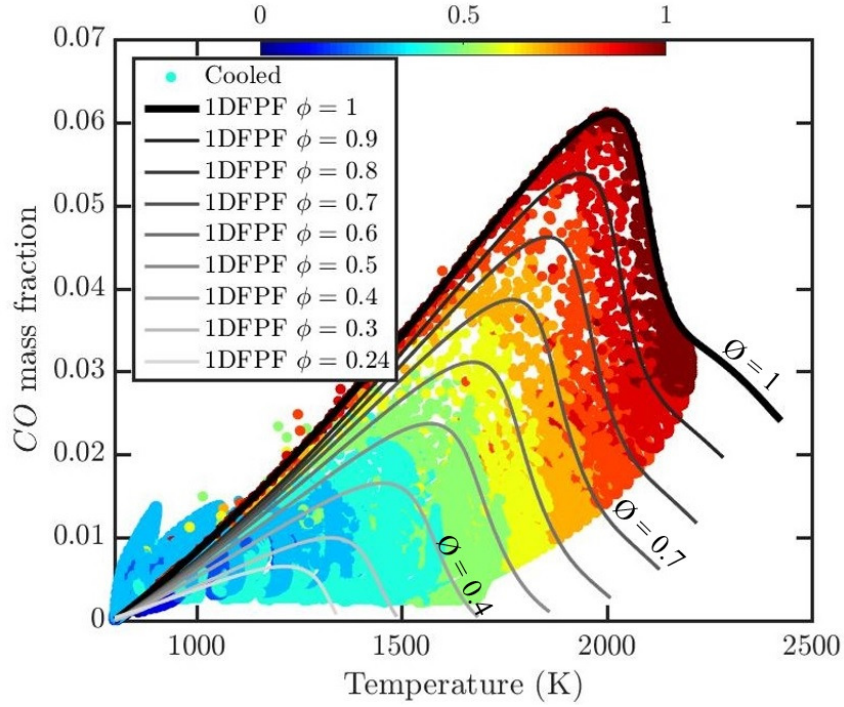


Figure 5.15: Scatter plots of CO mass fraction (Y_{CO}) against temperature (in K) for Case 5 coloured by ξ . Only the points in the near-wall, post-cooling hole window ($X^+ \geq 3$, $Y^+ \geq 1$) are considered for this analysis. 1D FPF results for several equivalence ratios are shown.

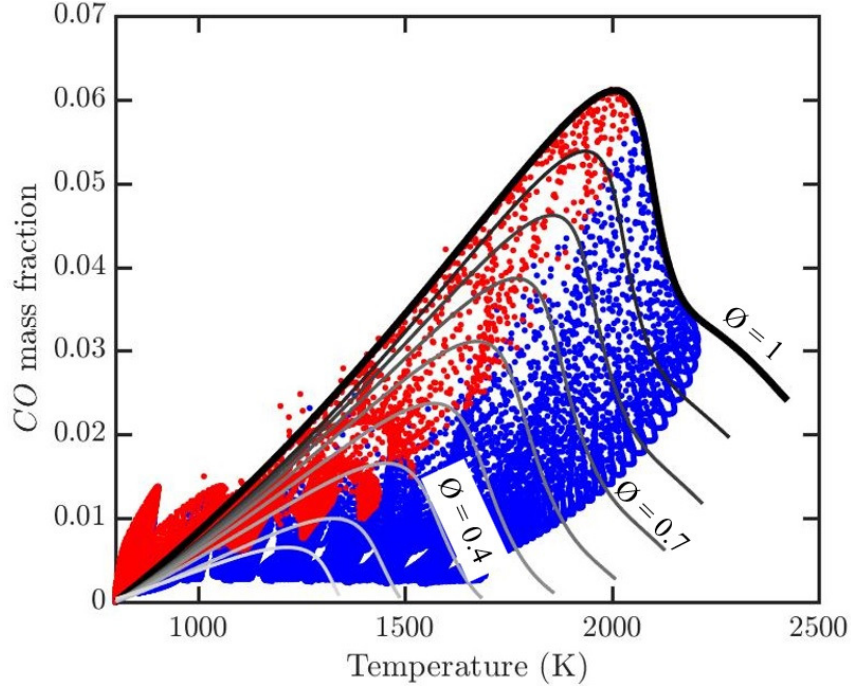


Figure 5.16: Scatter plots of CO mass fraction (Y_{CO}) against temperature (in K) for Case 5 in the window: $X^+ \geq 3$, $Y^+ \geq 1$, coloured by $R/|R|$ where R is the reaction rate term in the species transport budget analysis for CO . Red dots indicate a positive reaction rate term while the negative values are shown in blue. 1D FPF results for the same equivalence ratios as in Figure 5.15 are also shown.

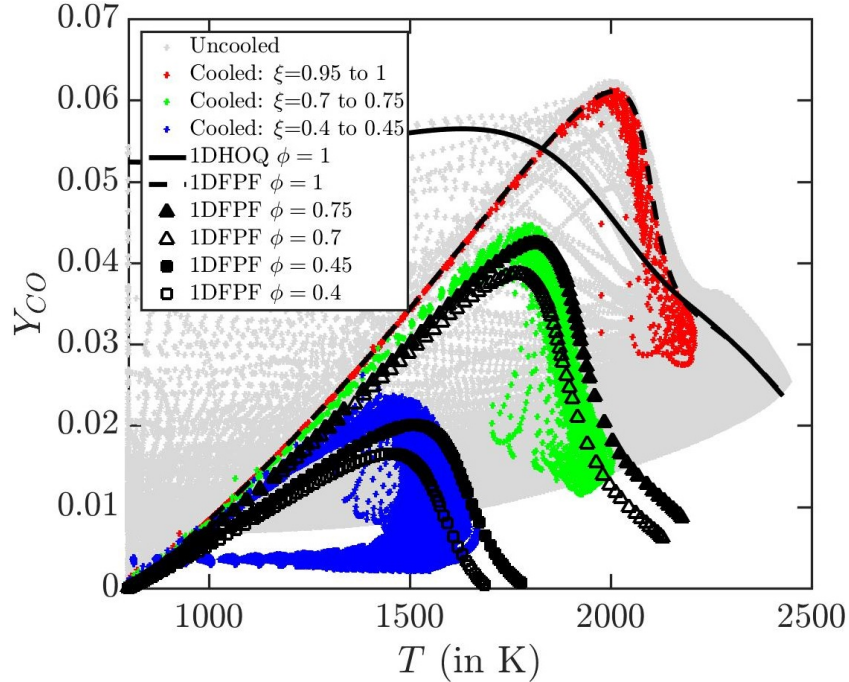


Figure 5.17: Scatter plots of CO mass fraction (Y_{CO}) against temperature (in K) for several bands of ξ for Case 5, in the near-wall, post-cooling hole window ($X^+ \geq 3$, $Y^+ \geq 1$). Relevant 1D HOQ and FPF results and the $Y_{CO} - T$ scatter plots for uncooled case are also shown.

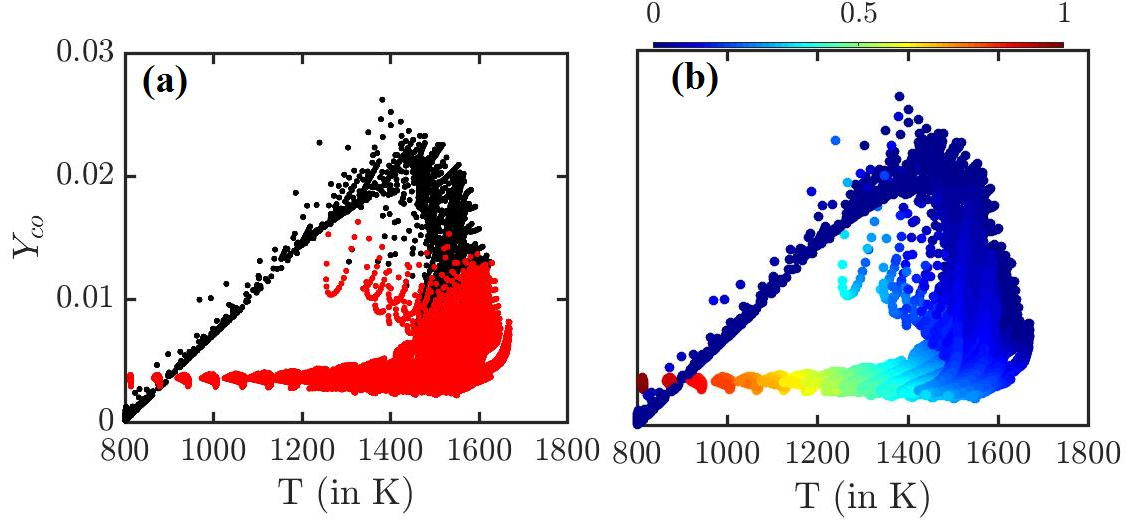


Figure 5.18: Y_{CO} - T scatter plots for Case 5 in the window: $X^+ \geq 3$, $Y^+ \geq 1$, for $\xi = 0.4 - 0.45$. The red dots in (a) indicate $c_{CO_2} > c'$. Subfigure (b) is coloured by normalised enthalpy deficiency.

To further investigate the approximately constant Y_{CO} as a function of temperature for $\xi = 0.4 - 0.45$, Figure 5.18 shows the scatter plot of Y_{CO} against temperature in the same near-wall, post-cooling hole window as shown in Figure 5.15. A threshold value of c_{CO_2} , denoted by c' identified earlier in Section 5.3.1 is used here. The points where $c_{CO_2} > c'$, shown in red in Figure 5.18(a), identifies this low Y_{CO} branch. Further inspection of these points show that this CO branch is located in the burnt gas region (about $X^+ > 5$), and is close to the wall (about $Y^+ > 1$). Also, since this region is away from the cooling hole ($X_{cool} = 3$) the effect of the coolant stream is likely to be less, possibly leading to a higher wall heat loss. To confirm this hypothesis, the points in Figure 5.18(b) are coloured by the normalised enthalpy deficiency ($h_{def,norm}$). Now, this CO branch can also be identified with high values of the normalised enthalpy deficiency. Although this indicates that the wall heat loss is important in predicting the near-wall CO due to FCAI, one should note that in a realistic effusion cooled combustor, where a sheet of coolant is expected to be formed near the wall, such a region of high wall heat loss is unlikely to be present.

To investigate the difference between the FPF solutions and the DNS data in the CO production branch (see Figure 5.17), an ideal chemical reactor available in CHEMKIN PRO [65] is used. In the above-mentioned production branch, a sto-

stoichiometric flame interacts with a stream of cold air, mixing to varying extents which is quantified by ξ . The FPF model assumes that the time scale is sufficiently long to form a laminar flame at a given equivalence ratio. However, this assumption can break down if the relatively fast cooling jet leads to very short residence time available for the reaction of the mixture before it leaves the monitoring window ($X^+ > 3, Y^+ > 1$). For example, this can occur when the flame tip is in the vicinity of the cooling hole. To mimic these conditions, a perfectly stirred reactor (PSR) configuration is used in CHEMKIN, as shown in Figure 5.19. This 0-D model assumes that the mixture is fully mixed and is only limited by reaction kinetics [65]. Such a model provides an effective tool to isolate the impact of residence time on CO production/oxidation in a similar approach to [39].

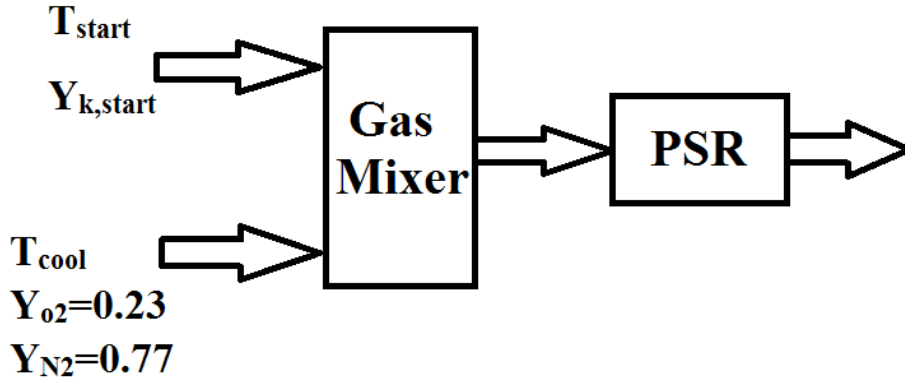


Figure 5.19: Schematic of the perfectly stirred reactor configuration.

As shown in Figure 5.19, two inlet streams are first mixed in a gas mixer and are then fed into the PSR. In the first stream, the conditions correspond to one point in the production branch of a stoichiometric 1D FPF, representing the flame before mixing with the coolant stream. This condition is referred as ‘the starting point’ in the rest of the discussion. The temperature and species mass fractions at this starting point are denoted by T_{start} and $Y_{k,start}$, respectively. Two such starting points, i.e. $T_{start} = 1796$ K and 1192 K are simulated. The second stream consists of air at the coolant inlet temperature (800 K), representing the coolant stream. A range of equivalence ratios for the mixture with two residence times t_{res} , as a factor of δ_{th}/V_{cool} where V_{cool} is the resultant coolant velocity, are considered.

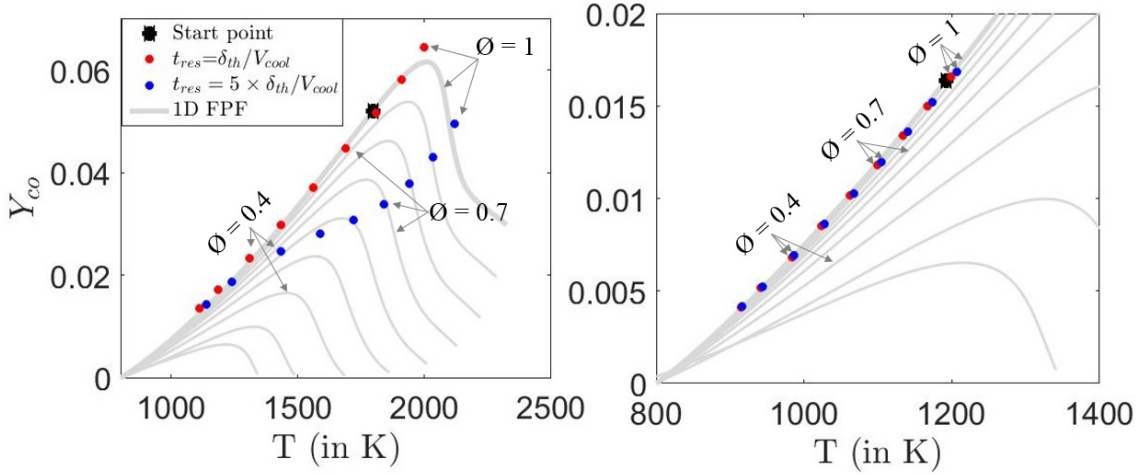


Figure 5.20: Thermochemical states of CO obtained using a PSR analysis, for two starting points, i.e. $T_{start} = 1796$ K (a) and 1192 K (b) and two residence times over a range of equivalence ratios. The starting points are marked in the plots using a black star. The 1D FPF solutions are also shown for reference

Figure 5.20(a) shows an increase in CO compared to that of the starting point when the equivalence ratio is above a certain point and the residence time is short. However, a decrease in CO is observed for lower equivalence ratios. This shows that providing additional oxygen when the temperature is still relatively high will promote production of CO whereas the opposite will occur at lower temperatures. For a longer residence time, a lower amount CO is generally present at the exit of the PSR for the high temperature starting point. However, for the lower T_{start} case shown in Figure 5.20(b), the results seem to be insensitive to the residence time for the cases considered. This is expected as the reactions are slower at lower temperatures.

These observations indicate that fast mixing of the cooling air with the stoichiometric flame front can lead to mixtures, featuring a higher amount of CO compared with the corresponding diluted flame. The inclusion of the effects of these mixing times can provide an improved modelling framework to predict CO in the production branch and is left for future work.

To summarise, the behaviour of the near-wall CO due to FCAI can be explained reasonably well using laminar flame solutions with a modified mixture fraction (ξ), particularly in the oxidation branch. This is an encouraging result, suggesting path-

ways for prediction of Y_{CO} near an effusion-cooled gas turbine wall. Considering the impact of relatively fast cooling jets on the flame tip and the heat loss to the wall on CO oxidation can lead to further improvement of this modelling approach.

