

# Flame Wall Interactions for Flames Diluted by Hot Combustion Products

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Submitted in total fulfilment of the requirements of the degree of  
Doctor of Philosophy

16th of March, 2021

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# Abstract

Flames diluted by combustion products can reduce emissions such as Carbon Monoxide (CO) and Oxides of Nitrogen ( $\text{NO}_x$ ) in industrial applications. In applications such as gas turbines, these flames are confined in a combustor and can interact with relatively cold walls. This interaction can quench the flame, producing incomplete combustion products. In this study, Flame-Wall Interaction (FWI) for methane/air flames diluted by hot combustion products was investigated using Direct Numerical Simulation (DNS).

One-Dimensional (1D) Head-On Quenching (HOQ) was first simulated to examine operating parameter effects on CO emissions from transient quenching processes. Average CO within the quenching region was used to evaluate these effects, and the species transport budget was used to investigate the dominant terms. At higher dilution levels, the peak average near-wall CO decreases, and the rate of near-wall CO reduction also decreases. At higher wall temperatures, the peak average near-wall CO and its reduction rate increases. The near-wall CO may be modelled under some conditions using only the integrated diffusion term.

Then, a two-Dimensional (2D) laminar V-flame was simulated in both steady and forced conditions. The changes in peak near-wall CO due to varying dilution level and wall temperature show similar trends to the 1D results. The exhaust CO is linked directly to the oxidation residence time, which is determined by the flame length. Due to the role of the flame length, the contribution of near-wall CO to the exhaust CO increases as dilution level or the wall temperature is reduced. Premixed flames can extinguish inside the cold-wall thermal boundary layer, which can leave high near-wall CO. This results in disproportionate levels of CO mass flux in the near-wall regions. The near-wall CO features large variations when the local

Damköhler number is greater than 0.1. Analysis of the CO transport budget shows that unlike 1D simulation, both convection and diffusion dominate the CO transport in the near-wall region, except for the case with autoignition at the wall.

Finally, a three-Dimensional (3D) turbulent V-flame in a channel was simulated with hot and cold walls. A main reaction zone in the central region supported by periodic bulk ignition events changes the position of volumetric reaction zones where CO is formed. Consistent with the 2D results, a lower wall temperature leads to a longer flame, thereby having more contribution to the exhaust CO. Near-wall turbulence-flame interaction creates wrinkled and streaky flame surfaces, and localizes the near-wall CO distribution. High mean of CO mass fraction locates in the free-stream where the free-stream autoignition happens, while the high RMS of CO mass fraction is present closer to the wall. 1D flame solutions might be sufficient for modelling CO in the free-stream region and some parts of the near-wall region but not closer to be adjacent to the wall. Turbulent mixing and diffusion contribute to this deviation. These results set a benchmark for future near-wall CO modelling.

# 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,

Bin Jiang

14<sup>th</sup> of March, 2021

# Acknowledgements

I would like to express my eternal gratitude to the following people for their support during this project, without which this thesis would not have been possible.

## **Financial**

The work presented in this thesis was supported by the University of Melbourne through the Research Training Program Scholarship and the scholarship from China Scholarship Council. The author acknowledges the generous support of the European Centre for Research and Advanced Training in Scientific Computation (CERFACS, <http://www.cerfacs.fr>), in providing the source code for NTMIX-CHEMKIN. In particular, the author thanks Dr. Benedicte Cuenot for her help with NTMIX-CHEMKIN. The research was supported by computational resources on the Australian NCI National Facility through the National Computational Merit Allocation Scheme and by resources at the Pawsey Supercomputing Centre.

## **Academic**

I would like to thank my primary supervisor Robert Gordon: his constant support and belief have made this project as well as financial supports. I thank my co-supervisor Mohsen Talei: his insights and inputs into the project have greatly improved its outcome, especially for the numerical resources. To my academic committee members Yi Yang and Michael Brear, their helpful feedback and advice greatly aided my growth as a researcher.

## **Research**

I am grateful to Davy Brouzet for his help in learning NTMIX-CHEMKIN. My thanks to Jacob Rivera and Rahul Palulli for helping me get started on the FWI

topic. I am thankful for Pavel Panek and Jen Zen Ho for helping me develop post-processing approaches.

### **Colleagues and Co-Workers**

To my co-workers in the Thermodynamics Laboratory and colleagues in the Melbourne Energy Institute, thank you for making my working environment productive and enjoyable, and for the lasting friendships that I have made during my time there.

### **Personal**

I thank my friends for carrying me through this time and helping me stay sane. I am grateful for my family, especially for my father Hanjun Jiang, my mum in the heaven and for my sisters Yanjiao, Yanping and Fei, whose endless love and tireless support was invaluable to completing this work.

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# Nomenclature

## Acronyms

|         |                                  |
|---------|----------------------------------|
| °C      | Degree Celsius                   |
| 0D      | Zero-Dimensional                 |
| 1D      | One-Dimensional                  |
| 2D      | Two-Dimensional                  |
| 3D      | Three-Dimensional                |
| AI      | Autoignition                     |
| ARC     | Analytically Reduced Chemistry   |
| BL      | Boundary Layer                   |
| CDC     | Colorless Distributed Combustion |
| DNS     | Direct Numerical Simulation      |
| EGR     | Exhaust Gas Recirculation        |
| FGM     | Flamelet Generated Manifold      |
| FLOX    | FLameless OXidation              |
| FLOXCOM | FLameless OXidation COMbustion   |
| FPF     | Freely Propagating Flame         |
| FWI     | Flame-Wall Interaction           |
| GT      | Gas Turbine                      |

|         |                                                 |
|---------|-------------------------------------------------|
| HOQ     | Head-On Quenching                               |
| IC      | Internal Combustion                             |
| JHC     | Jet in Hot Coflow                               |
| JICF    | Jet In Hot Cross-Flow                           |
| LEAF    | LEan Azimuthal Flame                            |
| LES     | Large Eddy Simulation                           |
| LHS     | Left-Hand Side                                  |
| MILD    | Moderate or Intense Low-oxygen Diluted          |
| NSCBC   | Navier-Stokes Characteristic Boundary Condition |
| OPPDIFF | Opposed-Flow Flame Model                        |
| PDF     | Probability Density Function                    |
| PF      | Premixed Flame                                  |
| PFR     | Plug Flow Reactor                               |
| ppm     | particle per million                            |
| QSS     | Quasi-steady state                              |
| RANS    | Reynolds-Averaged Navier-Stokes                 |
| REDIM   | REaction and DIffusion Manifold                 |
| RHS     | Right-Hand Side                                 |
| RMS     | Root-Mean Square                                |
| SWQ     | Side-Wall Quenching                             |
| UHC     | Unburned hydrocarbon                            |
| W(P)SR  | Well (Perfect) Stirred Reactor                  |

**Uppercase Roman**

|                      |                                  |     |
|----------------------|----------------------------------|-----|
| $\tilde{Y}_{CO,exh}$ | Average exhaust CO mass fraction | [-] |
|----------------------|----------------------------------|-----|

|            |                                                              |                                    |
|------------|--------------------------------------------------------------|------------------------------------|
| $C$        | Convection term in the species equation                      | $[\text{kg.m}^{-3}.\text{s}^{-1}]$ |
| $D$        | Diffusion term in the species equation                       | $[\text{kg.m}^{-3}.\text{s}^{-1}]$ |
| $H$        | Half channel width in 3D DNS                                 | $[\text{mm}]$                      |
| $L_f$      | Flame length in 2D simulation                                | $[\text{mm}]$                      |
| $MW$       | Molecular weight                                             | $[\text{g.mol}^{-1}]$              |
| $N_x$      | Number of grids along streamwise direction                   | $[-]$                              |
| $N_y$      | Number of grids along transverse direction                   | $[-]$                              |
| $N_z$      | Number of grids along spanwise direction                     | $[-]$                              |
| $Q_w$      | Wall heat flux                                               | $[\text{MW.m}^{-2}]$               |
| $R$        | Reaction term in the species equation                        | $[\text{kg.m}^{-3}.\text{s}^{-1}]$ |
| $T_b$      | Burned gas temperature                                       | $[\text{K}]$                       |
| $T_p$      | Time period of one cycle for the inlet forcing velocity      | $[\text{s}]$                       |
| $T_u$      | Unburned gas temperature                                     | $[\text{K}]$                       |
| $T_{wall}$ | Wall temperature                                             | $[\text{K}]$                       |
| $U$        | Streamwise velocity                                          | $[\text{m.s}^{-1}]$                |
| $U^+$      | Normalized streamwise velocity by the wall friction velocity | $[-]$                              |
| $X_\alpha$ | Mole fraction of species $\alpha$                            | $[-]$                              |
| $Y^+$      | Y coordinate in wall unit                                    | $[-]$                              |
| $Y_\alpha$ | Mass fraction of species $\alpha$                            | $[-]$                              |
| HRR        | Heat Release Rate                                            | $[\text{MW.m}^{-3}]$               |

#### Lowercase Roman

|            |                               |                 |
|------------|-------------------------------|-----------------|
| $\Delta x$ | grid spacing in $x$ direction | $[\mu\text{m}]$ |
| $\Delta y$ | grid spacing in $y$ direction | $[\mu\text{m}]$ |
| $\Delta z$ | grid spacing in $z$ direction | $[\mu\text{m}]$ |

|                      |                                                          |                         |
|----------------------|----------------------------------------------------------|-------------------------|
| $\tilde{m}_{CO,exh}$ | Average exhaust CO mass flux                             | [kg.s <sup>-1</sup> ]   |
| $c$                  | The speed of sound                                       | [m.s <sup>-1</sup> ]    |
| $c_{CH_4}$           | Progress variable based on CH <sub>4</sub> mass fraction | [-]                     |
| $c_p$                | Specific heat capacity                                   | [J.kg.K <sup>-1</sup> ] |
| $c_T$                | Progress variable based on temperature                   | [-]                     |
| $f$                  | Inlet forcing frequency in 2D DNS                        | [Hz]                    |
| $n_x$                | Streamwise component of flame normal                     | [-]                     |
| $n_y$                | Transverse component of flame normal                     | [-]                     |
| $n_z$                | Spanwise component of flame normal                       | [-]                     |
| $p$                  | Pressure                                                 | [atm]                   |
| $s_{L,0}$            | Adiabatic unstrained laminar flame speed                 | [m.s <sup>-1</sup> ]    |
| $t_Q$                | Quenching instant in 1D head-on quenching simulation     | [ms]                    |
| $u_\tau$             | Friction velocity at the wall in 3D DNS                  | [m.s <sup>-1</sup> ]    |
| $x$                  | Streamwise coordinate                                    | [-]                     |
| $y$                  | Wall normal coordinate                                   | [-]                     |
| $z$                  | Spanwise coordinate                                      | [-]                     |

### Greek Symbols

|                        |                                                    |                                        |
|------------------------|----------------------------------------------------|----------------------------------------|
| $\delta_{F,diffusive}$ | Diffusive flame thickness                          |                                        |
| $\delta_{ini,fw}$      | Initial flame-wall distance in 1D HOQ              | [mm]                                   |
| $\delta_{ini,tbl}$     | Initial thermal boundary layer thickness in 1D HOQ | [mm]                                   |
| $\delta_Q$             | Quenching distance                                 | [mm]                                   |
| $\delta_{th,0}$        | Thermal flame thickness                            | [mm]                                   |
| $\dot{\omega}$         | Production rate                                    | [kg.m <sup>-3</sup> .s <sup>-1</sup> ] |
| $\eta_k$               | Kolmogorov length scale                            | [μm]                                   |

|              |                                     |                                                 |
|--------------|-------------------------------------|-------------------------------------------------|
| $\lambda$    | Thermal conductivity                | $[\text{J.m}^{-1}.\text{k}^{-1}.\text{s}^{-1}]$ |
| $\nu$        | Kinematic viscosity                 | $[\text{m}^2.\text{s}^{-1}]$                    |
| $\Phi$       | Equivalence ratio                   | $[-]$                                           |
| $\rho$       | Density                             | $[\text{kg.m}^{-3}]$                            |
| $\tau_f$     | Flow through time in 3D DNS         | $[\text{s}]$                                    |
| $\tau_{F,0}$ | Flame time, $\delta_{th,0}/s_{L,0}$ | $[\text{s}]$                                    |
| $\zeta$      | Dilution level                      | $[-]$                                           |

### Subscripts

|                |                                 |
|----------------|---------------------------------|
| $(i)(j)(k)$    | Grid index                      |
| $(x)(y)(z)(t)$ | Spatial and temporal components |
| 0              | Initial time                    |
| $\alpha$       | Species                         |
| $\infty$       | Ambient conditions              |
| $ac$           | Acoustic quantity               |
| $ad$           | Adiabatic flame quantity        |
| $AI$           | Autoignition quantity           |
| $CL$           | Centreline quantity             |
| $F$            | Fuel-related quantity           |
| $flam$         | Flammability-limited quantity   |
| $in$           | Inlet quantity                  |
| $ini$          | Initial quantity                |
| $p$            | Period of time                  |
| $peak$         | Peak value                      |
| $Q$            | Quenching quantity              |



|                  |                                                      |
|------------------|------------------------------------------------------|
| <i>reactants</i> | Reactants-related quantity                           |
| <i>ref</i>       | Reference quantity                                   |
| <i>t(n)</i>      | Tangential or normal quantity along the flame normal |
| <i>target</i>    | Targeted quantity                                    |
| <i>u</i>         | Unburned-related quantity                            |
| <i>wall</i>      | Wall-related quantity                                |

### Superscripts

|          |                                                               |
|----------|---------------------------------------------------------------|
| '        | Fluctuating quantity regarding ensemble mean                  |
| *        | Non-dimensional quantity with reference value                 |
| +        | Non-dimensional quantity with wall units or friction velocity |
| <i>T</i> | Temperature dependent quantity                                |

### Operators and Symbols

|                   |                                            |
|-------------------|--------------------------------------------|
| –                 | Mixture-averaged quantity                  |
| $\delta$          | Kronecker delta                            |
| $\int$            | Integral operator                          |
| $  $              | Absolute operator                          |
| $\partial$        | Partial differential operator              |
| $\sum$            | Summation operator                         |
| $\sim$            | Statistically temporal and spatial average |
| <i>max.(min.)</i> | Maximum or minimum operator                |

### Non-dimensional numbers

|        |                                                                                            |
|--------|--------------------------------------------------------------------------------------------|
| $Da_f$ | Damköhler number in 2D DNS, defined as $\frac{1}{\tau_{F,0} f}$                            |
| $Fo$   | Fourier number, defined as $Max.(\bar{\nu} \frac{\Delta t}{\Delta h^2} \frac{1}{Re_{ac}})$ |
| $Pe$   | Peclet number, defined as $\frac{\delta_Q}{\delta_{F, diffusive}}$                         |

|           |                                                                                   |
|-----------|-----------------------------------------------------------------------------------|
| $Re$      | Reynolds number in 3D DNS, defined as $\frac{HU_{in}}{\nu}$                       |
| $Re_{ac}$ | Acoustic Reynolds number, defined as $\frac{a_{ref}\rho_{ref}L_{ref}}{\mu_{ref}}$ |
| $St$      | Strouhal number in 2D DNS, defined as $\frac{fL_f}{U_{in}}$                       |

# Chapter 1

## Introduction

### 1.1 Background and Motivation

Attempts to mitigate global warming are driving penetration of renewable energy in electrical generation systems. Due to increasing requirements for system stability, Gas Turbines (GTs) are essential in a high Variable Renewable Energy economy [1]. The dependence of renewable energy on natural weather and remote locations creates a variability in supply that can be supported by industrial gas turbines. However, this requires the industrial gas turbines to operate at part-load. These engines typically operate on natural gas as a fuel, and in 2018, natural gas consumption increased 4.6%, accounting for almost half of global energy demand growth [2].

#### 1.1.1 Gas Turbines Emissions at Part Load

Industrial gas turbines are designed to operate at peak power while maintaining low pollutant emissions. Part-load operation can lead to high CO emissions, as shown in Figure 1.1 [3]. At low loads,  $\text{NO}_x$  emission is low, largely due to the suppression of the thermal  $\text{NO}_x$  formation pathway. However, CO emission can quickly exceed legislated limits, which are typically between 10 to 25 ppm.

The chemical and physical processes for  $\text{NO}_x$  formation are largely understood for natural gas and other hydrocarbon fuels. However, the interaction of the various physical and chemical processes that influence the formation and oxidation of CO are

not as well understood. CO turndown, defined as the maximum power reduction where engine CO emissions remain below the legislated limits, is a main constraint for part-load operations [4].

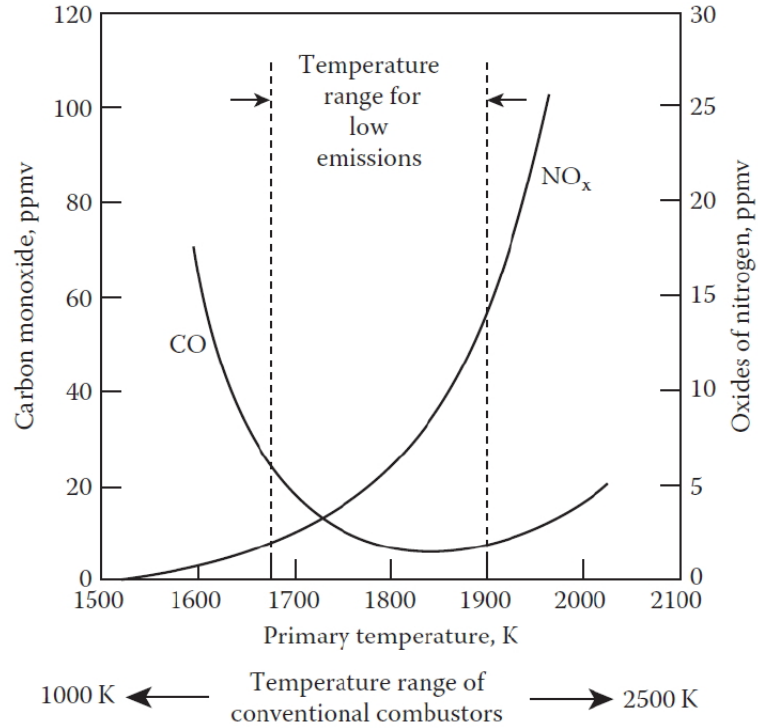


Figure 1.1: Trade-off between CO and NO<sub>x</sub> emissions at part-load conditions [3]

Three main hypotheses have been presented for high CO emissions at part load conditions:

1. Incomplete combustion due to either a rich fuel/air equivalence ratio, or insufficient residence times,
2. Poor fuel-air mixing causing localised rich mixture zones, forming pockets of high CO concentration,
3. Quenching of the flame due to wall heat transfer, or due to interaction with film/effusion cooling air.

It is the last of these which motivates this work.

### 1.1.2 Flames Diluted by Hot Combustion Products

One method to reduce emissions and extend the operating range of industrial engines is to dilute the flame. This is often achieved by using a portion of the exhaust gases of the flame as the diluent, which is known as Exhaust Gas Recirculation (EGR). In industrial gas turbines, low  $\text{NO}_x$  has been achieved by lowering or controlling combustion temperatures with steam addition, nitrogen dilution, lean premixed combustion and axial or radial staging of the combustion. Axial staging, where part of the fuel is injected later in the combustor into the hot combustion products, can lead to combustion regions of reduced oxygen concentration and temperatures above the autoignition temperature. In a diluted flame, peak temperatures are reduced, which reduces thermal  $\text{NO}_x$  formation and  $\text{CO}_2$  dissociation into CO. At extreme dilution levels, a combustion regime alternately known as Moderate or Intense Low oxygen Diluted (MILD) combustion [5], FLameless OXidation (FLOX) [6] or Col-orless Distributed Combustion (CDC) [7] can be achieved. It features autoignition stabilisation, lower peak temperatures, broadened reaction zones and low flame luminosity. This has been demonstrated to achieve low  $\text{NO}_x$  emissions experimentally and numerically, but can have unpredictably high CO emissions depending on the configuration.

### 1.1.3 Flame-Wall Interaction for Flames Diluted by Hot Combustion Products

Flames diluted by hot combustion products can often interact with combustor walls, which are generally colder than the temperature of the main reaction zone. This can affect the chemistry of the reaction zone by introducing heat loss and near-wall turbulence inside the velocity and temperature boundary layers. Further, the wall may attenuate CO oxidation, which may outweigh the advantage of low CO formation in diluted flames. The autoignition in diluted combustion can be inhibited by heat loss, the flame surface can be wrinkled by near-wall turbulence, and the flames can alter near-wall turbulence and heat the wall. These interactions are shown in Figure 1.2.

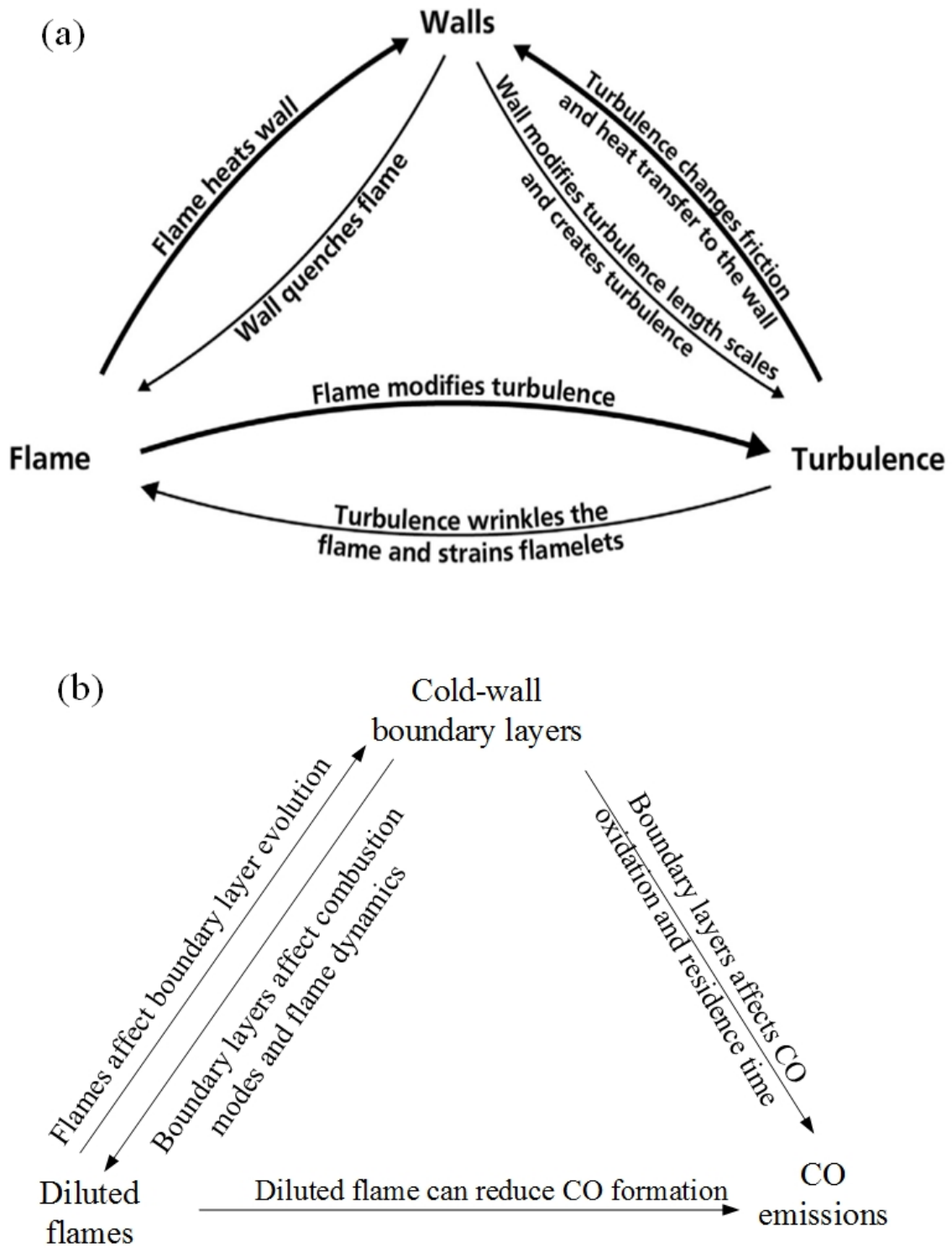


Figure 1.2: (a) Top: Relationships between flame, turbulence and wall[8, 9]. (b) Bottom: Diluted flames, wall and CO emissions. Modified from [8, 9].