5.4 Conclusions

This study examined the impact of flame-cooling air interaction (FCAI) on flame dynamics and CO emissions. Two-dimensional direct numerical simulations (DNSs) of an acoustically forced laminar flame interacting with a coolant jet issued from a relatively cold wall were performed. Cases with different blowing ratios, forcing frequencies, cooling hole positions and coolant type (air/ N_2) were considered. For $St = 1$, a long flame sheet was formed near the wall as a result of interaction with the coolant. This lean, diluted flame sheet was found to increase in length with increasing blowing ratio and with moving the cooling hole further upstream. The type of the coolant was found to have a negligible impact on the shape of this flame sheet. The annihilation of this flame sheet coincided with formation of a pocket of CO , which was then convected downstream while also diffusing towards the wall.

As expected, the mean wall heat flux in the effusion cooled cases were less than that in the uncooled case. An increase in blowing ratio, which introduces more coolant near the wall, further reduced the mean wall heat flux. In addition, a downstream shift in the cooling hole position reduced the wall heat flux. This was because the flame is further away from the wall-cooled region as the cooling hole moves downstream.

An analysis of the time-averaged CO mass fraction downstream of the cooling hole showed a negligible impact by the forcing frequency. Using air instead of nitrogen as the coolant reduced the CO emission by providing additional oxygen and therefore enhancing CO oxidation, as also shown in previous work [39]. Increasing the blowing ratio led to an increase of the CO emission away from the wall. This was attributed to the cooling air trajectory and the influence of the cooling jet on the overall flame dynamics. A similar effect was observed with a downstream movement of the cooling hole. Furthermore, the qualitative trend of the near-wall CO was attributed to the

CO pocket formed downstream of the cooling hole.

CO emission in the near-wall, post-cooling hole region was found to be a function of local temperature and a modified mixture fraction when a progress variable defined based on the CO_2 mass fraction is below a certain threshold. One-dimensional (1D) freely-propagating flame simulations with corresponding equivalence ratios to the level of dilution were found to reasonably describe the *CO* characteristics.

Chapter 6

Turbulent FWI and FCAI

6.1 Introduction

This chapter aims to extend flame-wall interaction (FWI) and flame-cooling air interaction (FCAI) studies undertaken in Chapters 4 and 5, respectively, to more realistic turbulent conditions. Three-dimensional (3D) direct numerical simulation (DNS) of a preheated, turbulent, premixed, methane/air flame is performed. The top wall is effusion cooled by injecting cooling air jets to simulate FCAI conditions while the bottom wall is uncooled, representing FWI conditions. The flame features and the effect of the flow-field on the flame and wall heat flux are discussed. The thermochemical states of CO are then examined, a CO modelling framework is proposed and evaluated using the DNS data.

This chapter is structured as follows. Section 6.2 outlines the major simulation parameters relevant to this chapter. The key flame features and their impact on the flow field are discussed in Section 6.3.1 whereas the results for the wall heat flux are presented in Section 6.3.2. The CO characteristics are explored in Section 6.3.3 and a CO model is proposed which is evaluated using the DNS data in Section 6.3.4.

6.2 Simulation parameters

This chapter studies a stoichiometric ($\phi = 1$), preheated ($T_u = 800$ K), premixed flame under turbulent flow conditions (inlet Mach number = 0.15 which corresponds to a jet Reynolds number of 3200). To remind the reader, a schematic of the computational domain of size $L_x^+ \times L_y^+ \times L_z^+ = 15 \times 2 \times 3$ is shown in Figure 6.1. The flame is anchored using a hot sheet imposed at $X^+ = 1$ from $Y^+ = 0.5$ to 1.5, as described in Section 3.5.4. Cooling air is fed through the top wall at several streamwise locations ($X^+ = 5, 6.5, 8, 9.5, 11, 12.5$ and 14) through slots of width 0.2, imposing unity blowing ratio. The simulations were run for four jet flow through times and the data of the last two flow through times were considered for the analysis.

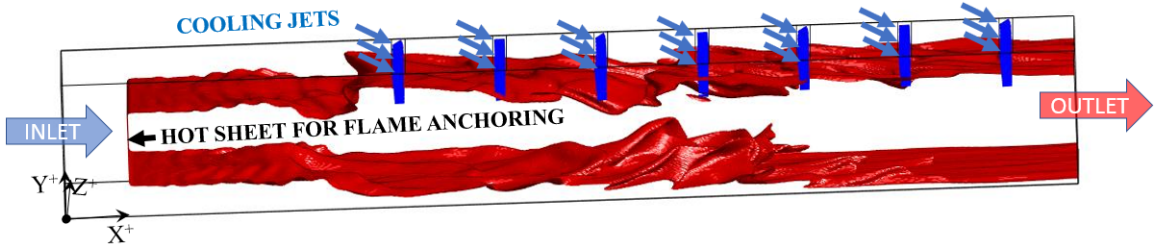


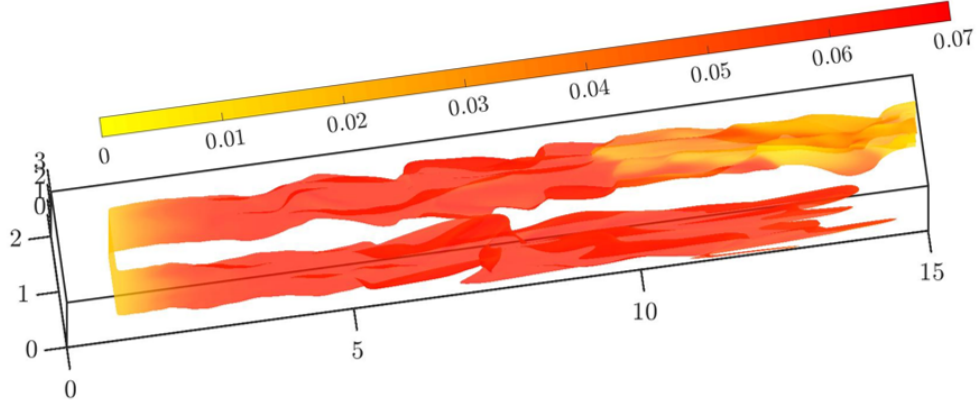
Figure 6.1: Computational domain.

6.3 Results and discussion

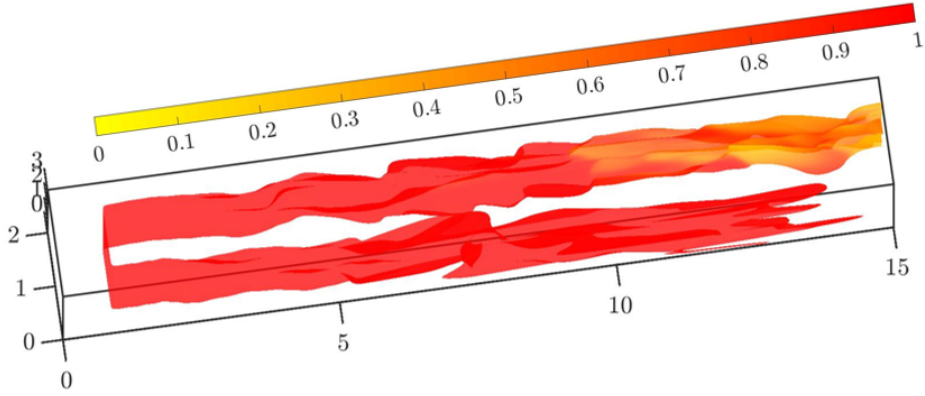
6.3.1 Flame dynamics

To visualise the flame, isosurfaces of the progress variable based on CO_2 mass fraction (see Section 5.2.1.2), $c_{co_2} = 0.5$, are presented in Figure 6.2 at one instant, coloured by Y_{CO} and ξ . Interaction of the flame with an uncooled wall, i.e. flame-wall interaction (FWI) occurs at the bottom wall while the flame interacts with the jets of cooling air at the top wall, representing flame-cooling air interaction (FCAI). Compared to the bottom wall, a region with less CO near the top wall closer to the exit of the domain is observed. This region corresponds to higher levels of dilution with the cooling air, as indicated by the lower values of ξ (see Figure 6.2(b)). Also, the flame appears to be longer near the effusion-cooled top wall unlike the bottom

wall where the flame seems to be quenched earlier. The reduction of CO emissions due to effusion cooling was also observed in the 2D laminar FCAI configuration (see Figure 5.17).



(a) Coloured by Y_{CO} .



(b) Coloured by ξ .

Figure 6.2: Isosurface of progress variable at $c_{co_2} = 0.5$ coloured by Y_{CO} and ξ at one instant.

The contours of c_{co_2} , heat release rate (HRR) and CO mass fraction (Y_{CO}) at one spanwise location, $Z^+ = 1.2$, for several instants are shown in Figures 6.3 to 6.5. As observed in Figure 6.2, the flame is longer near the top wall compared to the bottom wall, at all the instants. The regions where both HRR and Y_{CO} are low are observed downstream of the domain near the top wall. To confirm if this behaviour is limited to the chosen spanwise location and instants, the spanwise and time average of these parameters are shown in Figures 6.6 and 6.7.

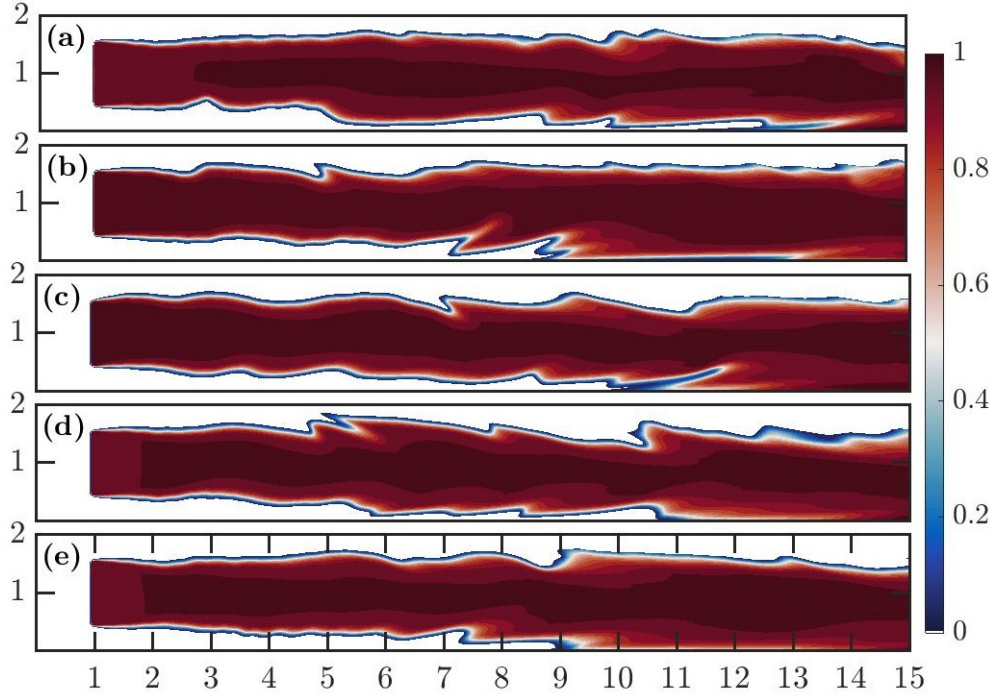


Figure 6.3: Contours of progress variable at several instants (shown as (a) to (e)) at one spanwise location, $Z^+ = 1.2$.

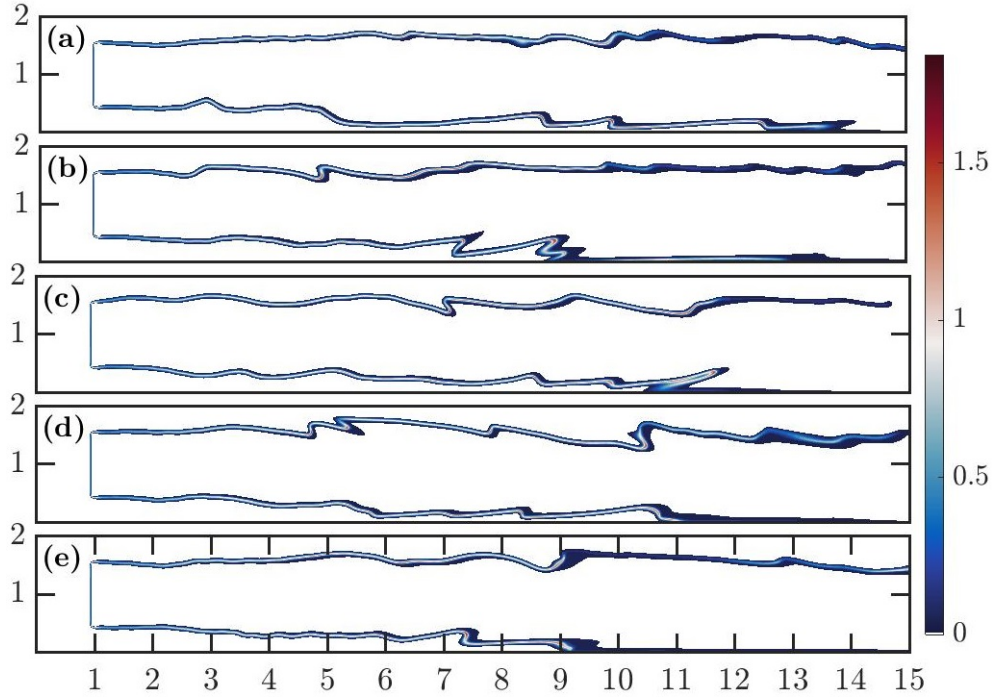


Figure 6.4: Contours of HRR normalised by the peak HRR in a 1D HOQ configuration at $Z^+ = 1.2$. Subfigures (a) to (e) show different instants.

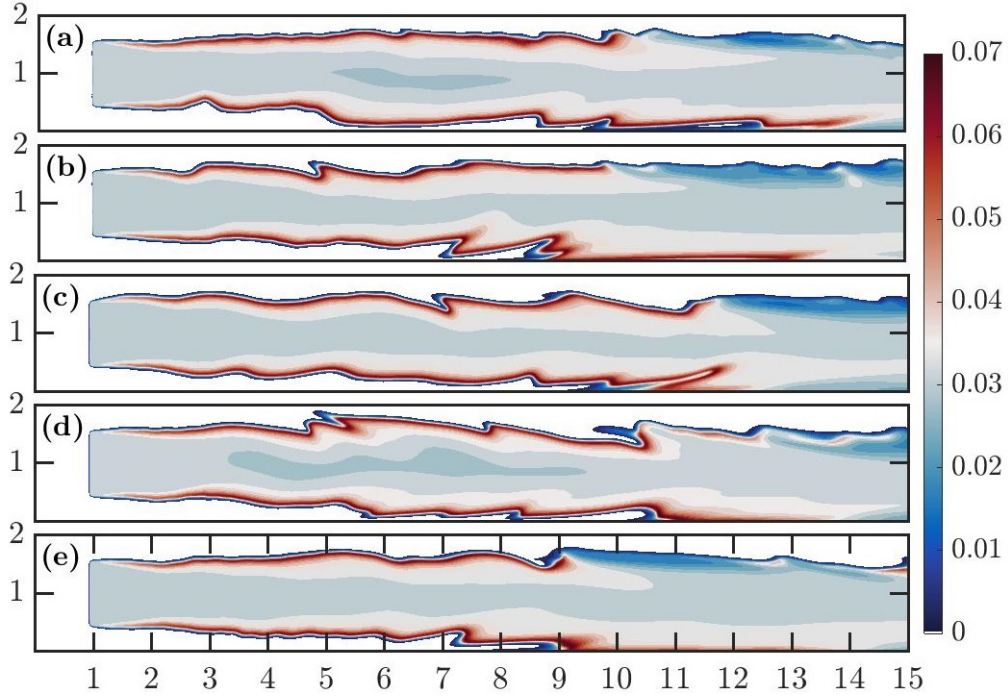


Figure 6.5: Contours of Y_{CO} at $Z^+ = 1.2$ at several instants.