## 1.2 Research Goals

Flame-Wall Interaction (FWI) for turbulent methane/air flames diluted by hot combustion products has not yet been investigated. Autoignition is strongly affected by local turbulence, and the near wall scales are so small as to make experimental investigation extremely challenging [10]. DNS of these effects can fully resolve the turbulence structures. Further, resolution of the near-wall and quenching chemistry is important to these interactions. The overall objective of this project is therefore to investigate the flame dynamics, combustion modes and near-wall CO characteristics in FWI for flames diluted by hot combustion products, using DNS with detailed chemistry. Laminar and turbulent flow conditions will be studied, across a variety of FWI configurations and conditions.

# Chapter 2

## Literature Review

### 2.1 Introduction

Flames diluted by combustion products can reduce emissions such as CO and NO<sub>x</sub>. In most applications, such as in gas turbine combustion, these flames are confined in a combustor and can interact with relatively cold walls. This interaction can quench the flame and may produce incomplete combustion products. In this chapter, the fundamentals of FWI and parametric influences on FWI behaviour and CO emissions are reviewed. Following this, the physics and chemistry of flames diluted by hot combustion products are reviewed, focusing on experimental and numerical studies into the emissions from MILD combustion. The most recent literature on FWI for diluted combustion is then reviewed. The gaps in this literature are summarised, followed by a proposal of research aims.

### 2.2 Flame-Wall Interaction (FWI)

This section reviews the foundations of FWI. Investigations into the effects on FWI behaviour of wall temperature, surface chemistry, pressure, and turbulence are reviewed. The findings and limitations of recent studies into CO emissions due to FWI are then discussed.



### 2.2.1 Basic Parameters of FWI

FWI is a two-way coupling process where flame and wall mutually interact. The flame alters the boundary layer features, while the wall quenches the flame by wall heat loss. Wall quenching can be divided into two geometric extremes: Head-On Quenching (HOQ), where flame propagation is perpendicular to the wall; and Side-Wall Quenching (SWQ), with the flame burning parallel to the wall. A schematic of these two quenching processes are shown in Figure 2.1 [8]. Literature also categorized the neither parallel nor perpendicular quenching into SWQ [9] or oblique-wall quenching [11].

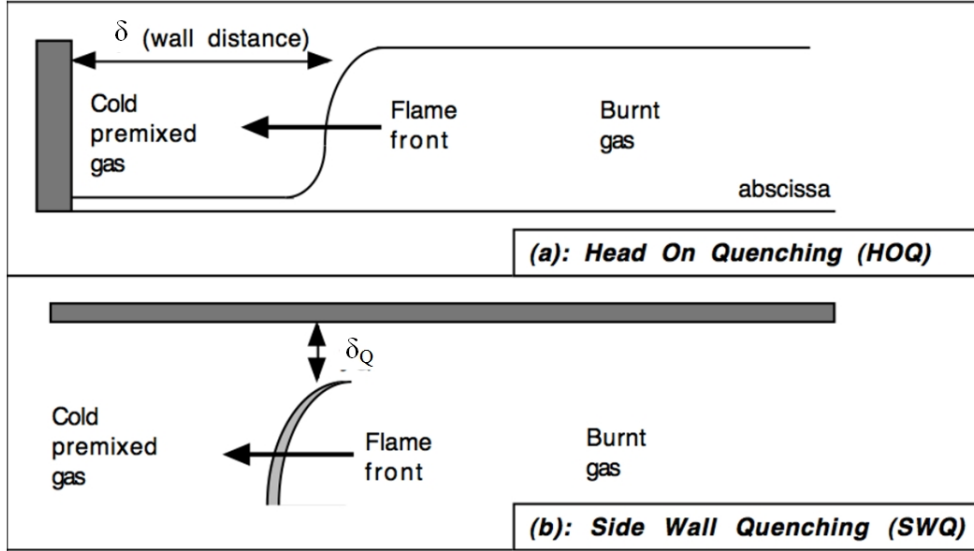


Figure 2.1: Schematic of Head-On Quenching (HOQ) (top) and Side-Wall Quenching (SWQ) (bottom). [8]

The quenching distance is of primary importance for the analysis of amplified heat flux during FWI. It is denoted  $\delta_Q$ , and defined as the minimum distance between the heat release zone of a premixed flame and the wall. Zirwes et al. studied the quenching distance of methane flame under different simulation setups, including 20 different chemical kinetic mechanisms, 1-3D dimensions, transport models, i.e. thermal diffusion, multi-component transport and Lewis number. The results showed that the Lewis number has the most dominant effect than other setting parameters [12]. Flame-wall distances are commonly non-dimensionalised by a flame thickness to obtain a local Peclet number ( $Pe$ ) [13]. At the quenching point, the minimum

$Pe$  number is

$$Pe_Q = \frac{\delta_Q}{\delta_{F, diffusive}} \quad (2.2.1)$$

where the diffusive flame thickness,  $\delta_{F, diffusive}$ , is used for the normalisation. The diffusive flame thickness is obtained by:

$$\delta_{F, diffusive} = \frac{\lambda_u}{\rho_u c_p s_{L,0}} \quad (2.2.2)$$

Where  $\lambda_u$  denotes the thermal conductivity of the unburned reactants,  $\rho_u$  is the reactant density,  $c_p$  is the specific heat capacity, and  $s_{L,0}$  is the adiabatic, unstrained laminar burning velocity.

For HOQ, the minimum Peclet number for methane/air flames is in the order of  $Pe_Q = 3.5 \pm 1$ . For SWQ, the minimum Peclet number is around 7.0 [13]. This number is almost independent of the equivalence ratio.

Time evolution in FWI was often normalized by the flame time [13]. The flame time,  $\tau_{F,0}$ , is defined as Equation 2.2.3.

$$\tau_{F,0} = \frac{\delta_{th,0}}{s_{L,0}} \quad (2.2.3)$$

where the  $s_{L,0}$  is the laminar, unstrained and adiabatic flame speed;  $\delta_{th,0}$  is the thermal flame thickness as shown in Equation 2.2.4.

$$\delta_{th,0} = \frac{T_{ad} - T_u}{max.(dT/dx)} \quad (2.2.4)$$

Wall heat flux,  $Q_w$ , is another important quantity in FWI, defined as

$$Q_w = \lambda \frac{dT}{dy}_{wall} \quad (2.2.5)$$

where  $\lambda$  is the thermal conductivity of the gas next to the wall, and  $(dT/dy)_{wall}$  is the wall-normal temperature gradient next to the wall.  $Q_w$  was generally normalized

by the flame power, defined as  $\rho_u Y_f s_{L,0} c_p (T_{ad} - T_u)$ .

### 2.2.2 Effects of Wall Temperature and Surface Chemistry on FWI

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, reducing  $\delta_Q$ . As a result, the wall heat flux increases, provided the wall temperature is much less than the adiabatic flame temperature.

Kosaka et al. studied the quenching distances at different wall temperatures experimentally with methane/air mixture in a V-flame configuration [14]. A decreasing quenching distance was observed at higher wall temperatures, yet this was coupled with a higher wall heat flux. In a non-reacting 1D heat transfer problem, higher  $T_{wall}$  should decrease the temperature gradient, leading to reduced wall heat transfer. This counter-intuitive result validates the findings of Boust et al. [15], who showed the same inverse proportionality between  $\delta_Q$  and wall heat transfer, even at higher  $T_{wall}$  [15].

The wall temperature alters the near-wall chemistry, and thus the quenching process. Westbrook et al. found that as the flame approaches the wall, heat loss in the flame activates exothermic radical recombination reactions that recombine radicals into less active species [16]. These low activation energy reactions form the major radical consumption pathway, as the temperature decreases due to heat loss.

Wall temperature also affects the surface reactivity. Three types of wall mechanisms were tested in a numerical study on wall reactivity effects on lean methane/air flames ( $\Phi = 0.2$  and  $0.4$ ) [17]:

- Inert wall: no surface reaction, and surface diffusion and Stefan velocity are zero. This condition isolates velocity and thermal boundary layer effects from catalytic wall effects.
- Recombination wall: this allows adsorption, recombination and desorption but without surface reactions. The heat release rate in the gas-phase is allowed as per [18]. The wall adsorbs active radicals (e.g. H, OH, O), and rejects them

as stable species (e.g.  $\text{HO}_2$ ,  $\text{H}_2\text{O}_2$ ). Surface diffusion and Stefan velocity are not zero.

- Catalytic wall: this allows recombination, adsorption, desorption and catalytic surface reactions. The surface diffusion and Stefan velocity are not zero.

They studied a 2D stationary boundary layer flow, where the pressures were set to 1 atm and 10 atm, and the wall temperatures were 600 K and 1200 K, corresponding to conditions in internal combustion engines and gas turbine engines, respectively. The wall could be regarded as chemically inert for lean combustion at  $T_{\text{wall}} = 600$  K. At a higher wall temperature (1200 K), the catalytic platinum surface retards homogeneous combustion of methane more than a recombination wall, indicated by a larger quenching distance.

These studies were extended by Kim et al., who used stoichiometric methane/air flames in a slot burner [19]. Figure 2.4 shows that the quenching distance is significantly affected by the surface temperature. Wall temperature has little effect up to 500 °C, after which the quenching distance rapidly reduces. A reactive wall surface delays this by about 100 K. Beyond 800 °C, the surface reactivity has almost no effect on the quenching distance for the alumina and quartz walls.

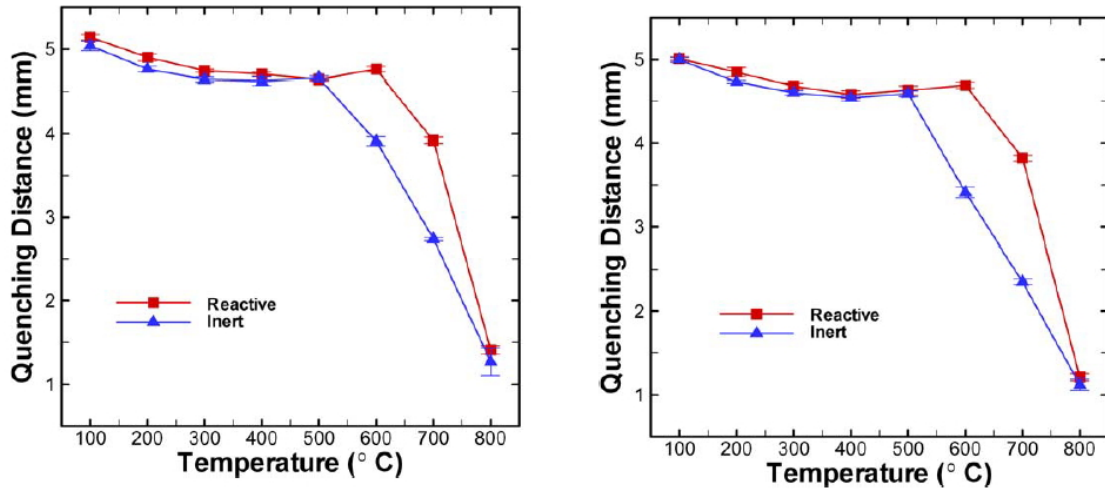


Figure 2.2: Quenching distance for reactive and inert alumina (left) and quartz (right) surfaces at different wall temperatures [19]

Popp, Smooke and Baum compared an inert wall with a catalytic platinum wall in a 1D HOQ for methane and propane/air flames [20]. Figure 2.3 shows that below 400

K wall temperature, the reactivity is negligible for methane, while above this the surface reactivity appears to play an increasingly important role on the wall heat flux. The numerical results tend to over-predict the wall heat flux compared to the experimental findings, as the heat loss to the surroundings (except for the wall) is not included in the computational studies. The experimental results exhibit little variation in this temperature range, consistent with [19].