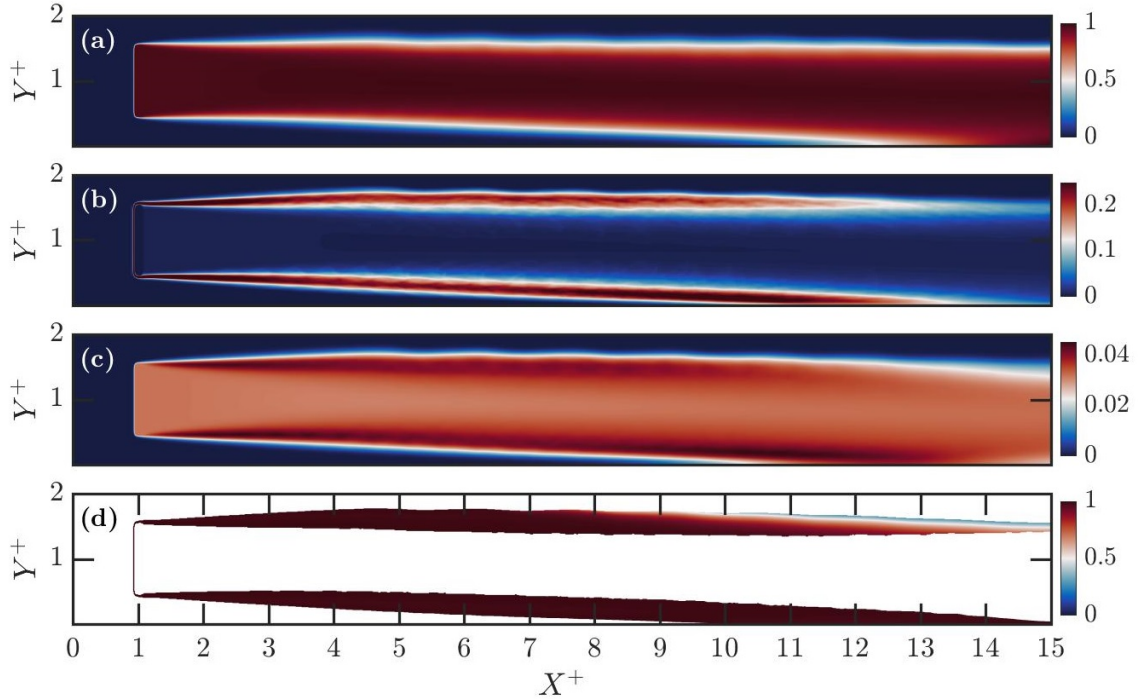


Figure 6.6: Contours of the following variables: (a) progress variable, (b) HRR , (c) Y_{CO} and (d) modified mixture fraction (ξ), averaged in the spanwise direction and in time. In (d), the contour plot is clipped to include only the region where $\overline{HRR}$ is more than 5% of the maximum $\overline{HRR}$.

Figure 6.6 shows several parameters averaged in the spanwise direction (Z^+) and in

time. The parameters averaged in the spanwise direction and time are denoted as $\overline{(\cdot)}$. Longer regions of relatively low $\overline{HRR}$ seen near the top wall for $X^+ > 10$ (see Figure 6.6(b)) coincide with the region of lower $\overline{Y_{CO}}$ (see Figure 6.6(c)) and lower ξ (see Figure 6.6(d)). Mixing with cooling air reduces $\overline{Y_{CO}}$ and this diluted flame features a lower $\overline{HRR}$. This is once again consistent with the observations from Chapter 5 (see Figures 5.5 and 5.17).

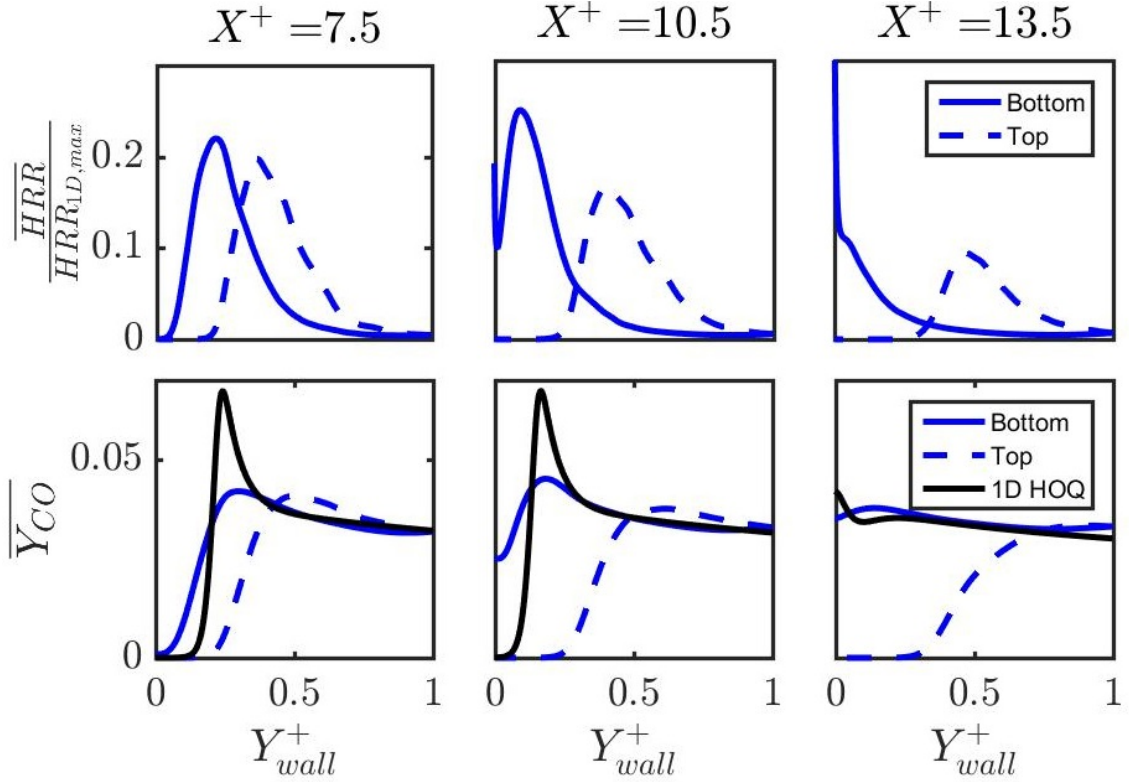


Figure 6.7: $\overline{HRR}$ and $\overline{Y_{CO}}$ at several streamwise locations versus non-dimensional distance from the wall (Y_{wall}^+). The top ($Y^+ \geq 1$) and bottom ($Y^+ < 1$) halves of the domain are indicated with dashed and solid blue lines, respectively. The $\overline{Y_{CO}}$ obtained from 1D HOQ simulation using SK mechanism is shown in black.

The variables $\overline{HRR}$ and $\overline{Y_{CO}}$ at three streamwise locations, $X^+ = 7.5, 10.5$ and 13.5 , are shown in Figure 6.7. The top ($Y^+ \geq 1$) and bottom ($Y^+ < 1$) halves of the domain are considered separately. The results are presented as a function of the non-dimensional, wall-normal distance from each wall (Y_{wall}^+). The $\overline{Y_{CO}}$ profiles from the 1D HOQ solutions obtained using the same premixture temperature (800 K) and pressure (1 atm) as the turbulent case are also presented in Figure 6.7 for several instants before and during quenching. The $\overline{Y_{CO}}$ profiles spread over a wider region of Y_{wall}^+ compared to the $\overline{Y_{CO}}$ profiles from the 1D HOQ results. This is expected as

a thicker average flame brush is present in a turbulent flame. However, the profiles of $\overline{HRR}$ and $\overline{Y_{CO}}$ near the bottom wall resemble those of 1D HOQ. The heat-release rate profiles near the top wall is qualitatively similar to that of a freely-propagating flame. As discussed earlier, the peak $\overline{HRR}$ and $\overline{Y_{CO}}$ near the top wall is less than that near the bottom wall and decreases further downstream. From $X^+ = 7.5$ to 13.5 the peak $\overline{HRR}$ and $\overline{Y_{CO}}$ decrease by about 50 % and 20 %, respectively.

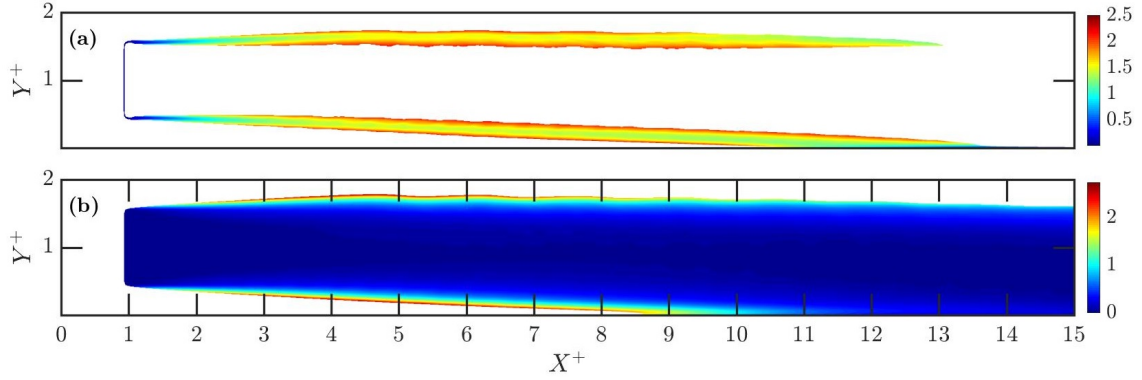


Figure 6.8: RMS HRR and Y_{CO} in the spanwise direction. These variables are also averaged in time and are normalised by $\overline{HRR}$ and $\overline{Y_{CO}}$. Only the points greater than $0.05 \times \overline{HRR}_{max}$ and $0.05 \times \overline{Y_{CO}_{max}}$, respectively, are shown.

The RMS values of HRR and Y_{CO} are shown in Figure 6.8, normalised by their local mean values. The points where the mean HRR and Y_{CO} are below 5% of their maximum values are not included. This is to ensure that the presented values are not unrealistically magnified due to normalisation by a low mean value. Figure 6.8 shows that downstream of the hot sheet ($X^+ = 1$), fluctuations of HRR and Y_{CO} increase initially which is likely due to the enhanced flame-turbulence interaction. Fluctuations of HRR and Y_{CO} decrease further downstream from about $X^+ > 10$, near the top wall. From Figure 6.6(d), this corresponds to the region where flame-cooling air mixing is stronger, indicated by regions of low values of $\bar{\xi}$. Thus, one may infer that the interaction of the flame with the sheet of cooling air is likely to reduce the fluctuations of the flame surface and Y_{CO} in the vicinity of the wall.

Figure 6.9 shows contours of vorticity magnitude at several instants at one spanwise location ($Z^+ = 1.2$). The flame is represented by an isoline of progress variable ($c_{co_2} = 0.5$). The flame features marked as B1, B2 and C1, causes the fresh gas to move away from the wall. They appear in regions with high vorticity values. Further

investigation of the evolution of such structures is discussed in Figure 6.10.

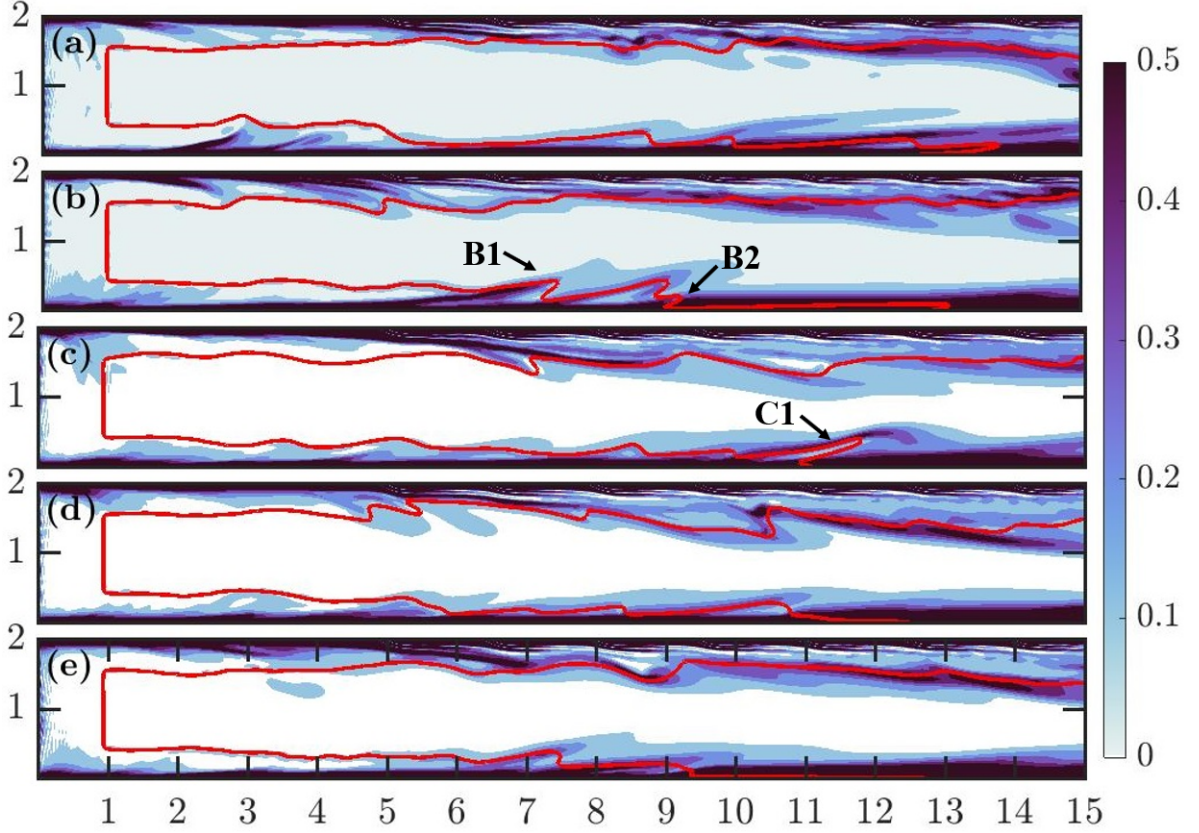


Figure 6.9: Contour plots of the magnitude of vorticity (non-dimensional) for several instants at $Z^+ = 1.2$. The flame position ($c_{co_2} = 0.5$) is marked in red. Certain structures, i.e. B1, B2 and C1, are marked for further discussion.

Figure 6.10 shows isosurfaces of progress variable ($c_{co_2} = 0.5$) at several instants between the snapshots shown in Figure 6.9(b) and 6.9(c). The time evolution of the structure B1 (see Figure 6.9) is illustrated, marked using black circles. From Figure 6.10(a) to 6.10(d), B1 becomes C1 which is a streak like feature marked in Figure 6.9. These “finger-like structures” have been observed in other DNS studies of FWI with simple chemistry [42]. They eventually collapse at the wall as they move further downstream and can subsequently influence the near-wall CO transport and wall heat flux.

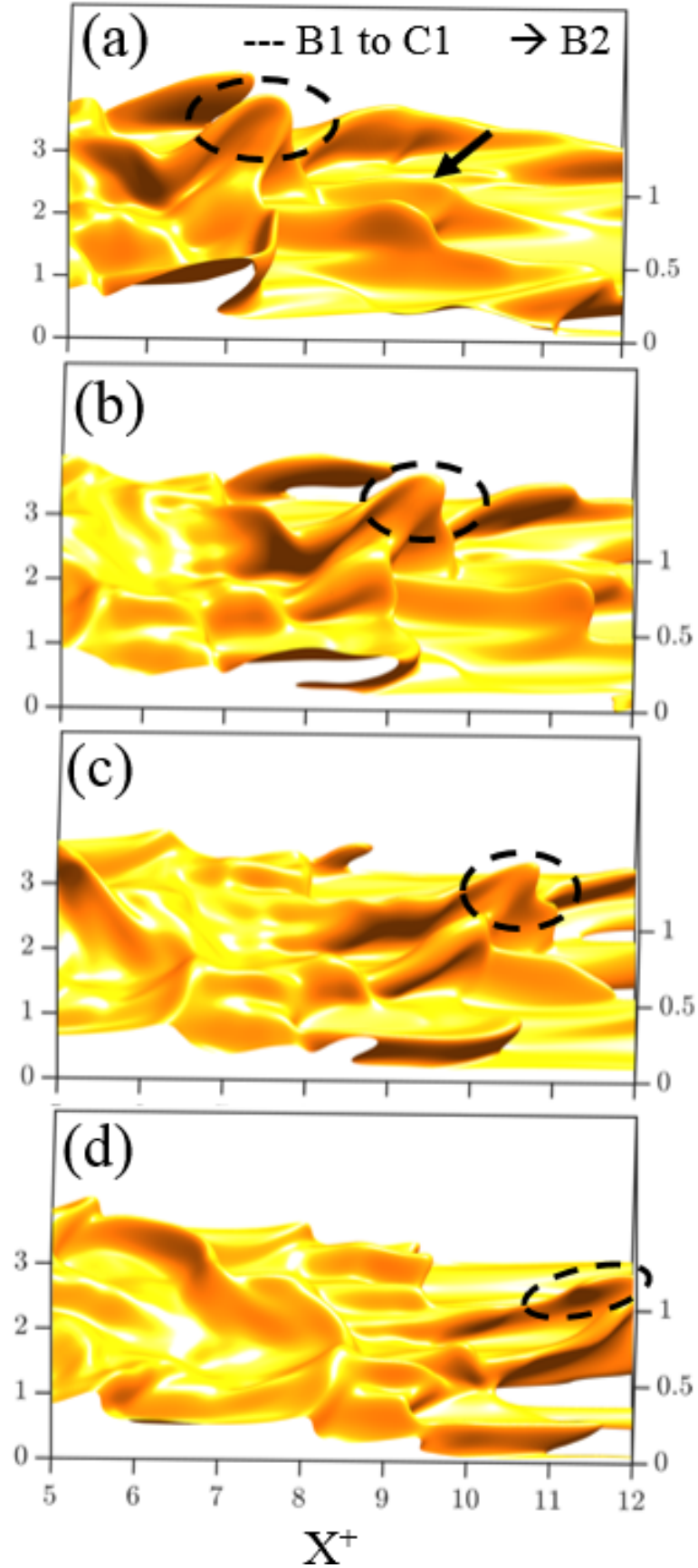


Figure 6.10: Time evolution of flame structures shown using $c_{co_2} = 0.5$ isosurfaces. The figure is stretched in Y^+ direction.

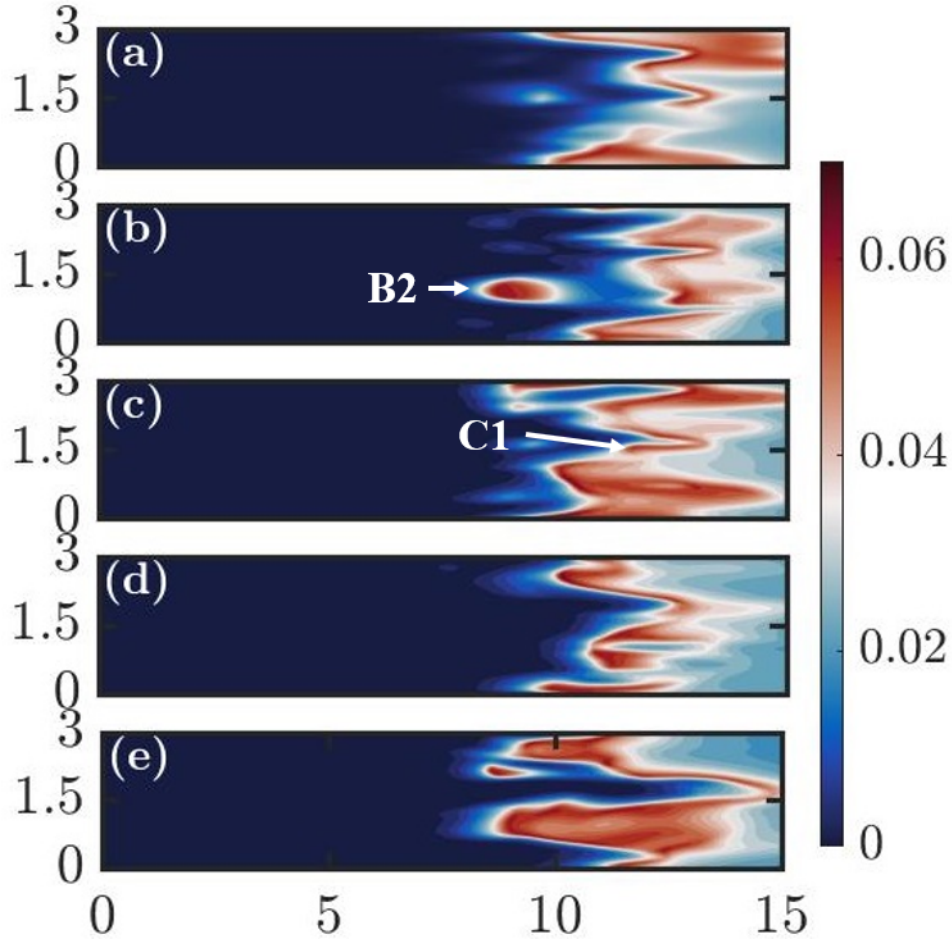


Figure 6.11: Contours of Y_{CO} at the bottom wall at several instants. Regions of interest (B2 and C1) are marked to show the effect of flame structures on CO at the wall.

Figure 6.11 shows snapshots of Y_{CO} at the bottom wall at several instants. The locations corresponding to the flame structures identified earlier are marked. These locations are where the flame structures interact with the wall, leading to high CO emissions. Also, as discussed earlier, such near-wall flame structures are also expected to influence the wall heat flux which is further discussed in Section 6.3.2.

6.3.2 Wall heat flux due to FWI

The wall heat flux to the top wall is found negligible due to the effect of cooling air which forms a protective sheet between the flame and the wall. Compared to the bottom wall, the wall heat flux to the top wall is an order of magnitude less and hence is not discussed in this section.

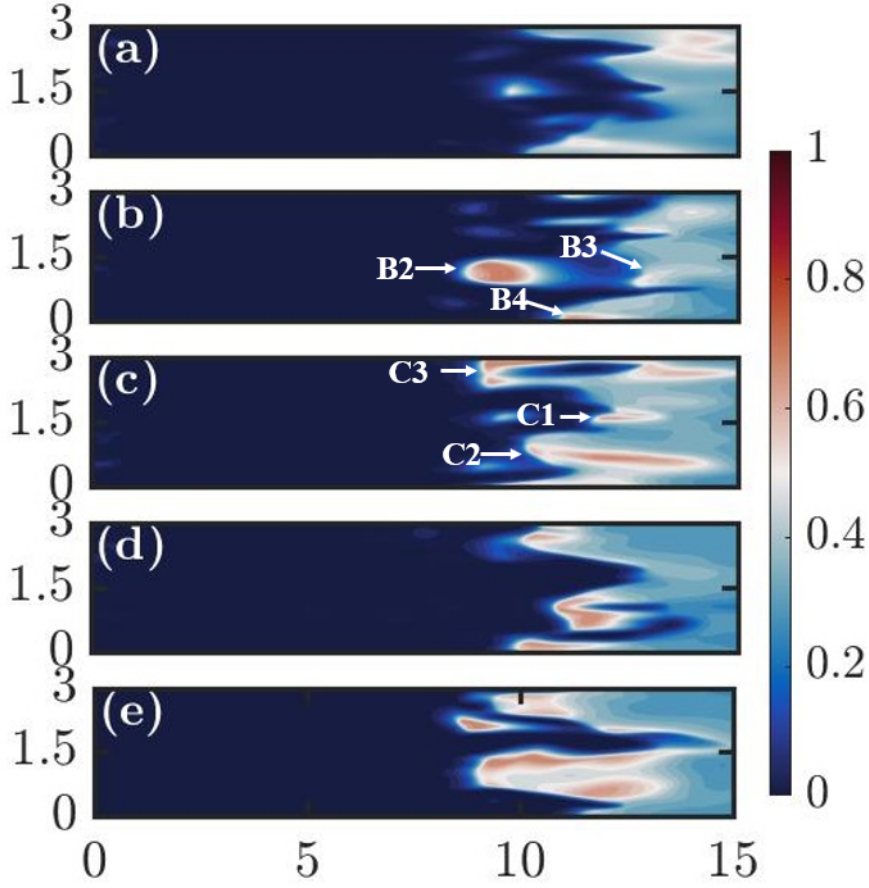
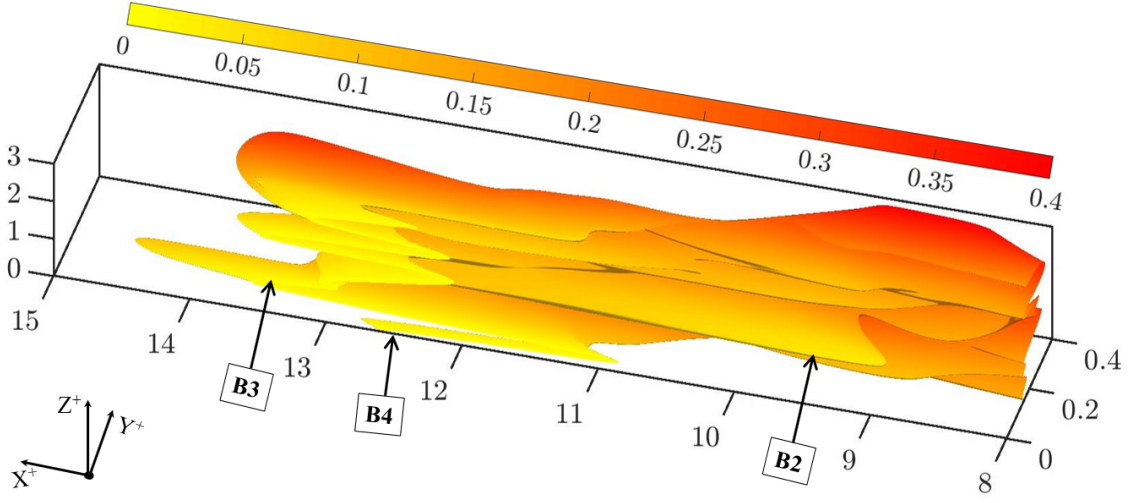


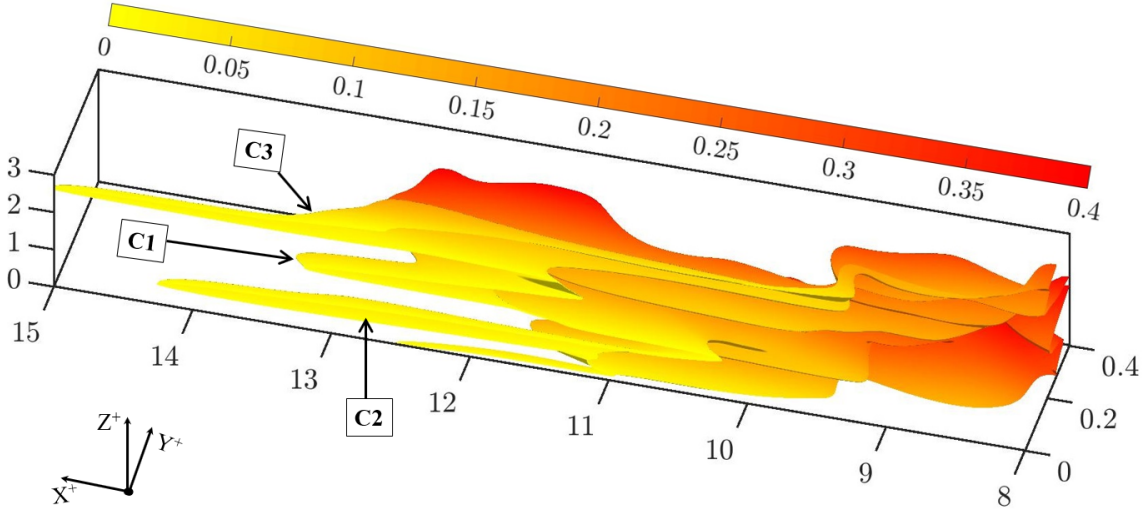
Figure 6.12: Wall heat flux (ϕ_{wall}) to the bottom wall at several instants, normalised by the peak ϕ_{wall} when a 2D laminar steady-state flame interacted with a non-effusion wall. Some regions of interest (B2 - B4, C1 - C3) are marked for discussion. The $X^+ - Z^+$ plane shown here is the bottom wall.

Figure 6.12 shows snapshots of the wall heat flux (ϕ_{wall}) to the bottom wall at several instants, normalised by the peak ϕ_{wall} in a 2D laminar steady-state configuration. Regions of high ϕ_{wall} are observed at the wall beyond $X^+ = 9$. This is expected as the flame approaches the wall in this region, as seen in Figure 6.6. Some of the high ϕ_{wall} regions observed at the bottom wall are marked as B2 - B4 and C1 - C3 as representative cases for further discussion. For better illustration of the flame at the marked regions, isosurfaces of progress variable ($c_{co_2} = 0.5$) at the chosen instants are shown in Figure 6.13. These isosurfaces are coloured by Y^+ to indicate the proximity of the flame to the bottom wall. The regions B2 - B4 and C1 - C3 are also shown. At location B2, the flame reaches closer to the wall for a small range of X^+ , see Figure 6.13(a). The other marked regions seem to be long streaks of flame which are closer to the wall contributing to the wall heat flux at the bottom

wall.



(a) Time corresponding to Figure 6.12(b)



(b) Time corresponding to Figure 6.12(c)

Figure 6.13: Isosurfaces of progress variable ($c_{co_2} = 0.5$) at different instants, coloured by Y^+ . Figures are stretched in the Y^+ direction. The domain is clipped in this region: $X^+ = 8$ to 15 ; $Y^+ = 0$ to 0.4 ; $Z^+ = 0$ to 3 .

6.3.3 Y_{CO} - T scatter plots

Figure 6.14 shows the thermochemical states of CO for all instants at $X^+ = 4.5, 7.5, 10.5$ and 13.5 . These scatter plots are coloured by the modified mixture fraction (ξ), as defined in Section 5.2.1.1. The top ($Y^+ \geq 1$) and the bottom ($Y^+ < 1$) halves of the domain, which represent FCAI and FWI conditions respectively, are shown

in the top and bottom rows of Figure 6.14. The temperature dependence of Y_{CO} in 1D FPF configuration for different equivalence ratios are also shown. The first column ($X^+ = 4.5$) in the top half represents the uncooled region as the cooling slots start from $X^+ = 5$ and hence show $\xi = 1$ indicating the unmixed condition. Similarly, most points in the bottom half of the domain are unmixed. As expected, the scatter plots at the bottom half resemble the thermochemical states of CO near a non-effusion cooled wall (see Figure 4.14). Importantly, $Y_{CO} - T$ dependence in the top half of the domain, at $X^+ = 7.5, 10.5$ and 13.5 , at different ξ are captured reasonably well by the corresponding 1D FPF results. This is particularly the case in the oxidation branch of CO while some differences are observed in the production branch, as also observed in Chapter 5 (see Figures 5.15 and 5.17). Furthermore, the horizontal branch of CO observed in Chapter 5 (see Figures 5.15 and 5.17) which was attributed to the wall heat loss is not observed in Figure 6.14. This is because of the difference in the cooling slot configuration. Multiple cooling slots form a sheet of cooling air thereby shielding the wall from the flame. As a result, the effect of the wall heat loss is not seen in the $Y_{CO} - T$ plots. To highlight these effects, Figure 6.15 shows these scatter plots for selected bands of ξ only, in the top half of the domain.

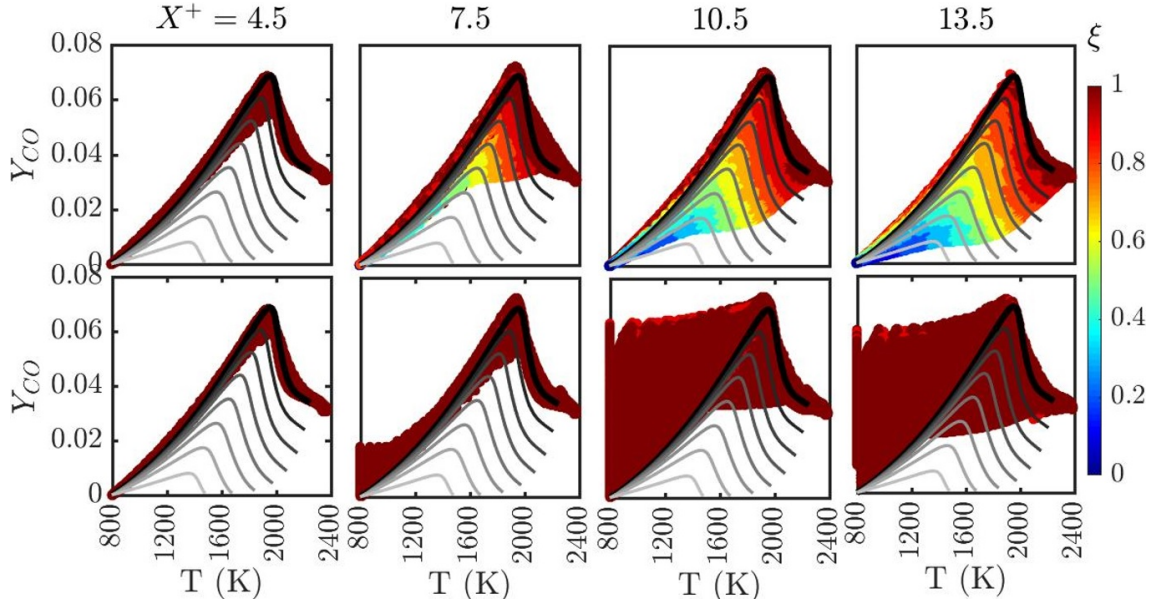


Figure 6.14: $Y_{CO} - T$ scatter plots for $X^+ = 4.5, 7.5, 10.5$ and 13.5 for all instants. The top and bottom rows of the figure indicate the top and bottom halves of the domain, i.e. $Y^+ \geq 1$ and $Y^+ < 1$, respectively. The plots are coloured with ξ . The line plots show 1D FPF results for a range of equivalence ratios.