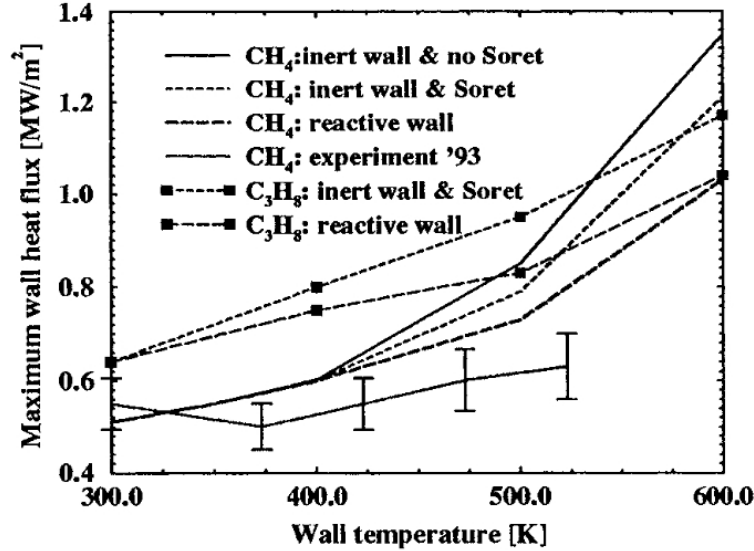


Figure 2.3: Variation of the dimensional maximum wall heat flux with wall temperature for a stoichiometric methane/air and propane/air flame [20]

Vlachos et al. used a recombination wall to check the role of wall quenching of radicals on the ignition and extinction of premixed CH<sub>4</sub>/air flames in a stagnation model [21]. They found that the removal of H, O and OH radicals retards the flame stability. The short residence time at high strain rate inhibits CO oxidation and promotes extinction.

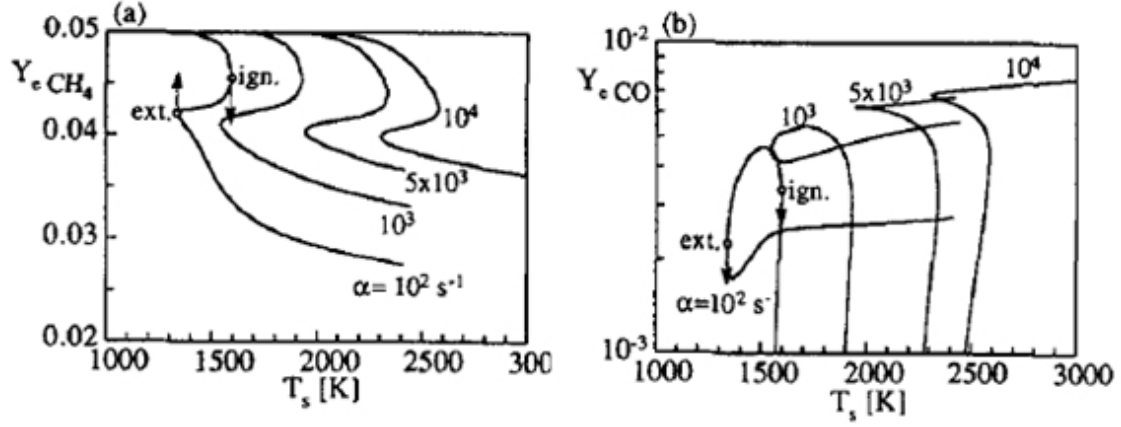


Figure 2.4: Wall temperature effects on  $\text{CH}_4$  and  $\text{CO}$  under different strain rates ( $\alpha$ ) at the outlet of a stagnation model [21].

Despite the surface chemistry effects at high wall temperature, some studies choose hot inert walls, even up to 1200 K  $T_{\text{wall}}$  [22–24]. One explanation is that consideration of surface chemistry for a given wall material may limit the generality of the results, as a number of wall materials may be used in practical combustors [24].

Egolfopoulos et al. studied wall temperature effects on the prediction of laminar flame speed in a stagnation model [25]. They found that at a low strain rate, the wall heat loss and H radical removal do not affect the flame speed, which attains the same value with opposed jet flames. Similarly, Narukawa et al. studied the flame displacement speed of methane/air flames at 300 K, 500 K, 700 K and 900 K wall temperatures in a 2D closed domain [26]. They found that the H radical removal from the surface chemistry reduces heat release rate at the wall. However, this region is closer to the wall than the quenching distance, as such it does not affect the near-wall flame displacement speed.

These stagnation model studies were initialised with the combustion products near the wall. Recently, Luo et al. studied the strain rates and wall temperature effects on  $\text{CO}$  thermochemical states with reactants next to the wall [27]. They found that compared with 300 K wall temperature, the strain rate does not affect the  $\text{CO}$  thermochemical state within the quenching region at 600 K wall temperature.

### 2.2.3 Effects of Pressure on FWI

As gas turbine combustion takes place at elevated pressures, it is important to understand the influence of pressure on FWI behaviour. These effects have been principally studied in HOQ and narrow-slot configurations. Several studies have shown power law relationships between pressure and quenching distance, e.g. [28, 29]. An inverse relationship between pressure and quenching distance was reported as a power-law relation where  $\delta_Q$  is inversely proportional to the  $n^{th}$  power of pressure. Westbrook et al. reported a power law for methane/air flames in the HOQ case as [16]:

$$\delta_Q = 0.5p^{-0.56} \quad (2.2.6)$$

where  $\delta_Q$  is the quenching distance in mm, and  $p$  is the pressure in atm. They also reported that the fuel remaining at  $t_Q$  is smaller at a higher pressure condition. The smaller quenching distance enhances the diffusion of the near-wall reactant into the reaction zone. Sotton et al. reported an inverse power of 1.27 for methane in the parallel plate configuration, but deviations from this were observed above 3 atm [28].

The impact on quenching distances is a combination of the effects of pressure on laminar flame speed, radical recombination reactions, heat transfer and density and as such needs to be carefully explored in the context of FWI. Not only are the scaling laws limited in configuration generality, they appear to be limited in range as well.

### 2.2.4 Turbulent Flame-Wall Interaction

Turbulent FWI brings the addition of turbulent eddies to the dynamics of laminar FWI. These eddies introduce flame stretch, and they can interact with or disrupt the heat and mass transfer processes in the flame reaction zone and can induce the ejection of burnt and unburned gases into and out from the wall. As a flame approaches the wall, the local viscosity increases, and this can also dampen the near-wall turbulence.

Early investigations on turbulent FWI used 3D DNS with single-step chemistry.

Bruneaux et al. conducted 3D back-to-back turbulent premixed FWI in a channel [30]. They found that horseshoe vortexes push the flame towards the wall, while fresh gases escaped from the wall in finger-like structures. To quantify the effects of turbulence, they used a 1D stagnant FWI model. The results led to the development of a FWI model based on flame surface density [31].

To achieve statistically stationary FWI, Alshaalan and Rutland simulated 3D turbulent FWI with single-step chemistry in a Couette flow with a hot spot in the domain to anchor the flame [32]. They observed that the probability of the four quadrants of the near-wall Reynolds stresses change as flame approaches the wall by comparing constant and variable density simulations. This changed the turbulent production term into a destruction term, demonstrating the effects of the flame on the turbulence. They found that the high-speed streaks increase flame stretch but decrease the heat transfer, while low-speed streaks have the opposite effect. They also found turbulence pushing the flame towards the wall, increasing the wall heat flux, and the law-of-the-wall scaling becomes 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. To further study the unsteady effects from turbulent streaks on wall heat flux, they conducted a simplified 2D DNS with forced inlet wall-normal velocity. They found that, as the wall-normal velocity increased from negative to zero, an upstream flame motion was observed and closer to the wall and further increased the wall heat flux.

Janiski et al. measured the turbulent boundary layer evolution during FWI [33]. The flame suppresses the turbulent boundary layer during quenching, while the ‘new’ boundary layer grows much faster than the cold boundary layer upstream the quenching point. They also reported that the flow field does not change significantly with stoichiometry. Their study further confirms the turbulent destruction during FWI reported by Alshaalan and Rutland [32].

Lai and Chakraborty conducted 3D turbulent HOQ with one-step chemistry [34]. They studied the Lewis number effects on wall heat flux, the mean reaction rate and the scalar dissipation rate. This led to a modification of a closure of mean reaction rate using the scalar dissipation rate. This modification was further validated with



detailed chemistry [35]. Recently, Zhao, et al. identified two types of flame front and flame speed characteristics in the above 3D HOQ configuration with one-step chemistry[36]. Based on the relation between the flame normal and wall normal, they identified entrained and HOQ flame fronts, and the entrained flame fronts are more common within the quenching region. They also conducted oblique-wall quenching with one-step chemistry, as HOQ does not consider the evolution of a turbulent boundary layer [11]. It was found that the minimum flame-wall distance in oblique-wall quenching is smaller than the HOQ.

Gruber et al. conducted 3D turbulent SWQ DNS in a channel with  $H_2$ /air with detailed chemistry [24]. A flame anchor was imposed in the domain to create a  $H_2$ /air V-flame, with  $T_{wall} = 750$  K. It was reported that radical recombination reactions near the wall contribute around 70% of HRR, and these reactions combine with vorticity, resulting in high wall heat flux. In addition, they found a regime change from the thin flamelet to wrinkled flame, due to thickening and reduced flame speed near the wall. However, the flame speed does not drop to zero close to the wall, due to diffusion. They demonstrated that the turbulent length and time scales have strong correlation with the wall heat flux. Figure 2.5 also shows that the flow exhibits ‘quasi-laminarization’ downstream the flame tip. Recent work by Palulli et al. on methane/air flames confirmed that radical recombination reactions are responsible for the majority of wall HRR even for hydrocarbon flames [37].

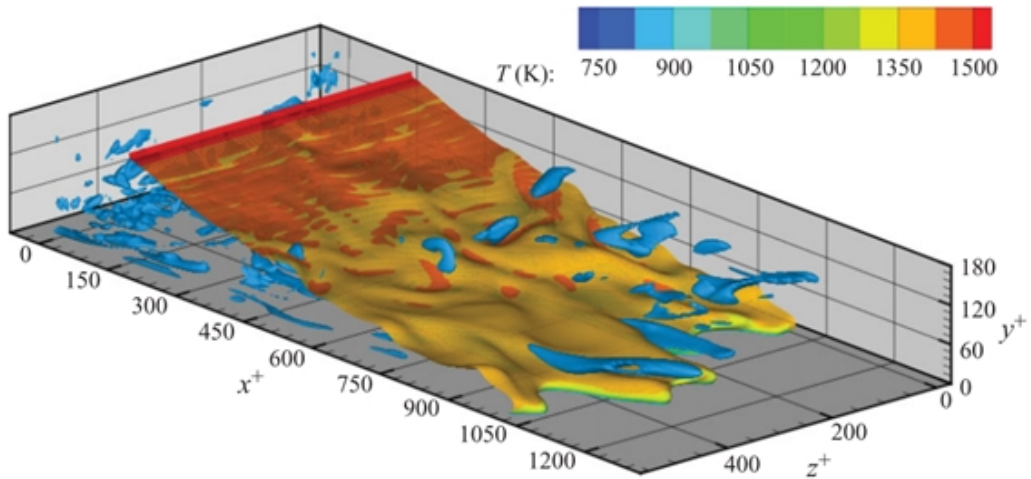


Figure 2.5: Instantaneous flame surface marked with progress variable of  $H_2$  at  $c = 0.7$  colored by the local temperature and iso-surface of the vorticity magnitude (blue). [24]

Heinrich et al. studied 3D SWQ V-flame with LES with methane/air flames [38]. His numerical setup was validated on the SWQ experiments from TU Darmstadt, with turbulence statistics in both non-reacting and reacting cases, including mean/RMS velocities [33]. This is the only FWI numerical study with experimental validation. They studied the probability of HOQ and SWQ modes based on the flame-wall angle. Furthermore, they categorized three types of flame movements, including downstream, upstream and jump-like movements. The jump-like movements deviated the SWQ to HOQ regime and attain maximum wall heat flux, which increases the difficulty of statistical modelling of these regions.