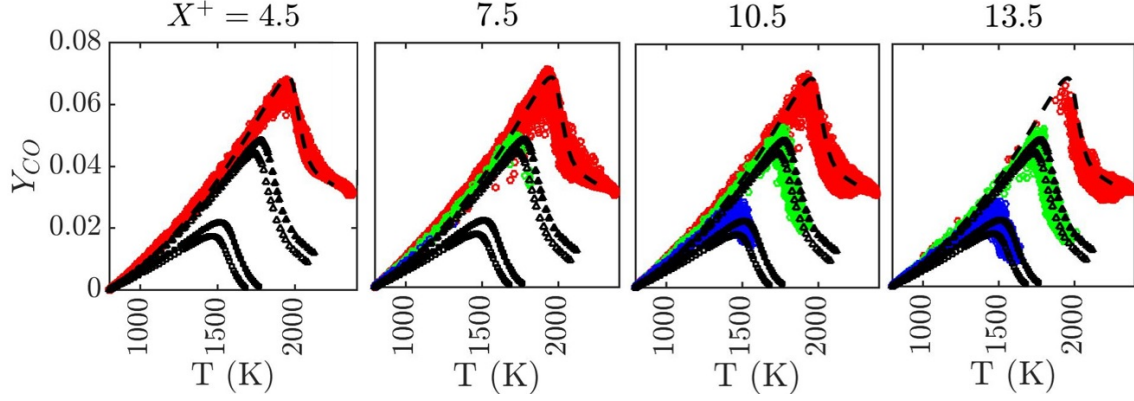


Figure 6.15: Y_{CO} - T scatter plots for $\xi = 0.95 - 1$ (red), $\xi = 0.7 - 0.75$ (green) and $\xi = 0.4 - 0.45$ (blue) at $X^+ = 4.5, 7.5, 10.5$ and 13.5 for all instants, for the top ($Y^+ \geq 1$) half of the domain. The 1D FPF results with the corresponding equivalence ratio, i.e. $\phi = 1$ ($\blacksquare$), $\phi = 0.75$ ($\blacktriangle$), $\phi = 0.7$ ($\triangle$), $\phi = 0.45$ ($\blacksquare$) and $\phi = 0.4$ ($\square$), are also shown.

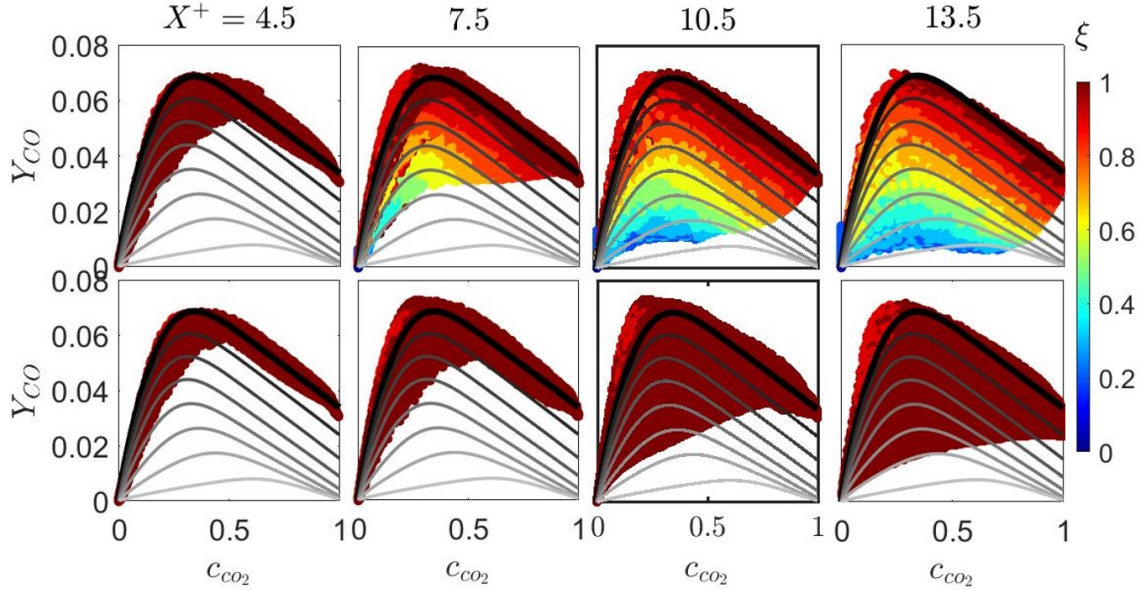


Figure 6.16: c_{CO_2} - Y_{CO} scatter plots for $X^+ = 4.5, 7.5, 10.5$ and 13.5 for all instants for $Y^+ \geq 1$ (top row) and $Y^+ < 1$ (bottom row). The plots are coloured with ξ . The 1D FPF results are shown for several equivalence ratios.

The scatter plots presented in Figure 6.16 show the variation of Y_{CO} with progress variable (c_{CO_2}) at $X^+ = 4.5, 7.5, 10.5$, and 13.5 for all instants under FCAI ($Y^+ \geq 1$) and FWI ($Y^+ < 1$) conditions. The scatter plots are coloured by ξ and the corresponding 1D FPF solutions are shown for comparison. Similar to the observations in Figure 6.14, the Y_{CO} - c_{CO_2} dependence is also captured reasonably well by the 1D FPF solutions. This indicates that either temperature or c_{CO_2} could be used along

with ξ to estimate CO under FCAI conditions. In this study, temperature and ξ are used for CO estimation.

6.3.4 CO model evaluation

It is possible from the results of the previous section that the CO mass fraction close to the top wall can be estimated using 1D FPF results, if the local temperature (T_{local}) and mixture fraction (ξ_{local}) are known. This model for estimation of Y_{CO} is referred to as ‘ CO model’ in the remainder of this thesis. To examine to what extent T_{local} and ξ_{local} can determine local CO in this configuration Y_{CO} - T data is tabulated for 1D FPFs for stoichiometries ranging from 0.3 to 1. The CO mass fraction is interpolated at T_{local} and ξ_{local} where T_{local} at a given stoichiometry is a proxy for the local progress variable. The 1D FPF simulations were performed using the same chemical mechanism as that used in the DNS (SK mechanism, see Section 3.6). At very low equivalence ratios (< 0.3) where the 1D FPF simulations could not be performed, Y_{CO} is set to zero in the model.

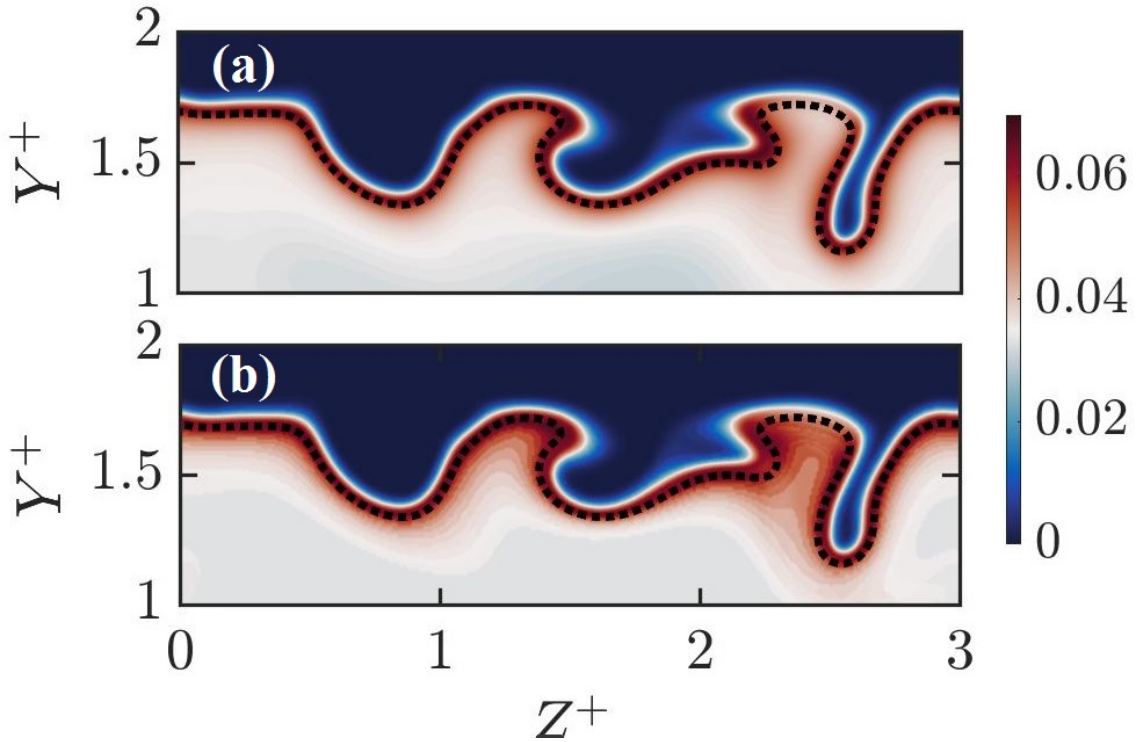


Figure 6.17: The contour of Y_{CO} at $X^+ = 7.5$ (a) from DNS and (b) from the CO model, at one instant. The black dotted line shows $c_{CO_2} = 0.5$.

Figures 6.17 and 6.18 show the values of Y_{CO} obtained from DNS and those estimated

using the CO model, for one instant, at $X^+ = 7.5$ and 13.5 , respectively. The flame front ($c_{co_2} = 0.5$) is also indicated on these plots. Importantly, the qualitative trend of Y_{CO} seen in the DNS results is reproduced by the CO model. To further evaluate the performance of the model, Y_{CO} obtained from both the DNS data and the CO model are averaged in the spanwise direction and in time. These results are presented as functions of $\overline{c_{co_2}}$ and Y^+ in Figures 6.19 and 6.20 at $X^+ = 7.5$ and 13.5 , respectively. Once again, a good agreement is observed between the results of the CO model and DNS. A more quantitative examination of the performance of the model at several streamwise locations is presented in Figure 6.21.

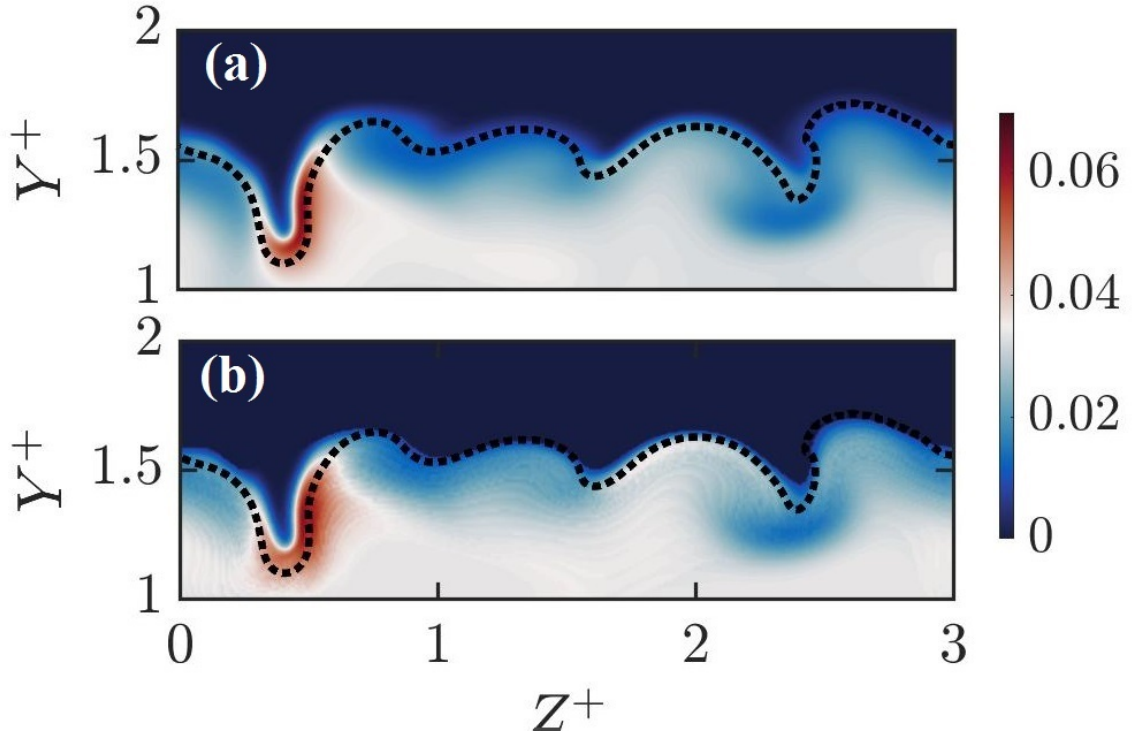


Figure 6.18: The CO mass fraction at $X^+ = 13.5$ (a) from DNS and (b) from the CO model, at one instant. The black dotted line shows $c_{co_2} = 0.5$.

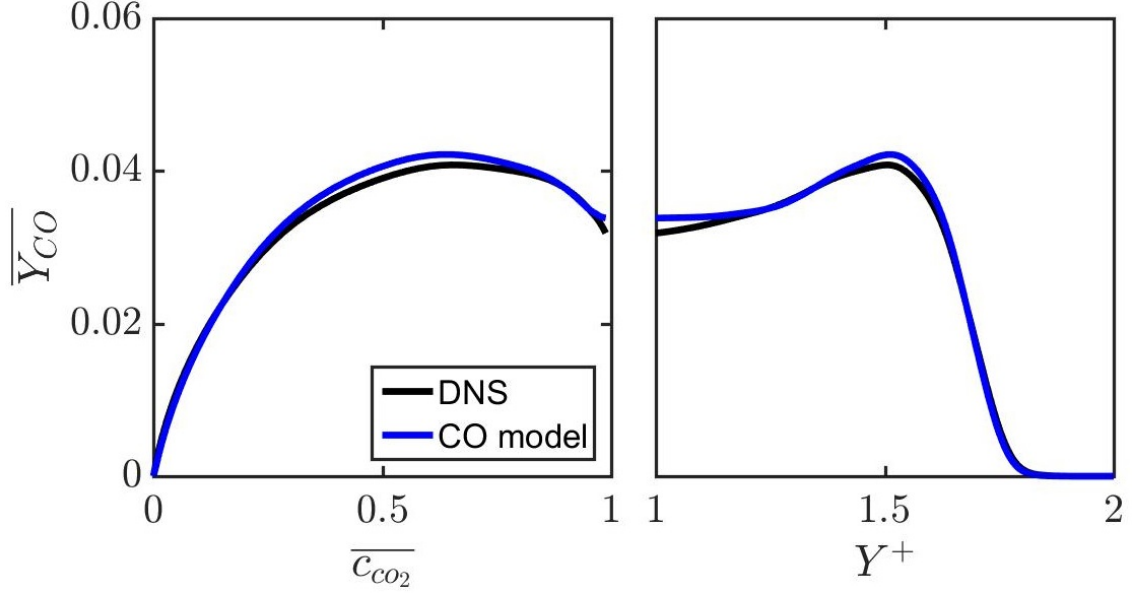


Figure 6.19: The DNS (black) and modelled (blue) Y_{CO} at $X^+ = 7.5$ averaged in the spanwise direction and in time ($\overline{Y_{CO}}$), as a function of $\overline{c_{CO_2}}$ (left) and Y^+ (right).