Ahmed et al. simulated a 3D turbulent FWI of stoichiometric methane/air flames with one-step chemistry [39]. Isothermal and adiabatic wall boundaries were compared. They found that the flame surface near the adiabatic wall is more wrinkled than near an isothermal wall, as shown in Figure 2.6. They explained this flame shape by examining the heat loss effects on the dilatation rate near the wall. An isothermal wall introduces a heat loss and attenuates the turbulent flame intensity. The adiabatic wall boundary condition should then be considered to be insufficient for high fidelity simulation of FWI.

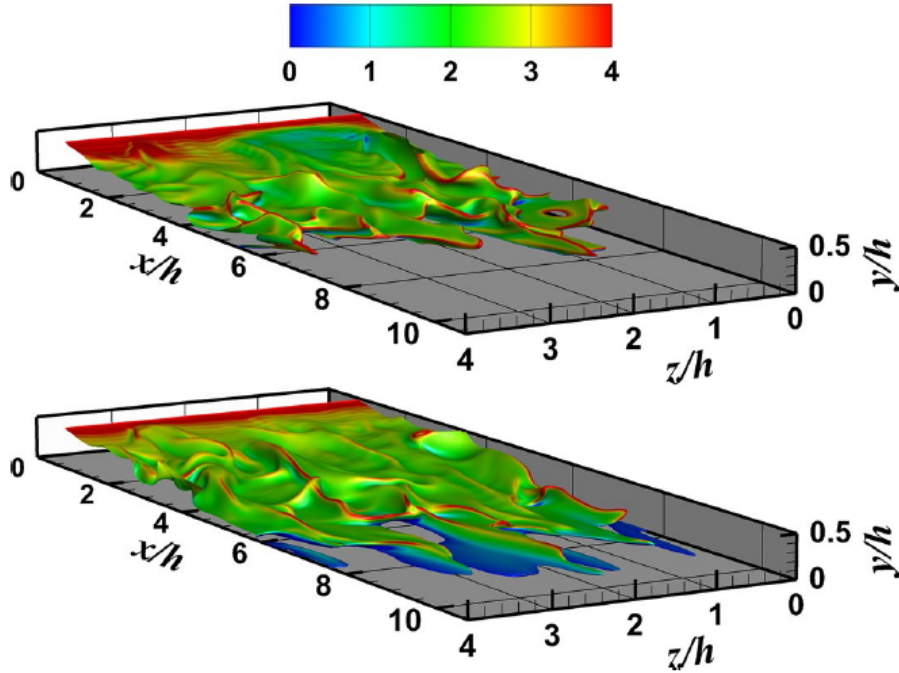


Figure 2.6: Bottom half of the instantaneous turbulent flames represented by flame front iso-surface coloured by normalised dilatation rates for adiabatic (top) and isothermal (bottom) walls [39]

It is clear that 3D DNS is required to appropriately investigate near-wall turbulence and turbulent boundary layer effects in FWI [40]. The finest experimental resolutions are still of order of the quenching distance. However, the detailed resolution near the wall constrains the simulation fidelity due to the high cost. Similar to the surface chemistry discussion, detailed kinetics near the wall, coupled with turbulence, is required to capture all the relevant physics related to emissions from FWI. For the simplest hydrocarbon, methane, such kinetics test the limits of 3D DNS, and only very few studies have appeared for near-wall 3D turbulent DNS of methane with detailed kinetics.

### 2.2.5 CO Emissions and FWI

One of the primary motivations in investigating FWI is the potential for contribution to exhaust emissions. It is hypothesized that the flame quenching and reduced oxidation processes near the wall can contribute to significant exhaust CO. CO behavior was first examined numerically in a HOQ simulation in [41]. They compared CO/CO<sub>2</sub> mechanisms at 300 K and 600 K as shown in Figure 2.7. The following reaction becomes non negligible at 600 K wall temperature:



Not only is this observation important for wall temperature effects, but such third-body reactions are often sensitive to pressure effects as well, and third-body efficiencies of some combustion products can be much higher than the reactant gases.

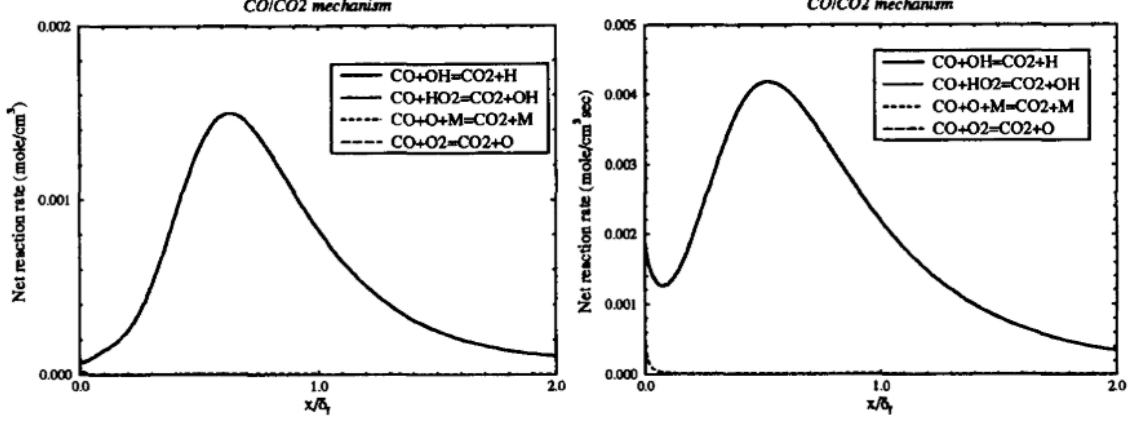


Figure 2.7: Net production rate at quenching instant. Left figure is at 300 K wall temperature, and the right figure is at 600 K wall temperature [41].

In HOQ experiments, Mann et al. conducted both laminar and turbulent HOQ in a stagnation burner with methane/air [42]. They found that high CO region in statistically stationary turbulent HOQ is closer to the wall than in laminar steady results. This is attributed to turbulent eddies pushing the heat release zones closer to the wall. Also, the transient HOQ leads to higher near-wall CO than steady stagnation results. A full understanding of the influence of these mechanisms motivated the work of Rivera et al. and Palulli et al. and require further investigation to determine their role in exhaust CO emission [37, 43]. Palulli et al. conducted a forced 2D laminar premixed methane/air SWQ simulation, which features statistically stationary FWI [37]. Detailed chemistry with the GRI3.0 chemical kinetics mechanism was used [44]. The excitation is generated with a sinusoidal velocity at the inlet with different frequencies, non-dimensionalized as the Strouhal number ( $St$ ),

$$St = \frac{f L_f}{U_{in}} \quad (2.2.8)$$

where  $f$  is the forcing frequency,  $L_f$  is the maximum streamwise distance between the flame front and the inlet, and  $U_{in}$  is the maximum inlet convective velocity.

Temperature-CO scatter plots are plotted at an intermediate forcing frequency,  $St = 1$ , from a moving window around the flame tip in the right of Figure 2.8. Combined with the HRR contour on the left figure of Figure 2.8, it shows that a Freely Propagating Flame (FPF) and HOQ are the two extreme conditions during SWQ,

with the SWQ manifolds lying between these two boundaries when the bulk flame is a preheated, premixed flame. This work used undiluted reactant and was without autoignition. At highly diluted condition, autoignition may affect the reaction zone response to the forcing and the flame length.

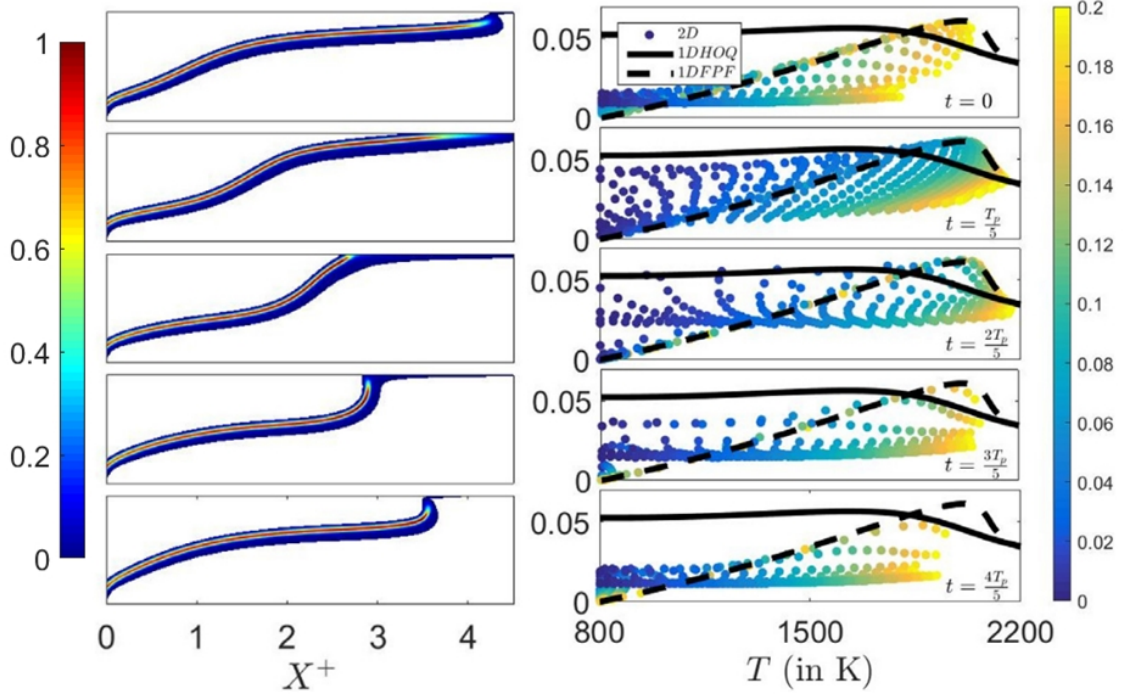


Figure 2.8: Left: HRR contours at several instants with the same time interval during one cycle for forcing frequencies,  $St = 1$ .  $T_p$  is the cycle period of the inlet velocity. Right: Scatter plots of Temperature versus CO mass fraction in a window with a width of 10 times of thermal flame thickness on either side of the flame tip and a height of 2 times of thermal flame thickness from the wall.  $T$ -CO plots of 1D HOQ and 1D FPF are also shown for reference. The points are coloured by the distance from the wall [37]

Ganter et al. recently conducted 2D laminar methane/air SWQ simulation [45]. They reported that the diffusion is more dominant in the near-wall CO transport than the reaction as shown in Figure 2.9. For some flames, the integral of the diffusion term in Lagrangian coordinates can predict the observed near-wall CO.