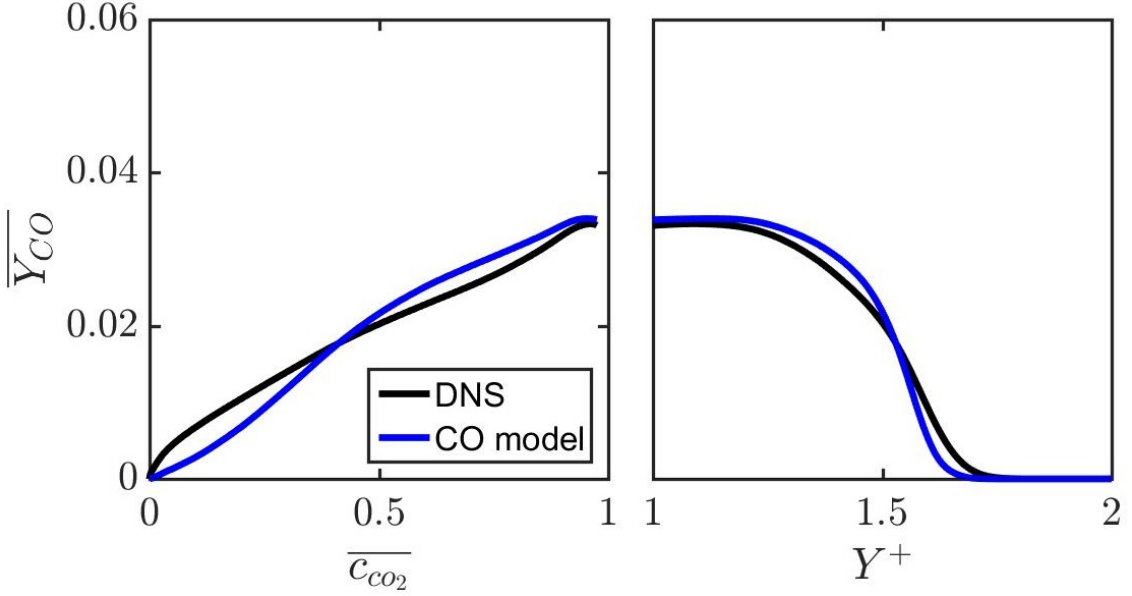


Figure 6.20: The DNS (black) and modelled (blue) Y_{CO} at $X^+ = 13.5$ averaged in the spanwise direction and in time ($\overline{Y_{CO}}$), as a function of $\overline{c_{CO_2}}$ (left) and Y^+ (right).

To compare the percentage difference between the integrated Y_{CO} values obtained from DNS and from the CO model at several X^+ locations, a variable Δ_{model} is defined as follows:

$$\Delta_{model} = \left(\frac{\tilde{Y}_{CO,DNS} - \tilde{Y}_{CO,model}}{\tilde{Y}_{CO,DNS}} \right) \times 100, \quad (6.3.1)$$

where,

$$\tilde{Y}_{CO} = \frac{\iint \int_{Y^+=1}^2 (\rho Y_{CO}) dY^+ dZ^+ dt}{\iint \int_{Y^+=1}^2 \rho dY^+ dZ^+ dt} \quad (6.3.2)$$

The subscripts ‘DNS’ and ‘model’ refer to the data obtained from DNS and the *CO* model, respectively. Note, the integration is performed in time, in the spanwise direction and in the wall-normal direction from $Y^+ = 1$ to 2. A positive value of Δ_{model} indicates that the *CO* model under-predicts $\tilde{Y}_{CO}$ while a negative value indicates overestimation of $\tilde{Y}_{CO}$ by the model.

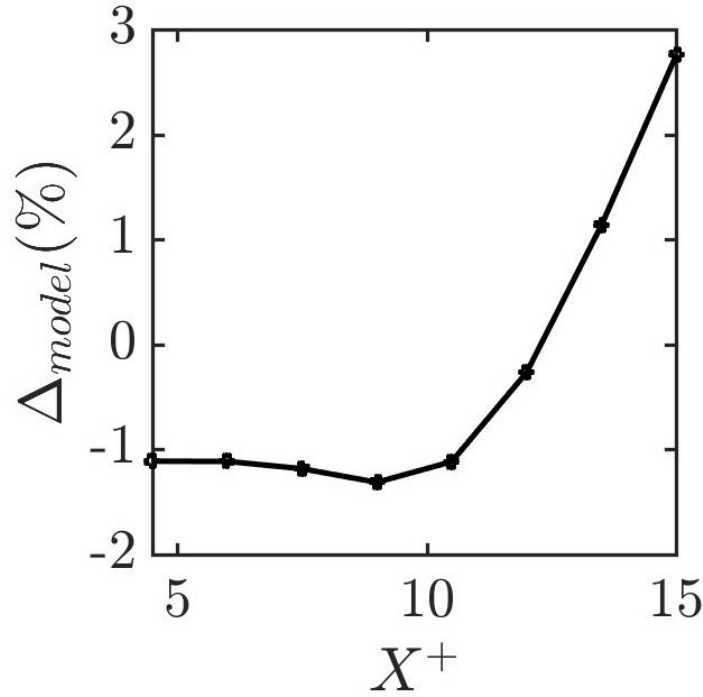


Figure 6.21: Evaluation of the *CO* model by comparing with the DNS data at several streamwise locations. The variable Δ_{model} , defined in Equation 6.3.1, is presented as a function of X^+ .

Figure 6.21 shows the variation of Δ_{model} along the streamwise direction from $X^+ = 4.5$ to 15. While $X^+ = 4.5$ is a location upstream of all the cooling slots, $X^+ = 15$ is at the outlet of the domain. Importantly, Figure 6.21 shows that the absolute value of Δ_{model} is within 3% indicating that the *CO* model compares well with the DNS data quantitatively. Although this result is promising, the accuracy of this model needs to be further assessed for turbulent flames in different parts of the regime diagram and necessary adjustments are to be made to improve its accuracy under

those conditions.

6.4 Conclusions

This study investigated the flame dynamics, wall heat flux and CO emission characteristics of a turbulent, premixed flame interacting with a sheet of cooling air at the top wall and with an uncooled bottom wall. This enables flame-cooling air interaction (FCAI) and flame-wall interaction (FWI) to be simulated at the same time. A longer flame with reduced CO mass fraction at its tail was observed near the top wall compared to the bottom wall. The tail of this flame was leaner due to mixing with the cooling air. Also, the fluctuations in the heat release rate and CO mass fraction were relatively low in the region where the flame interacted with the sheet of cooling air.

Finger-like flame features near the bottom wall were formed due the interaction of turbulent structures with the flame surface, initially moving away from the wall and eventually collapsing at the wall. These structures were found to create regions of high Y_{CO} at the wall and large wall heat flux.

The thermochemical states of CO near the effusion-cooled top wall at several stream-wise locations were captured by 1D freely-propagating flame (FPF) results reasonably well. The analysis of the CO thermochemical states presented a framework to predict near-wall CO due to FCAI. The CO mass fraction corresponding to the local temperature and dilution level at any chosen point was estimated using the 1D FPF results. A comparison of this estimated Y_{CO} to the DNS results confirmed that the qualitative and quantitative behaviour of Y_{CO} was well predicted by the model. Planned future work will evaluate the performance of this model in different turbulent combustion regimes with necessary improvements to be made under those conditions.

Chapter 7

Conclusions and future work

7.1 Summary of findings

This thesis studied a preheated, premixed methane/air flame in the context of flame-wall interaction (FWI) and flame-cooling air interaction (FCAI) using direct numerical simulation (DNS). A preheated mixture of methane and air at 800 K, comparable to the temperature at the compressor outlet of a gas turbine (GT) was used. Methane was used as the fuel since it is the major component in natural gas and is a common fuel in GTs for power generation.

Chapter 4 investigated the flame behaviour, wall heat transfer and near-wall CO emissions in a 2D forced laminar flame configuration. The near-wall *CO* transport mechanisms were explored using a species transport budget analysis where the contribution of convection, molecular diffusion and reaction terms to the near-wall *CO* transport were analysed. Laminar FCAI was the subject of research in Chapter 5 where the effects of injection of coolant jets through the combustor wall were parametrically studied in a 2D computational domain. The impact of FCAI on flame behaviour, near-wall *CO* and wall heat flux were explored. A model to predict the near-wall *CO* due to FCAI was proposed. The effects of FWI and FCAI under turbulent flow conditions were explored in a 3D computational domain in Chapter 6 where the above-mentioned model was also evaluated under a more realistic turbulent condition.

The major findings of this research are summarised below:

1. **In an acoustically forced laminar premixed flame interacting with a relatively cold wall, a range of FWI configurations from SWQ to a combination of HOQ and SWQ can occur depending on the forcing frequency.**

To study transient FWI, a laminar flame subject to velocity perturbations at the inlet was studied for a range of forcing frequencies. Such an analysis helps to isolate different flow time-scales and study their effects on the flame dynamics separately. The forcing frequency was non-dimensionalised based on the flame length under steady state conditions and the maximum convective velocity at the inlet to obtain a non-dimensional number called Strouhal number (St). The flame was largely unaffected at the highest frequency of excitation ($St = 8.3$), behaving like a steady flame while the flame displayed a SWQ behaviour at the lowest excitation frequency ($St = 0.5$). The flame showed a combination of HOQ-like and SWQ-like characteristics at unity St .

2. **Low-activation energy, exothermic reactions involving reactive radicals contribute to about 50% of the near-wall HRR when a preheated methane/air flame interacts with a relatively cold wall.**

The significance of low-temperature chemistry near a relatively cold wall was systematically studied by quantifying the contributions of individual reactions to the overall HRR at the wall. The low-activation energy, exothermic reactions involving reactive radicals, collectively known as radical recombination reactions, contributed to about 50% of the overall HRR at the wall, at the quenching instant for unity St . This underlines the importance of low-temperature chemistry in understanding of the near-wall HRR in a preheated, premixed methane/air flame.

3. **Convection and diffusion dominate the near-wall CO transport in**

transient FWI.

Near-wall CO transport mechanisms were investigated using species transport budget analysis [35]. The contributions of mass convection (C), molecular diffusion (D) and reaction rate (R) terms to the rate of change of CO were quantified. Convection and diffusion of CO were found to be significant in the near-wall region. For instance, during HOQ-like behaviour of the flame, CO diffusion was dominant while movement of the flame in the streamwise direction coincided with a significant contribution from the convection term. The reaction rate term was insignificant near the flame tip in the vicinity of the wall.

4. **A combination of factors including flame tip dilution, trajectory of coolant jet, formation and transport of CO pockets influence the near-wall CO characteristics due to FCAI.**

The interaction of laminar and turbulent premixed flames with cooling air was investigated. This interaction makes the flame tip leaner and longer compared with the FWI cases. Also, the CO mass fraction was lower in this region. The trajectory of coolant jet was found to vary depending on the position of the cooling hole and on the blowing ratio (BR), i.e. the ratio of mass flux of the coolant to that of the inlet premixture. This change of the trajectory controls the extent of the near-wall region which is influenced by the cooling air, affecting CO both near the wall and away from it. For instance, for high BR , the near-wall region influenced by coolant jet was smaller compared to the lower BR cases. An increase in BR , which reduces the wall heat flux increased the overall CO emissions. Furthermore, the interaction of the coolant jet with the flame leads to the formation of CO pockets downstream of the flame. The transport of such CO pockets influenced the near-wall CO characteristics.

5. **Near-wall CO characteristics due to FCAI can be modelled as a function of temperature and a modified mixture fraction, using a**

set of computationally inexpensive 1D simulations.

Based on the thermochemical states of CO observed in the laminar and turbulent cases, this thesis proposed a framework to predict the near-wall CO due to FCAI, using simple 1D simulations. To quantify the extent of mixing with the cooling air, a modified mixture fraction (ξ) was defined. Here, the mixture fraction definition proposed by Bilger [64] was modified such that $\xi = 1$ refers to the stoichiometric condition of the inlet premixture and $\xi = 0$ indicates pure cooling air. One-dimensional, unstrained, freely propagating flame simulations for equivalence ratios corresponding to the local value of ξ were performed. The CO mass fraction corresponding to the local temperature in the computational domain was then estimated using these 1D solutions. This modelling framework showed encouraging results and provided a basis for further improvement.

6. **Under turbulent FWI conditions, the collapse of certain flame structures at the wall leads to regions of high CO and wall heat flux.**

Under turbulent flow conditions, formation of flame structures were observed in the regions with high vorticity magnitude. Such flame structures were found near both effusion-cooled (FCAI) and non-effusion cooled (FWI) walls. However, these structures were closer to the non-effusion cooled wall and hence influenced the near-wall parameters more strongly. The propagation of one of these structures was analysed using 3D isosurfaces of the flame. It was observed that as these structures reach near the wall, they create local regions at the wall where wall heat flux and CO are high.

7.2 Recommendations for future work

1. **Investigate CO emissions due to FWI and FCAI at higher Re .**

For the next step, a DNS dataset simulating FWI and FCAI under a higher

Reynolds number than that considered in this study can be produced. This dataset can provide further information on the impact of parameters such as Karlovitz number on the flame dynamics as well as *CO* emissions.

2. **Improve the *CO* model to predict the near-wall *CO* due to FCAI by including the effects of flame stretch and wall heat loss.**

To further improve the near-wall *CO* model proposed in this thesis, the contribution of phenomena like flame stretch and wall heat loss can be studied and included in the model. From the literature, flame stretch and wall heat loss are known to influence *CO* predictions in a gas turbine combustor [67].

3. **Study the effect of blowing ratio on the near-wall *CO* under turbulent conditions.**

The effect of blowing ratio on the wall heat flux and *CO* emissions was found to be important. Although an increase in *BR* decreased the wall heat flux, high values of *BR* adversely affected *CO* emissions. While the former is important to reduce the thermal stress on the combustor walls, the latter is undesirable. The increased *CO* at a high *BR* was attributed to the cooling jet trajectory which affected the near-wall region influenced by the coolant jet. An improved understanding of the *BR* effects on *CO* can be achieved by investigating this effect in a turbulent flame.

4. **Investigate the effect of the near-wall *CO* characteristics on the exhaust *CO*.**

The exhaust *CO* in a gas turbine is highly relevant to the gas turbine industry. Therefore, the entire *CO* journey from where it is formed in the combustor to where it leaves the gas turbine needs to be considered to improve our understanding of the exhaust *CO* emissions. The study conducted in this thesis needs to be extended to examine the impact of the near-wall *CO* character-

istics on the exhaust CO . One should note that the high computational cost incurred by DNS limits the size of the problem that can be considered. This means that lesser expensive computational techniques such as large eddy simulations or other low order models need to be used to simulate the entire CO journey in a gas turbine.

Bibliography

- [1] International Energy Agency (IEA), World Energy Outlook 2018 - Executive Summary, pp. 1–11, 2018.
- [2] International Energy Agency (IEA), World Energy Outlook 2017 - Executive Summary, pp. 1–13, 2017.
- [3] N. E. Klarmann, *Modeling Turbulent Combustion and CO Emissions in Partially-Premixed Conditions Considering Flame Stretch and Heat Loss*. PhD thesis, 2019.
- [4] A. H. Lefebvre and D. R. Ballal, *Gas turbine combustion: alternate fuels and emissions*. CRC press, Boca Raton, 2010.
- [5] A. Dreizler and B. Böhm, Advanced laser diagnostics for an improved understanding of premixed flame-wall interactions, *Proceedings of the Combustion Institute*, vol. 35, pp. 37–64, 2015.
- [6] A. Gruber, R. Sankaran, E. R. Hawkes, and J. H. Chen, Turbulent flame-wall interaction: a direct numerical simulation study, *Journal of Fluid Mechanics*, vol. 658, pp. 5–32, 2010.
- [7] R. Haghighi, *Towards understanding multicomponent chemistry interaction using direct numerical simulation*. PhD thesis, (Doctoral dissertation, Technische Universität), 2015.
- [8] T. J. Poinso, D. C. Haworth, and G. Bruneaux, Direct simulation and modeling of flame-wall interaction for premixed turbulent combustion, *Combustion and Flame*, vol. 95, pp. 118–132, 1993.
- [9] J. Sotton, B. Boust, S. A. Labuda, and M. Bellenoue, Head-on quenching of

- transient laminar flame: heat flux and quenching distance measurements, *Combustion and Flame*, vol. 177, pp. 1305–1322, 2005.
- [10] R. Friedman and W. C. Johnston, The wall-quenching of laminar propane flames as a function of pressure, temperature, and air-fuel ratio, *Journal of Applied Physics*, vol. 21, no. 8, pp. 791–795, 1950.
- [11] R. Friedman and W. C. Johnston, Pressure dependence of quenching distance of normal heptane, iso-octane, benzene, and ethyl ether flames, *The Journal of Chemical Physics*, vol. 20, no. 5, pp. 919–920, 1952.
- [12] M. Bellenoue, T. Kageyama, S. A. Labuda, and J. Sotton, Direct measurement of laminar flame quenching distance in a closed vessel, *Experimental Thermal and Fluid Science*, vol. 27, pp. 323–331, 2003.
- [13] C. K. Westbrook, A. A. Adamczyk, and G. A. Lavoie, A numerical study of laminar flame wall quenching, *Combustion and Flame*, vol. 40, pp. 81–99, 1981.
- [14] P. Popp, M. Smooke, and M. Baum, Heterogeneous/homogeneous reaction and transport coupling during flame-wall interaction, *Symposium (International) on Combustion*, vol. 26, pp. 2693–2700, 1996.
- [15] L. Connelly, T. Ogasawara, D. Lee, R. Greif, and R. F. Sawyer, Fall meeting, *Combustion Institute/Western States Section, Stanford, CA, Paper N. WSCI*, pp. 77–93, 1993.
- [16] D. Haworth, Numerical simulations of Lewis number effects in turbulent premixed flames, *Journal of Fluid Mechanics*, vol. 244, 1992.
- [17] C. J. Rutland and A. Trouvé, Direct simulations of premixed turbulent flames with nonunity Lewis numbers, *Combustion and Flame*, vol. 94, pp. 41–57, 1993.
- [18] J. Lai and N. Chakraborty, Effects of Lewis number on head on quenching of turbulent premixed flames: a direct numerical simulation analysis, *Flow, Turbulence and Combustion*, vol. 96, no. 2, pp. 279–308, 2016.
- [19] T. Häber and R. Suntz, Effect of different wall materials and thermal-barrier coatings on the flame-wall interaction of laminar premixed methane and

- propane flame, *International Journal of Heat and Fluid Flow*, vol. 69, pp. 95–105, 2018.
- [20] M. Saffman, Parametric studies of a side wall quench layer, *Combustion and Flame*, vol. 55, pp. 141–159, 1984.
- [21] R. Owston, V. Magi, and J. Abraham, A numerical study of thermal and chemical effects in interactions of n-heptane flames with a single surface, *Combustion and Flame*, vol. 148, pp. 127–147, 2007.
- [22] K. T. Kim, D. H. Lee, and S. Kwon, Effects of thermal and chemical surface–flame interaction on flame quenching, *Combustion and Flame*, vol. 146, no. 1, pp. 19–28, 2006.
- [23] P. Popp and M. Baum, Analysis of wall heat fluxes, reaction mechanisms, and unburnt hydrocarbons during the head-on quenching of a laminar methane flame, *Combustion and Flame*, vol. 108, no. 3, pp. 327–348, 1997.
- [24] J. Lai, M. Klein, and N. Chakraborty, Direct Numerical Simulation of Head-On Quenching of Statistically Planar Turbulent Premixed Methane-Air Flames Using a Detailed Chemical Mechanism, *Flow, Turbulence and Combustion*, vol. 101, no. 4, pp. 1073–1091, 2018.
- [25] M. Mann, C. Jainski, M. Euler, B. Böhm, and A. Dreizler, Transient flame–wall interactions: Experimental analysis using spectroscopic temperature and *CO* concentration measurements, *Combustion and Flame*, vol. 161, pp. 2371–2386, 2014.
- [26] A. Singh, M. Mann, T. Kissel, J. Brübach, and A. Dreizler, Simultaneous measurements of temperature and *CO* concentration in stagnation stabilized flames, *Flow, Turbulence and Combustion.*, vol. 90, pp. 723–739, 2013.
- [27] C. Jainski, M. Reißmann, B. Böhm, J. Janicka, and A. Dreizler, Sidewall quenching of atmospheric laminar premixed flames studied by laser-based diagnostics, *Combustion and Flame*, vol. 183, pp. 271–282, 2017.
- [28] H. Kosaka, F. Zentgraf, A. Scholtissek, L. Bischoff, T. Häber, R. Suntz, B. Albert, C. Hasse, and A. Dreizler, Wall heat fluxes and *CO* formation/oxidation

- during laminar and turbulent side-wall quenching of methane and DME flames, *International Journal of Heat and Fluid Flow*, vol. 70, pp. 181–192, 2018.
- [29] J. E. Rivera, R. L. Gordon, and M. Talei, Flame-wall interaction of a forced laminar premixed propane flame: Flame dynamics and exhaust *CO* emissions, *Proceedings of the Combustion Institute*, vol. 37, pp. 1083–1090, 2019.
- [30] H. Kosaka, *Experimental Investigation of Flame-Wall Interaction by Laser-based Diagnostics*. PhD thesis, 2019.
- [31] S. Ganter, A. Heinrich, T. Meier, G. Kuenne, C. Jainski, M. C. Reißmann, A. Dreizler, and J. Janicka, Numerical analysis of laminar methane – air side-wall-quenching, *Combustion and Flame*, vol. 186, pp. 299–310, 2017.
- [32] B. Jiang, R. L. Gordon, and M. Talei, Head-on quenching of laminar premixed methane flames diluted with hot combustion products, *Proceedings of the Combustion Institute*, vol. 37, pp. 793–801, 2019.
- [33] S. Ganter, C. Straßacker, G. Kuenne, T. Meier, A. Heinrich, U. Maas, and J. Janicka, Laminar near-wall combustion: Analysis of tabulated chemistry simulations by means of detailed kinetics, *International Journal of Heat and Fluid Flow*, vol. 70, pp. 259–270, 2018.
- [34] A. Heinrich, S. Ganter, G. Kuenne, C. Jainski, A. Dreizler, and J. Janicka, 3D Numerical Simulation of a Laminar Experimental SWQ Burner with Tabulated Chemistry, *Flow Turbulence and Combustion*, vol. 100, pp. 535–559, 2018.
- [35] R. L. Gordon, A. R. Masri, S. B. Pope, and G. M. Goldin, Transport budgets in turbulent lifted flames of methane autoigniting in a vitiated co-flow, *Combustion and Flame*, vol. 151, pp. 495–511, 2007.
- [36] M. K. Razdan, J. T. McLeroy, and W. E. Weaver, Retrofittable dry low emissions combustor for 501-K industrial gas turbine engines, in *International Gas Turbine and Aeroengine Congress and Exposition. American Society of Mechanical Engineers*, 1994.
- [37] K. Smith and A. Fahme, Back Side-Cooled Combustor Liner for Lean-Premixed

- Combustion, in *International Gas Turbine and Aeroengine Congress and Exhibition*. American Society of Mechanical Engineers, 1999.
- [38] G. E. Andrews and M. N. Kim, The Influence of Film Cooling on Emissions for a Low NO_x Radial Swirler Gas Turbine Combustor, in *ASME Turbo Expo 2001: Power for Land, Sea, and Air*, 2001.
- [39] J. E. Rivera, R. L. Gordon, D. Brouzet, and M. Talei, Exhaust CO emissions of a laminar premixed propane – air flame interacting with cold gas jets, *Combustion and Flame*, vol. 210, pp. 374–388, 2019.
- [40] S. M. Correa, Carbon monoxide emissions in lean premixed combustion, *Journal of Propulsion and Power*, vol. 8, no. 6, pp. 1144–1151, 1992.
- [41] T. M. Alshaalan and C. J. Rutland, Turbulence, scalar transport, and reaction rates in flame-wall interaction, *Symposium (International) on Combustion*, vol. 27, no. 1, pp. 793–799, 1998.
- [42] G. Bruneaux, K. Akselvoll, T. J. Poinso, and J. H. Ferziger, Flame-wall interaction simulation in a turbulent channel flow, *Combustion and Flame*, vol. 107, pp. 27–44, 1996.
- [43] T. Alshaalan and C. J. Rutland, Wall heat flux in turbulent premixed reacting flow, *Combustion Science and Technology*, vol. 174, no. 1, pp. 135–165, 2002.
- [44] M. Baum, T. J. Poinso, D. C. Haworth, and N. Darabiha, Direct numerical simulation of $H_2/O_2/N_2$ flames with complex chemistry in two-dimensional turbulent flows, *Journal of Fluid Mechanics*, vol. 281, no. 1, pp. 1–32, 1994.
- [45] C. Jimenez, B. Cuenot, T. Poinso, and D. Haworth, Numerical Simulation and Modeling for Lean Stratified Propane-Air Flames, *Combustion and Flame*, vol. 128, pp. 1–21, 2002.
- [46] C. Jiménez, A. Haghiri, M. J. Brear, M. Talei, and E. R. Hawkes, Sound generation by premixed flame annihilation with full and simple chemistry, *Proceedings of the Combustion Institute*, vol. 35, pp. 3317–3325, 2015.
- [47] C. Jiménez and V. N. Kurdyumov, Propagation of symmetric and non-

- symmetric lean hydrogen-air flames in narrow channels: Influence of heat losses, *Proceedings of the Combustion Institute*, vol. 36, pp. 1559–1567, 2017.
- [48] D. Brouzet, *Investigation of Direct Combustion Noise in Turbulent Premixed Jet Flames Using Direct Numerical Simulations*. PhD thesis, 2020.
- [49] G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eite-
neer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, William
C. Gardiner, Jr., Vitali V. Lissianski, and Z. Qin, GRI-MECH 3.0,
<http://www.me.berkeley.edu/grimech/>.
- [50] M. D. Smooke, I. K. Puri, and K. Seshadri, A comparison between numerical
calculations and experimental measurements of the structure of a counterflow
diffusion flame burning diluted methane in diluted air, *Symposium (Interna-
tional) on Combustion*, vol. 21, pp. 1783–1792, 1986.
- [51] J. D. Anderson, *Computational Fluid Dynamics*. New York: McGraw-Hill,
1995.
- [52] T. J. Poinso and S. K. Lele, Boundary conditions for direct simulations of
compressible viscous flows, *Journal of Computational Physics*, vol. 101, pp. 104–
129, 1992.
- [53] A. Andreini, R. Becchi, B. Facchini, A. Picchi, and A. Peschiulli, The effect of
effusion holes inclination angle on the adiabatic film cooling effectiveness in a
three-sector gas turbine combustor rig with a realistic swirling flow, *Interna-
tional Journal of Thermal Sciences*, vol. 121, pp. 75–88, 2017.
- [54] P. K. Yeung and S. B. Pope, Lagrangian statistics from direct numerical simula-
tions of isotropic turbulence, *Journal of Fluid Mechanics*, vol. 207, pp. 531–586,
1989.
- [55] R. D. Moser, J. Kim, and N. N. Mansour, Direct numerical simulation of turbu-
lent channel flow up to $Re_\tau=590$, *Physics of Fluids*, vol. 11, no. 4, pp. 943–945,
1999.
- [56] T. Passot and A. Pouquet, Numerical Simulation of Compressible Homogeneous

- Flows in the Turbulent Regime, *Journal of Fluid Mechanics*, vol. 181, pp. 441–466, 1987.
- [57] A. Smirnov, S. Shi, and I. Celik, Random flow generation technique for large eddy simulations and particle-dynamics modeling, *Journal of Fluids Engineering*, vol. 123, pp. 359–371, 2001.
- [58] S. Lee, S. K. Lele, and P. Moin, Simulation of spatially evolving turbulence and the applicability of Taylor’s hypothesis in compressible flow, *Physics of Fluids A: Fluid Dynamics*, vol. 4, pp. 1521–1530, 1992.
- [59] A. Gruber, *Direct Numerical Simulation Of Turbulent Combustion Near Solid Surfaces*. PhD thesis, 2006.
- [60] H. Choi and P. Moin, On the space-time characteristics of wall-pressure fluctuations, *Physics of Fluids A: Fluid Dynamics*, vol. 2, pp. 1450–1460, 1990.
- [61] M. Talei, E. R. Hawkes, and M. J. Brear, A direct numerical simulation study of frequency and Lewis number effects on sound generation by two-dimensional forced laminar premixed flames, *Proceedings of the Combustion Institute*, vol. 34, no. 1, pp. 1093–1100, 2013.
- [62] M. Talei, M. J. Brear, and E. R. Hawkes, A comparative study of sound generation by laminar, combustng and non-combustng jet flows, *Theoretical and Computational Fluid Dynamics*, vol. 28, pp. 385–408, 2014.
- [63] S. R. Turns, *An introduction to combustion 2nd ed.* McGraw Hill Boston., 2000.
- [64] R. W. Bilger, The structure of turbulent nonpremixed flames, *Symposium (International) on Combustion*, vol. 22, pp. 475–488, 1988.
- [65] R. Kee, F. Rupley, J. Miller, M. Coltrin, J. Grcar, E. Meeks, H. Moffat, A. Lutz, G. Dixon-Lewis, M. Smooke, J. Warnatz, G. Evans, R. Larson, R. Mitchell, L. Petzold, W. Reynolds, M. Caracotsios, W. Stewart, P. Glarborg, C. Wang, and O. Adigun, CHEMKIN-PRO 15131, *Reaction Design*, San Diego, 2013.
- [66] T. Panitz and D. T. Wasan, Flow attachment to solid surfaces: The Coanda effect, *AIChE Journal*, vol. 18, no. 1, pp. 51–57, 1972.
- [67] N. Klarmann, B. T. Zoller, and T. Sattelmayer, Numerical modeling of CO-

- emissions for gas turbine combustors operating at part-load conditions, *Journal of the Global Power and Propulsion Society*, vol. 2, pp. 376–387, 2018.
- [68] R. Palulli, B. Jiang, J. E. Rivera, M. Talei, and R. L. Gordon, Direct Numerical Simulation of Flame-Wall Interaction for a Forced Laminar Flame, in *20th Australasian Fluid Mechanics Conference*, 2016.
- [69] B. Cuenot, B. Bedet, and A. Corjon, NTMIX3D user’s guide manual, *Preliminary Version 1*, 1997.
- [70] A. Bourlioux, B. Cuenot, and T. J. Poinso, Asymptotic and numerical study of the stabilization of diffusion flames by hot gas, *Combustion and Flame*, vol. 120, no. 1, pp. 143–159, 2000.
- [71] M. Talei, M. J. Brear, and E. R. Hawkes, Sound generation by laminar premixed flame annihilation, *Journal of Fluid Mechanics*, vol. 679, pp. 194–218, 2011.
- [72] M. Talei, M. J. Brear, and E. R. Hawkes, A parametric study of sound generation by premixed laminar flame annihilation, *Combustion and Flame*, vol. 159, no. 2, pp. 757–769, 2012.

Appendix

Appendix A

Direct Numerical Simulation of FWI for a Forced Laminar Flame using Single-step Chemistry

A.1 Introduction

This section investigates the flame-wall interaction of a two-dimensional (2D) laminar premixed flame using direct numerical simulation (DNS) using a single-step chemistry model. The flame is excited by velocity perturbations at the inlet for a range of forcing frequencies. The flame behaviour is closely analysed by using the contours of various parameters. This qualitative inspection is followed by determination of the Peclet number (Pe) in each case, in order to understand the nature of the flame quantitatively. A combination of the qualitative and quantitative methods is used to provide more clarity on the various mechanisms involved in the flame-wall interaction.

Results shown in this appendix have been presented to the 20th Australasian Fluid Mechanics Conference [68].

A.2 Numerical method

A 2D domain as shown in Figure A.1 was used with 800 equally spaced grid points in the streamwise direction and 120 grids in the transverse direction. The number of grid points was chosen such that there are at least 10 grid points within the flame thickness. The upper boundary is the wall and is at the same temperature as the inlet. Inlet to the domain is at $X^+ = X/L_{ref} = 0$ from $Y^+ = 0.2$ to 1.2, where L_{ref} is the width of the inlet. A symmetry condition is applied to the bottom boundary. The flame is anchored at $X^+ = 0$ from $Y^+ = 0$ to 0.2, using tanh functions for both mass fraction and temperature. A parabolic velocity profile, corresponding to ducted laminar flows is induced at the inlet from $Y^+ = 0.2$ to 1.2. Sinusoidal velocity perturbations at 25% of the mean inflow velocity are provided at the inlet corresponding to $St=0.01, 0.015, 0.02, 0.025, 0.03, 0.04, 0.05, 0.1$, where $St = fL_{ref}/a_{ref}$ is the non-dimensional number corresponding to the frequency of excitation, f . The variable a_{ref} is the speed of sound in the fresh gas. Non-reflecting outflow at the right boundary was imposed using Navier-Stokes Characteristic Boundary Condition (NSCBC) [52]. The flame position was defined by the points where the reaction rate is maximum.