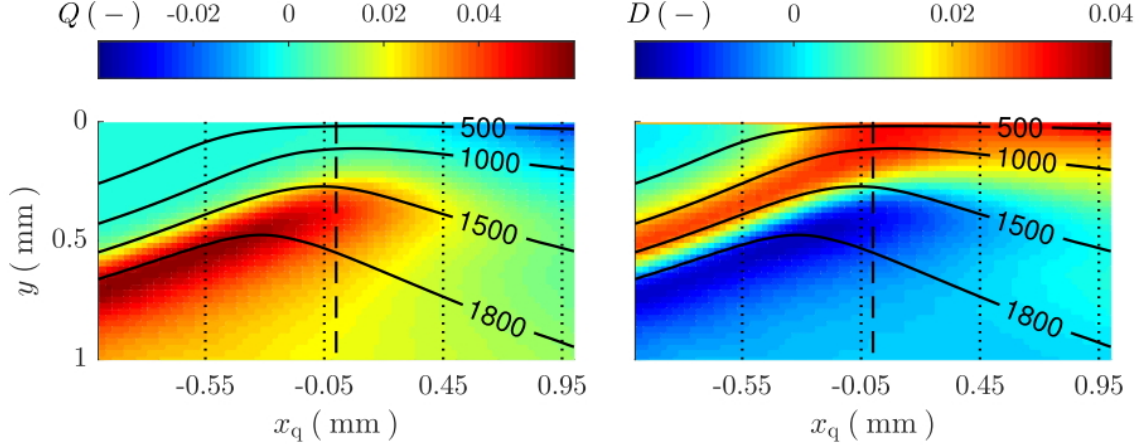


Figure 2.9: Integrated source term,  $Q$ , (left); integrated diffusion term,  $D$ , (right) with temperature isolines (K) (Solid black line), quenching point position (dashed black line) and streamwise positions (dotted black line).[45]

Klarmann et al. investigated stretch and heat loss effects on combustion and CO emissions for a model GT combustor, to improve CO emission modelling [46–48]. They modified the Flamelet-Generated Manifold (FGM [49]) model by adding stretch and heat loss to the tabulated flamelets and extracting a local Favre-averaged stretch and heat loss from the CFD as an input. A correction factor as a function of stretch and heat loss was attained which was used to modify the reaction source term. This correction affects the species distribution in the flame, such as CO.

To then refine the treatment of CO specifically, three zones are modelled separately: the in-flame zones; the post-flame zones; and the quenching zones. The pre-flame zones were ignored. The in-flame zone is treated with the modified FGM model. A Damköhler number based on CO oxidation rate and flow timescale was used as the criterion for the transition from the in-flame to post-flame CO modelling. The CO burnout in the post-flame zones has a longer timescale than the formation and is dominated by the CO oxidation reaction:



Therefore, they added a CO transport model with treatment for burnout based on Eq. 2.2.9 in the post-flame zones. In this reaction, OH has a much faster creation rate than the CO consumption rate and is treated as being at equilibrium as a

function of mixture fraction.

The transition from post-flame zone to quenching zone is defined by the timescale ratio of OH formation and oxidation. In the quenching zone, OH has an equivalent formation rate to CO burnout and thus cannot be treated as equilibrium. However, OH is dominated by five key reactions whose reactants can be treated as equilibrium. Therefore, OH formation rate was then tabulated as a function of mixture fraction.

The CO model predicted CO well in part-load conditions of fuel-staged combustor. Neglecting heat loss leads to high CO in the in-flame zone and significant underestimation of CO in the post-flame zone, as the CO formation and oxidation rates are higher at high temperatures. Without the quenching zone model, CO is also underestimated, as OH is not at equilibrium. This model approach demonstrated reduced performance in quenching with lean burnout. Such non-equilibrium OH in lean burnout may also exist in FWI.

A similar FGM approach was tested by Ganter et al. in a 2D SWQ simulation [50]. In their approach, the scalar dissipation rate in the enthalpy direction was treated as zero, which inhibits CO diffusion in that dimension. This leads to up to 80% underestimation of near-wall CO compared to detailed chemistry. However, an improved tabulated chemistry based on 1D HOQ, REaction-Diffusion Manifold (REDIM [51]) overall performed well for CO and temperature prediction. Variances of around 12 % were attributed to the gradients of CO<sub>2</sub> and enthalpy in HOQ being 30 % higher than for SWQ. This indicates that an improved understanding of the detailed kinetic response during FWI may significantly improve the fidelity of near-wall CO modelling.

Efimov, de Goey and van Oijen recently improved the FGM treatment of FWI for CO modelling [52]. They used 1D laminar HOQ to generate a 3D Quenching Flamelet Manifold (QFM). A rate of enthalpy loss dimension was added in the QFM by tabulating 1D flames with different inlet velocity and temperature. This 3D QFM predicted CO in 2D laminar SWQ well, however, has not been extended to turbulent FWI.

None of these studies have considered flames diluted by hot combustion products.

There are three additional effects that may impact CO modelling:

1. Local exhaust gas dilution may add another dimension to the tabulated manifold.
2. At high dilution level, the reactants can autoignite, which may challenge the validity of neglecting the preheating zone.
3. Diluted flames may extinguish due to increased minimum flammable temperatures. This may also affect the assumption of equilibrium OH in the post-flame CO burn-out.

In experimental study, Kosaka et al. measured the CO in the burner mentioned above in SWQ experiments with DME [53]. They defined a CO oxidation timescale based on a 1D FPF flame, and a heat transfer timescale was calculated based on the thermal conductivity and heat capacity. Comparing the adiabatic and non-adiabatic conditions in Figure 2.10, CO oxidation shifts to low temperature region when the heat transfer timescale is shorter than the CO oxidation. They conducted non-adiabatic flame modelling by adding an energy sink term into the 1D energy conservation equation. This sink term accounts for the effective energy loss experienced by the flame, as a result of the wall heat transfer. The non-adiabatic flame simulations show decreasing post-flame CO concentration, as the post-flame gas temperature decreases with wall heat loss. After considering non-adiabatic effects in a 1D simulation, the temperature-CO scatter matches the 3D data better than in the adiabatic condition, as shown in Figure 2.11. Despite this, their results still do not account for the large CO concentrations that they and Jainski et al. measured near the wall [54].



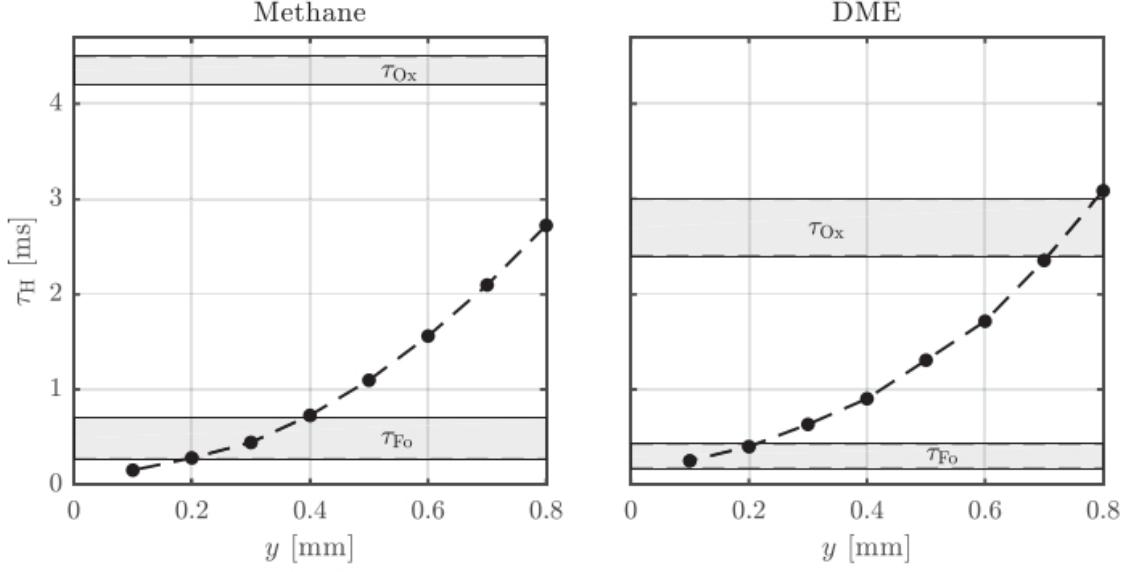


Figure 2.10: Estimated timescales of wall heat transfer (dots), CO oxidation (upper shaded region) and CO formation (lower shaded region), for stoichiometric methane (left) and DME (right) flames [53]

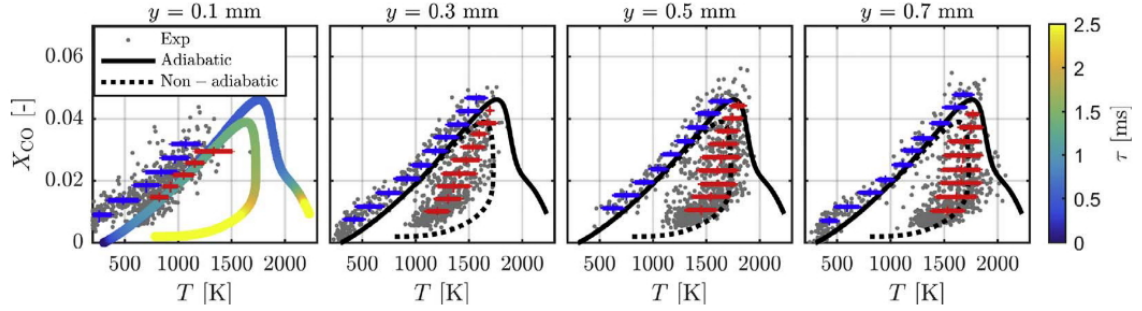


Figure 2.11: Scatter plots of gas-phase temperature and CO mole fractions. Conditional mean (blue and red dots) and root-mean square, (error bar) of experimental data are compared to the results obtained from 1D laminar flame calculations with (dotted line) and without wall heat transfer (solid line). For the wall-normal distance,  $y = 0.1$  mm, laminar flame simulations are colour-coded; the different colours represent time duration from start of the simulation. All data recorded at 330 K wall temperature. [53]

To study cooling rate effects on FWI, Rivera et al. [55] studied laminar SWQ with a controllable cooling rate. They found that a higher cooling rate leads to lower semi-local CO, while far downstream the CO is not affected. They also found that the forcing frequency and amplitude do not affect the quenching distance and the semi-local locations, indicating the CO cannot be modelled by the quenching distance only, unlike the wall heat flux.

Rivera et al. also studied temperature and residence time effects on CO oxidation and exhaust CO at atmospheric pressure [55]. The CO oxidation time ( $t_{cool}$ ), defined as the time from the peak CO ( $Y_{CO,peak}$ ) to a threshold defined as [53].

$$Y_{CO} = Y_{CO,equilibrium} + 0.1(Y_{CO,peak} - Y_{CO,equilibrium}) \quad (2.2.10)$$

Three CO oxidation timescales were used as references:  $\tau_{Ad}$  is the CO oxidation timescale of the adiabatic case from FPF solution (4.1 ms);  $\tau_{EGC}$  is the CO oxidation timescale of the exhaust-gas-cooling case from 1D DNS by implementing a heat loss term from [53] (7.4 ms);  $\tau_{GT}$  is the approximated residence time of gas turbine combustor, estimated to be 20 ms [4]. Figure 2.12 shows that temperatures between 1200 K to 1800 K range have both low equilibrium levels of CO and very fast oxidation chemical time scales, leading to very low CO. Above 1800 K, the CO oxidation is controlled by the high equilibrium CO value at this temperature. Below 1200 K, the CO oxidation rate decreases with decreasing the temperature, leading to high exhaust CO. This is supported by Correa, who studied exhaust CO along a 2D laminar boundary layer [56]. The results showed that the post-flame non-equilibrium CO at 1100 K wall temperature can quickly reach equilibrium and does not contribute high exhaust CO. In this regards, relatively cool walls may have a significant impact on exhaust CO.