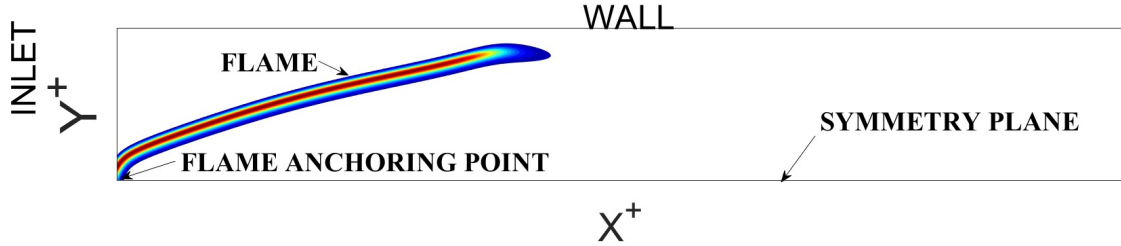


Figure A.1: The computational Domain.

The DNS code NTMIX [69] was used to conduct the simulations. NTMIX is a high-order accurate solver that has been used to perform DNS of reactive flows using a single-step chemistry e.g. [70–72]. It features a sixth-order compact scheme for spatial derivatives, combined with a third-order Runge–Kutta time integrator. The non-dimensional parameters used are $Re=(a \times L/\nu)_{ref}$, $Pr = (C_p\mu/\lambda)_{ref}$, $Sc = (\nu D)_{ref}$, $Le = Sc/Pr$, $Da = (D\Lambda/s_L^2)_{ref}$, $s_L^* = (s_L/a)_{ref}$ where ν is the kinematic viscosity, C_p is the specific heat at constant pressure, λ is the thermal conductivity,

μ is the dynamic viscosity, ρ is the density, D is the mass diffusion coefficient, Λ is the pre-exponential factor, s_L is the laminar flame speed, Re is the acoustic Reynolds number, Pr is the Prandtl number, Sc is the Schmidt number, Le is the Lewis number, Da is the Damkohler number, δ_L is the flame thickness and s_L^* is the non-dimensional laminar flame speed. The subscript ‘ref’ refers to unburnt gas properties which are treated as the reference condition. The heat release by the flame and the activation energy are measured by α and β respectively. The input parameters used in the simulation are $Re=2000$, $Le=1$, $Pr=0.75$, $s_L/a_{ref}=0.016$, $T_b/T_u=4$, $\alpha=0.75$, $\beta=8$. The variables T_u and T_b refer to the unburnt and burnt gas temperatures respectively. These parameters are taken for a typical premixed flame simulated in Ref. [8].

A.3 Results and discussions

Simple 1D transient simulation was performed initially, for the case of head-on quenching. The Peclet number (Pe) defined as the distance (y) of the flame from the wall, normalised by the reference flame thickness (δ_L), i.e. $Pe=y/\delta_L$ was calculated. Quenching (minimum Pe in the domain) was found to occur at a $Pe = 3.6$. 2D DNS was then conducted for the case of a steady flow. The contours of temperature and reaction rate for 2D steady flow are shown in Figure A.2. The minimum Pe in this case was found to be 4.35 which is close to that in the 1D head-on quenching.

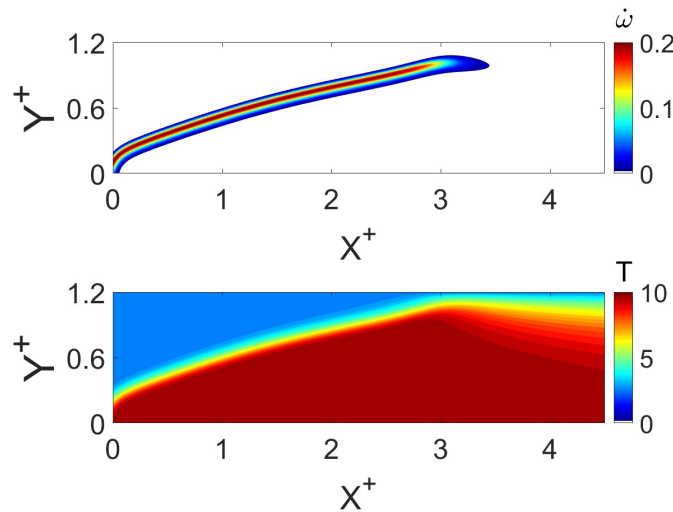


Figure A.2: Contours of reaction rate and temperature (steady flame).

Figure A.3 shows that at high frequency of excitation ($St=0.1$), the flame does not respond strongly to the incoming velocity perturbations. The Pe number varies from 4.35 to 4.6, while the minimum Pe in the case of steady flame was found to be 4.35. This is expected as the flame position changes slightly in this case. At an intermediate frequency of excitation ($St=0.025$), the flame is closest to the wall at $t=0$, with a Pe of 3.6 which is close to the value corresponding to head-on quenching (HOQ), reported earlier. At this instant, the flame has a long tail, parallel to the wall, making the flame-wall interaction more like a 1D head-on quenching. After extinction of this long tail, the flame starts to move backward with Pe number increasing until $t=3(T/5)$. The flame then starts to move forward as the forcing of the inlet velocity goes into the positive side of the cycle. As illustrated in Figure A.4, the flame continues to move away from the wall until the Pe number reaches its maximum value of 7. This value corresponds to the side-wall quenching (SWQ), as reported in the literature [8]. Afterwards, the flame developed a longer tail, while moving closer to the wall and the cycle starts again. The main observation from the flame behaviour at $St=0.025$ is that flame-wall interaction involves a combination of HOQ and SWQ. In the case of low frequency of excitation ($St=0.01$), the flame moves away from the wall from $t=0$ to $t=2(T/5)$ as Pe changes from 4.1 to 5.1, and moves towards the wall from $t = 3(T/5)$ onwards. At each value of Pe , the flame brushes along the X^+ direction, which is why there are multiple data points with the same Pe number (not all data points are shown for clarity). The minimum Pe in this case is 4.1, which is less than the value for steady flames ($Pe = 4.35$). This indicates that the flame moves closer to the wall than a steady flame.

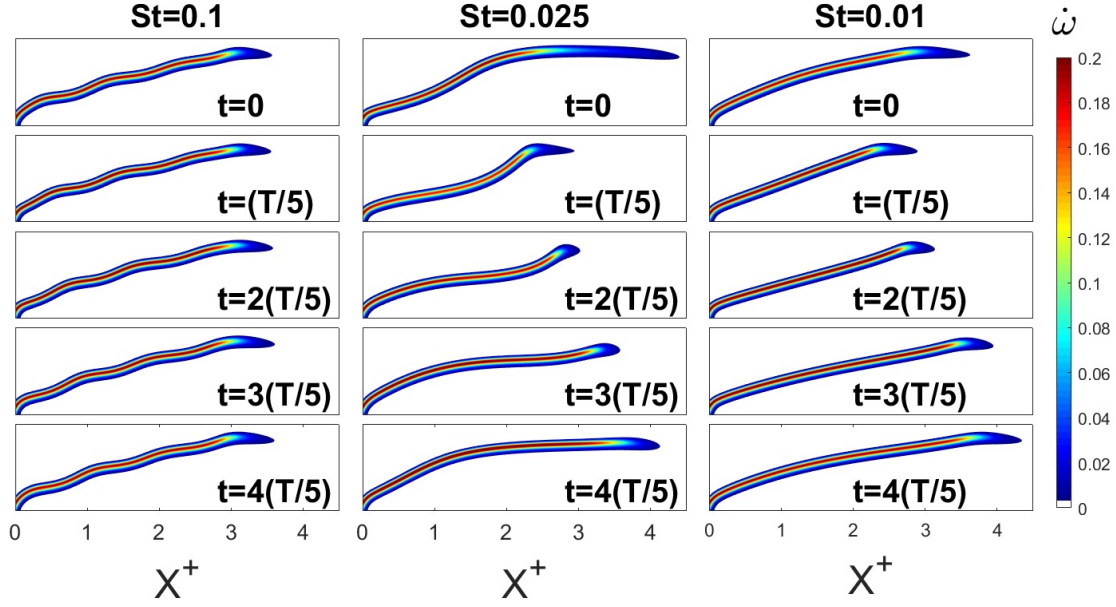


Figure A.3: Snapshots of reaction rate contours at various times for $St = 0.01, 0.025$ and 0.1 respectively.

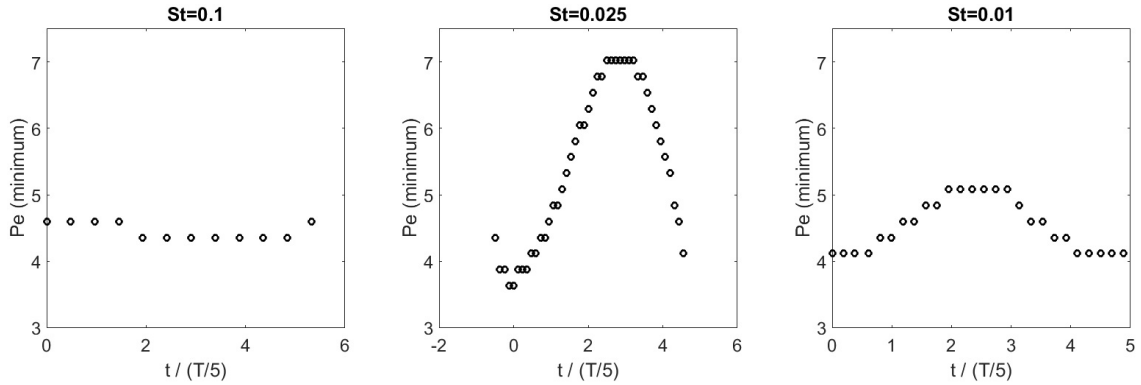


Figure A.4: Minimum Pe number (minimum in the domain) versus time for $St = 0.01, 0.025$ and 0.1 respectively.

The time-averaged mean and root mean square (RMS) values of wall heat flux (ϕ_{mean} and ϕ_{rms}), for different St , are plotted against X^+ in Figure A.5. For clarity, only the plots of three selected frequencies are shown. Decreasing the excitation frequency spreads out the heat flux profile. In addition, higher RMS values are observed at lower excitation frequencies. This is expected since the flame travels a larger distance against the wall as the excitation frequency decreases. The RMS values of up to 50% of the mean values can be observed at low excitation frequencies showing a high level of heat flux fluctuations. The peak of the mean heat flux is located downstream of flame whereas the peak RMS is located closer to the inlet.

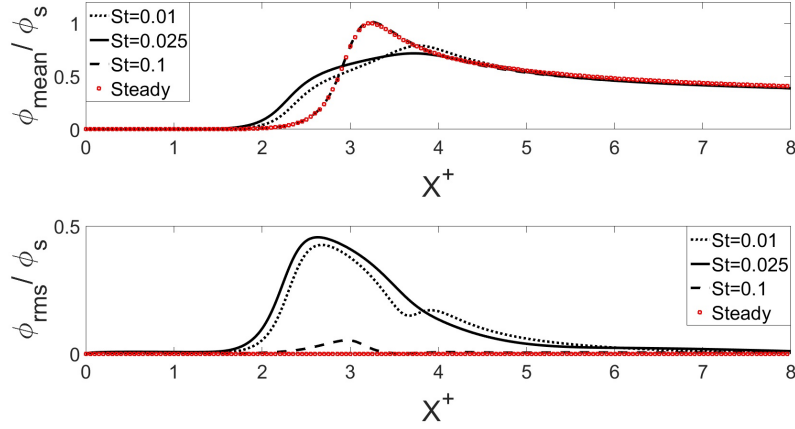


Figure A.5: Mean and rms wall heat flux vs direction of flow (X^+) for different St (ϕ_s : maximum wall heat flux for steady flame).

The variation of wall heat flux ϕ with time observed at the X^+ locations corresponding to maximum ϕ_{mean} and ϕ_{rms} were named $\phi_{t,\text{@maxmean}}$ and $\phi_{t,\text{@maxrms}}$, respectively. The mean with respect to time was deducted from $\phi_{t,\text{@maxmean}}$ and $\phi_{t,\text{@maxrms}}$, expressing the fluctuation of these two variables as $\phi'_{t,\text{@maxmean}}$ and $\phi'_{t,\text{@maxrms}}$. Also, the total wall heat flux ϕ_{total} for each time was calculated by integrating ϕ over X^+ . The mean with respect to time was deducted from ϕ_{total} , and the fluctuation of total wall heat flux, was expressed as ϕ'_{total} . The Fourier transforms of $\phi'_{t,\text{@maxmean}}$, $\phi'_{t,\text{@maxrms}}$ and ϕ'_{total} were obtained to calculate the amplitudes of these fluctuations, as shown in Figure A.6.

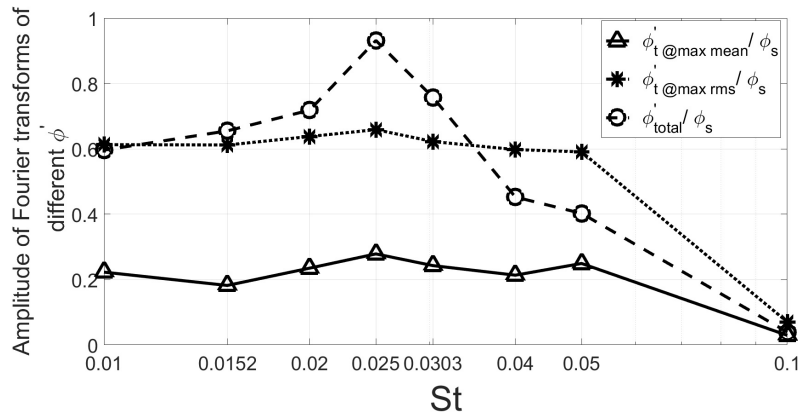


Figure A.6: Amplitude of Fourier transforms of different ϕ' , plotted in log-linear scale (ϕ_s : maximum wall heat flux for steady flame).

The trend observed in this Figure A.6 is consistent with what was reported earlier in the literature [6]. ϕ'_{total} shows a stronger variation with respect to the excitation fre-

quency compared with $\phi'_{t,@maxmean}$ and $\phi'_{t,@maxrms}$. This suggests that the analysis of the wall heat flux at a single point may not be appropriate in the case of flame-wall interaction of forced flames. Figure A.6 shows that at high excitation frequencies, ϕ'_{total} , $\phi'_{t,@maxmean}$ and $\phi'_{t,@maxrms}$ converge to similar small values because the flame does not respond strongly to the incoming velocity perturbations. At an intermediate frequency, $St = 0.025$, the maximum amplitude for the heat flux is observed. In particular, ϕ'_{total} is much higher than $\phi'_{t,@maxmean}$. At this frequency, $\phi'_{t,@maxmean}$ and $\phi'_{t,@maxrms}$ also show a peak. As discussed earlier, both HOQ and SWQ play a role during flame wall interaction for this case. At the lowest frequency of excitation, a comparable amplitude for ϕ'_{total} and $\phi'_{t,@maxrms}$ is observed. This is expected as the flame is mostly brushing against the wall at this frequency. Therefore, ϕ'_{total} will be mainly dominated by $\phi'_{t,@maxrms}$.

A.4 Conclusions

The present work investigated the flame behaviour near walls by studying the interaction of unsteady laminar premixed flames with a constant temperature wall. Two-dimensional DNSs of a forced flame were carried out for a range of excitation frequencies. To reduce the computational cost, a single-step chemistry model was used. The flame behaviour was analysed in detail at $St = 0.01$, 0.025 and 0.1 . While the flame did not respond strongly at high frequency, it showed a brushing action at low frequency. The flame behaviour for intermediate frequencies showed a combination of head-on quenching and side-wall quenching. This behaviour resulted in significantly different trend of total wall heat flux from that of the wall heat flux calculated using conventional methods. This suggests that more consideration must be given to this calculation in order to appropriately characterise the flame behaviour.