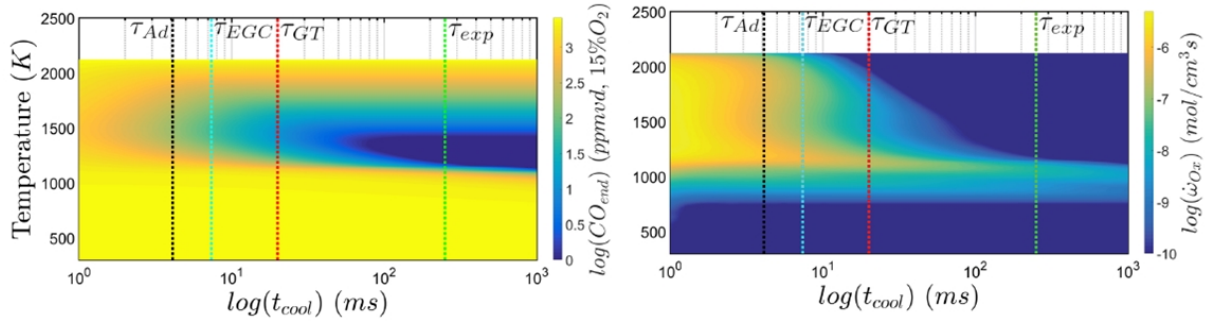


Figure 2.12: Contours of CO (left) and CO production rate (right) in logarithmic colourbars at different temperatures and cooling residence time ( $t_{cool}$ ) [55]

It is clear from the recent work on CO in FWI that the competing kinetics, timescales and physical processes are not fully resolved and have a leading effect on the final CO from wall regions.

## 2.3 Flames Diluted by Hot Combustion Products

Dilution with EGR is common in reciprocating and constant pressure engines to reduce  $\text{NO}_x$ . As noted in the Introduction to this thesis, high levels of EGR can lead to MILD combustion [5], also known as FLOX [6] or CDC [7]). This section will review dilution approaches and their effects, laboratory scale MILD combustors, diluted combustion in a gas turbine context, and the literature on exhaust CO from such burners.

### 2.3.1 Diluted and MILD Flames

#### 2.3.1.1 Dilution Approaches and Diluents Effects

Flames can be diluted with purely inert gases, water or with mixed compositions from combustion products. When diluting with combustion products, it is possible to achieve dilution with external or internal EGR. External EGR is usually accompanied with a cooling of the combustion products, which can also lead to a change in the equilibrium composition of the recirculated gases, most notably a reduction in the minor species and radical concentrations. Internal recirculation (within the combustion chamber) can be achieved quasi-adiabatically, or with some cooling, depending on the flow path of the product gases. No matter the approach taken, the objective is a reduction in the reaction rates of the combustion, which reduces the peak temperatures of the flame fronts, and lowers  $\text{NO}_x$  formation. This can occur through a reduction in oxygen concentration, changes in the specific heat of the mixture, and cooling from the diluent gases [5]. It is common to approach EGR combustion as at least partially premixed, where the reacting charge has been mixed with the exhaust gases prior to combustion .

The approach followed in this work was first developed by Sidey et al., who approximated internal hot combustion product recirculation numerically with an instantaneous, adiabatic mixing [57]. This case was proposed to be relevant to the rapid EGR found in a gas turbine context, where mixing is much faster than the flow timescale. This mixing process couples dilution and preheating. The undiluted re-

actants were at 298 K, and these were reacted in a freely propagating premixed flame to produce combustion products, taken at the equilibrium post-flame region.

A dilution level,  $\zeta$ , was defined as the mass flow rate ratio of the hot combustion products to the total mixture. Figure 2.13 shows that the reactant temperature increases and the  $O_2$  concentration decreases with increasing dilution level. This mixing approach maintains an almost constant enthalpy across the entire dilution range from  $\zeta = 0$  to 1.

$$\zeta = \frac{\dot{m}_{products}}{\dot{m}_{products} + \dot{m}_{reactants}} \quad (2.3.1)$$

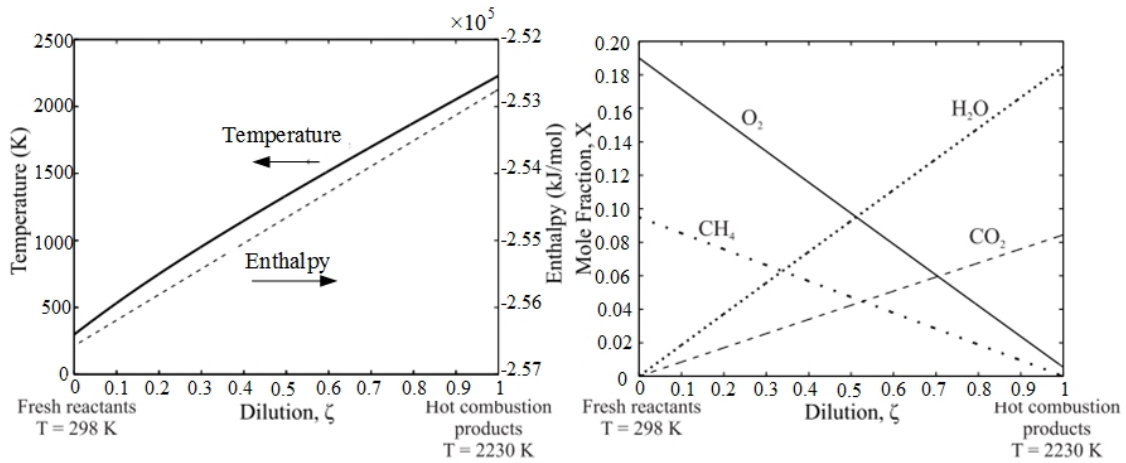


Figure 2.13: Temperature (left) and mass fraction (right) under adiabatic mixing.

The effects of the EGR species have been investigated by several authors, and can be separated into the effects of the major combustion product species, the reduction of oxygen, and the effects of the minor species and radicals. The species can affect the mixture reactivity, as well as the physical and thermodynamic properties of the gas.

The major species in hydrocarbon EGR are  $H_2O$ ,  $CO_2$  and  $N_2$ . While  $N_2$  is typically present in undiluted combustion, the effects of the other two products should be noted.  $CO_2$  and  $H_2O$  have three main effects [4]:

1. The molar specific heats of the triatomic molecules  $CO_2$  and  $H_2O$  are higher compared to  $N_2$ .

Therefore, at a constant equivalence ratio,  $\text{CO}_2$  and  $\text{H}_2\text{O}$  in the reactants reduce the flame temperature. Dally et al. reported that, in a fuel stream diluted with either  $\text{N}_2$  or  $\text{CO}_2$ , a furnace can achieve low  $\text{NO}_x$  and an invisible flame [58]. However, more  $\text{N}_2$  than  $\text{CO}_2$  was needed, because of the higher heat capacity of  $\text{CO}_2$ .

2. The transport properties of  $\text{CO}_2$ ,  $\text{H}_2\text{O}$  and  $\text{N}_2$ , including thermal conductivity, diffusivity and viscosity, are different from hydrocarbon fuels.

The viscosity affects the flow field and turbulence, thermal conductivity affects the heat transfer, and the diffusivity affects the availability of reactant and oxidiser during combustion.

$\text{CO}_2$  has around 20 % less binary diffusivity with  $\text{O}_2$  compared with  $\text{N}_2$  at 2000 K temperature, while the thermal conductivity and viscosity are equivalent to  $\text{N}_2$ . At around 1500 K temperature,  $\text{H}_2\text{O}$ 's binary diffusivity with  $\text{O}_2$  is around 30 % higher than  $\text{N}_2$  and  $\text{CO}_2$ , and the thermal conductivity of  $\text{H}_2\text{O}$  is double that of  $\text{N}_2$  and  $\text{CO}_2$ , while the dynamic viscosity is comparable to  $\text{N}_2$  and  $\text{CO}_2$ .

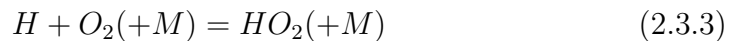
Owston, et al. found that adding  $\text{N}_2$  to reactants, both near-wall thermal conductivity and temperature gradient decrease, which reduce wall heat flux [23].

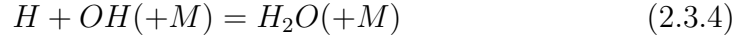
3.  $\text{CO}_2$  and  $\text{H}_2\text{O}$  alter the concentration of the  $\text{H}/\text{OH}/\text{O}$  radical pool, increasing the  $\text{OH}$  concentration while decreasing the  $\text{O}$  and  $\text{H}$  concentration.

$\text{CO}_2$  affects the partitioning of  $\text{H}/\text{OH}/\text{O}$  by shifting the  $\text{CO}$  oxidation reaction, Eq. 2.2.9, which affects combustion processes, including pollutant and  $\text{CO}$  formation.  $\text{H}_2\text{O}$  changes the radical pool through:



and radical recombination is affected through:





The third body efficiency of  $H_2O$  is 16 times higher than  $N_2$  and 4.3 times larger than  $CO_2$ , and these reactions compete with the main chain branching reaction,



All of these effects may be important in FWI for dilute hydrocarbon flames, particularly as highly reactive radicals and intermediate species in the hot products can alter the ignition behaviour significantly, as reported by Sidey et al. and Doan and Swaminathan [57, 59]. While low  $O_2$  and high  $H_2O$  and  $CO_2$  decrease flame temperature and inhibits thermal  $NO_x$ , less  $O_2$  tends to reduce the  $OH$  and  $O$ , while high  $H_2O$  and  $CO_2$  could increase  $OH$ . These changes can have different or even contradictory effects on the radical pool concentration that affects  $CO$  emissions.

### 2.3.1.2 MILD Combustion

Cavaliere and de Joannon provide a definition for MILD combustion as: “*A combustion process when the inlet temperature of the reactant mixture is higher than mixture self-ignition temperature, whereas the maximum allowable temperature increase with respect to inlet temperature during combustion is lower than mixture self-ignition temperature (in Kelvin).*” [5]. Which is to say that the process is stabilised through autoignitive mechanisms, but lacks the heat release rate to trigger thermal runaway.

Figure 2.14 shows a laminar MILD combustion in a simulation of a jet in hot coflow with methane/air mixture [60]. The left figure shows MILD combustion, while the right figure is a premixed flame. The reaction zone is more distributed in the MILD combustion. As MILD combustion is autoignited, the combustion mode was examined by plotting the species transport budget for  $OH$  as shown in Figure 2.15. At  $4 \text{ m.s}^{-1}$  conditions, an autoignition mode exists, indicated by negligible streamwise diffusion term ( $D_x$ ), while it switches to premixed combustion with increasing the inlet velocity to  $30 \text{ m.s}^{-1}$ . The fully unsteady species transport budget can be found in the Numerical Methods Chapter, Section 3.2.4.

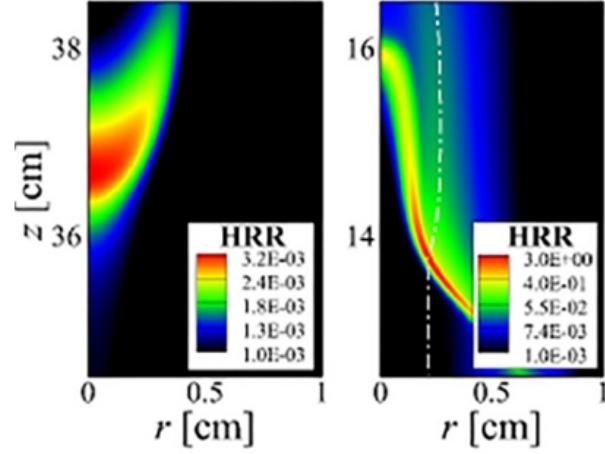


Figure 2.14: Isocontour of HRR ( $\text{J} \cdot \text{mm}^{-3} \cdot \text{s}^{-1}$ ) for autoignited laminar lifted methane/hydrogen jet flames with  $U_0 = 4$  (left) and  $15 \text{ m} \cdot \text{s}^{-1}$  (right). The dash-dotted line represents the stoichiometric mixture fraction iso-line [60].

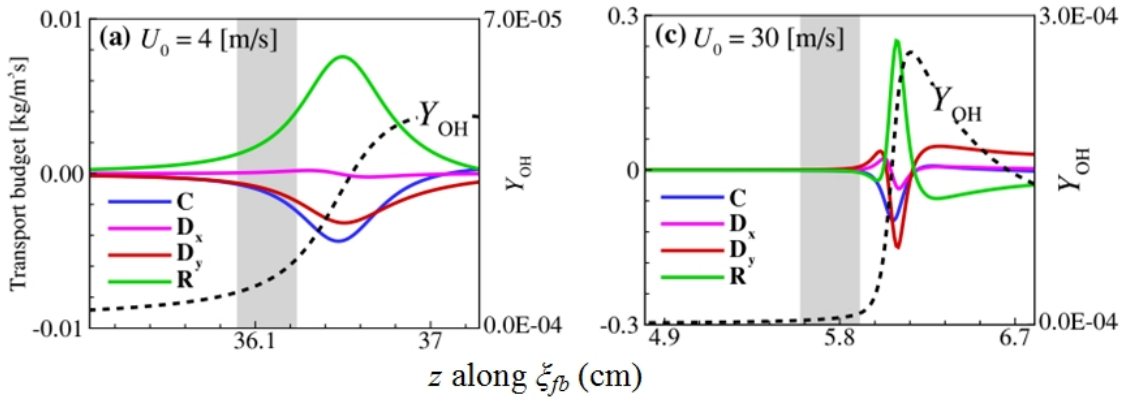


Figure 2.15: Species transport budget of OH on the flame with different inlet velocities. (a)  $4 \text{ m} \cdot \text{s}^{-1}$ ; (b)  $30 \text{ m} \cdot \text{s}^{-1}$ . Adapted from [60]

A turbulent EGR-type MILD combustion is shown in Figure 2.16 [61]. It shows coexisting reaction-dominated and propagation-dominated regions. This is mainly induced by the initial inhomogeneous mixing field in their study. They considered turbulent mixing in the dilution and attained an inhomogeneous mixing field from undiluted to purely product states. A threshold is defined to determine the combustion mode,  $B^+ = |C - D| - |R|$ , where the  $C$ ,  $D$  and  $R$  are from the transport equation with normalized temperature.  $B^+ < -1.5$  was defined as a reaction-dominated region; a region with  $B^+ > 1.5$  was dominated by flame propagation; the rest was entangled with these two combustion mode.

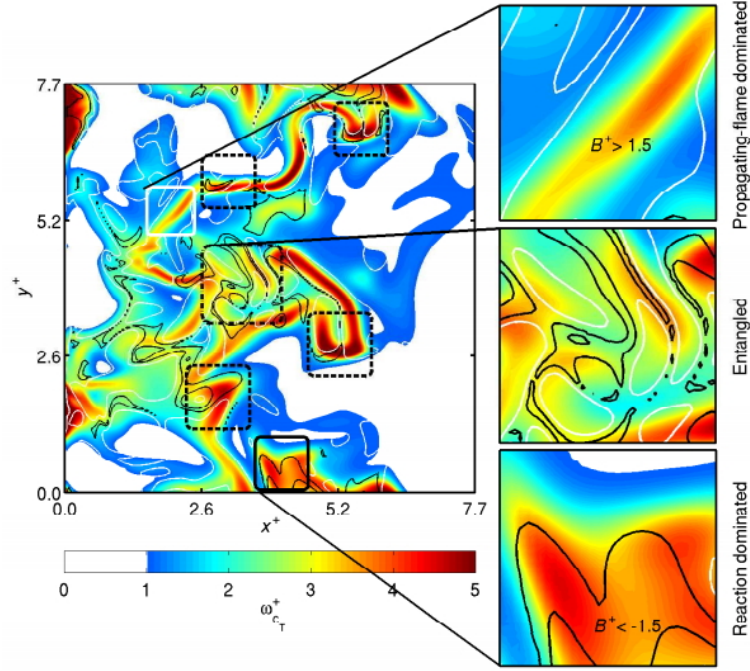


Figure 2.16: DNS contour of reaction rate with three combustion modes, including reaction-dominated ( $B^+ = -1.5$ , white contour lines), propagating-flame dominated ( $B^+ = 1.5$ , black contour lines)

and entangled regions. Reaction rate is defined on the progress variable with temperature.  $B^+$  is defined as  $|C - D| - |R|$ . [61]

## 2.3.2 Diluted Flames in Gas Turbines Context

### 2.3.2.1 Experimental Studies

Diluted combustion in an industrial gas turbine can be established with internal recirculation or a staged combustor. In a staged combustor, hot combustion products from the primary combustor ensures the secondary stage works at high combustion efficiency and stability. Additional stages add degrees of freedom to the system, and therefore allow a better control of temperatures, emissions and thermo-acoustics [3]. The FLameless OXidation COMbustion (FLOXCOM) [62], LEan Azimuthal Flame (LEAF) combustor [63] and CDC [64] use internal recirculation, and FLOX [65] and Ansaldo GT26/36 [66] uses the staged concept. The exploration of MILD for gas turbine combustion is inspired by the successful application of MILD combustion in furnaces. Unlike a furnace, a gas turbine generally has less residence time for mixing, and significantly higher pressure, which enhances the chemical kinetics.



Zanger et al. reported the successful operation of a FLOX-based combined heat and power system designed for natural gas in a staged micro gas turbine as shown in Figure 2.17 (a) [65]. They reported significant CO emissions of about 700 ppmvd @15% $O_2$  at part load. It was hypothesised that at part load conditions, the reaction zone is more distributed and extends to the exit. Near the exit, the cooling air quenches the reaction and increases the CO.

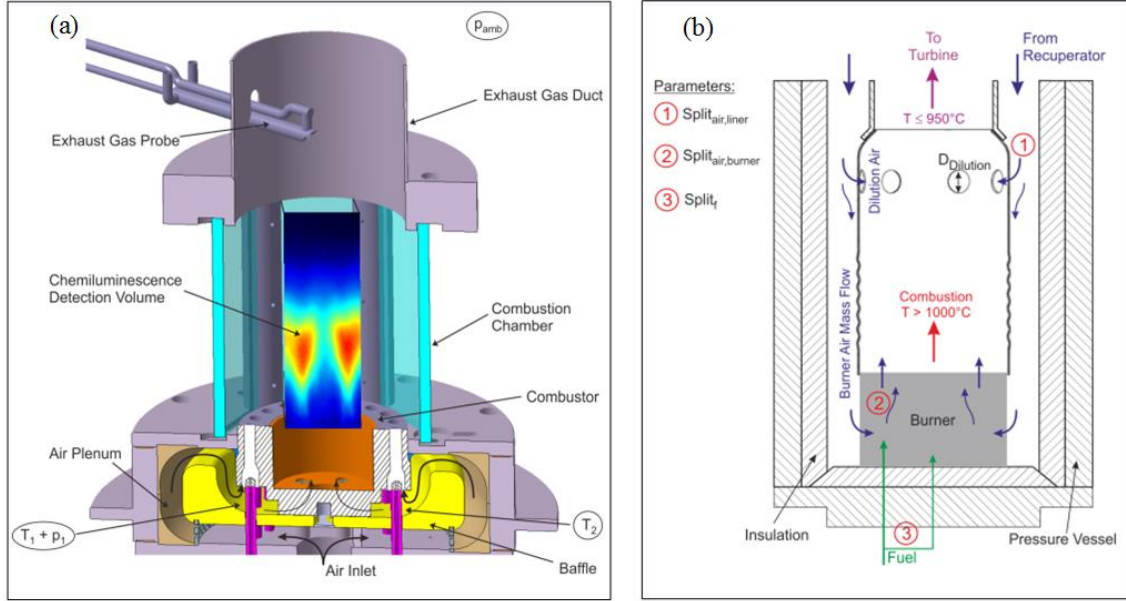


Figure 2.17: (a) Schematic of the FLOX-based combustor; (b) different paths of process air and fuel flow in the micro gas turbine chamber [65]

Khalil and Gupta [67] developed a high thermal intensity combustor producing ultra-low  $NO_x$  and CO emissions which is applicable for stationary GTs. One of their premixed CDCs is shown in Figure 2.18. The tube extension inside the combustor increased the residence time, and promoted a stronger swirl, resulting in a more efficient combustion. The reaction zone (marked with  $OH^*$ ) can be close to the wall, due to this tangential injection and swirling flow. This increases the probability of FWI.

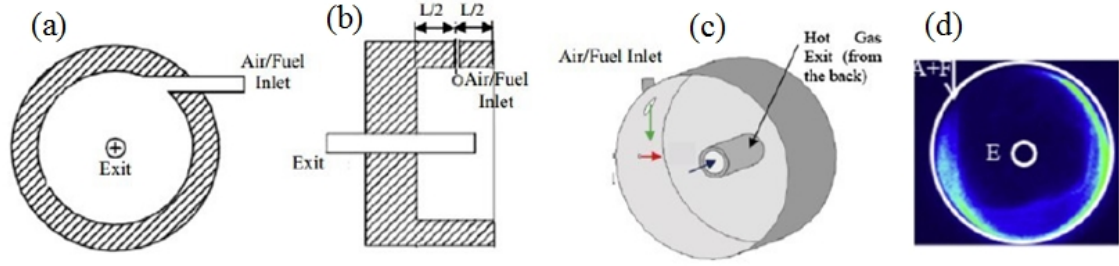


Figure 2.18: Premixed CDC combustor (a: top section at middle location, b: front section at cylinder axis, c: 3D model, d: OH\* marked reaction zone) [67]

The high thermal efficiency of MILD combustion helps downsize GT burners. Gupta reported that to achieve the same heat release intensity the size of MILD combustor can be reduced by 30% [68]. Arghode and Gupta developed three CDC combustors sizes with same length and different diameters resulting in heat release intensity of 20, 30 and 40 MW.m<sup>-3</sup>.atm [64]. They reported that increasing the heat release intensity from 20 to 40 MW.m<sup>-3</sup>.atm at equivalence ratio of 0.5, the CO @15%O<sub>2</sub> increases from 150 to 450 ppm. They speculated that the reason could be lower residence time associated with higher heat release intensity.

These efforts to implement MILD combustion in the context of gas turbines highlight that the approaches tend to increase FWI and reduce residence time. In many cases, while low NO<sub>x</sub> has been achieved, low CO has not, and this could be from a lack of understanding or control of the CO formation and oxidation pathways. Further, as MILD combustion relies on autoignitive processes to stabilise, it needs to be investigated whether the cold walls are inhibiting autoignition and transitioning the combustion to a preheated, premixed propagation, and what effect this has on the CO behaviour of these mixtures.

### 2.3.2.2 Numerical Studies

Experimental iteration to optimise CO is prohibitive in these industrial geometries, and hence numerical simulation is relied on to predict temperature, velocity and species distributions. The fidelity of the numerical models is essential for such approaches to be beneficial, and the prediction of CO continues to be problematic. These burners have been studied numerically with Reynolds-averaged Navier-Stokes

(RANS), Large Eddy Simulation (LES), and DNS [64, 69, 70]. The secondary combustor of the Ansaldo GT26 was simulated with LES to understand the high exit CO at the part-load condition [69]. They used tabulated chemistry and the stochastic fields model for turbulence-chemistry interaction. Figure 2.19 shows that the main reaction zone at a lower load (LP1) moves more downstream than at high load (LP3). The high CO region at LP1 is closer to the wall. The main reaction zone is widened at low load and increases the contact area of the reaction zone and the wall. A high CO tail (200 to 400 ppm) along the wall exists at LP1, and it was hypothesised that the interaction between the reaction zone and the wall was responsible. This high CO region at low load is consistent with the FLOX burner mentioned in Section 2.3.2.1 [65].

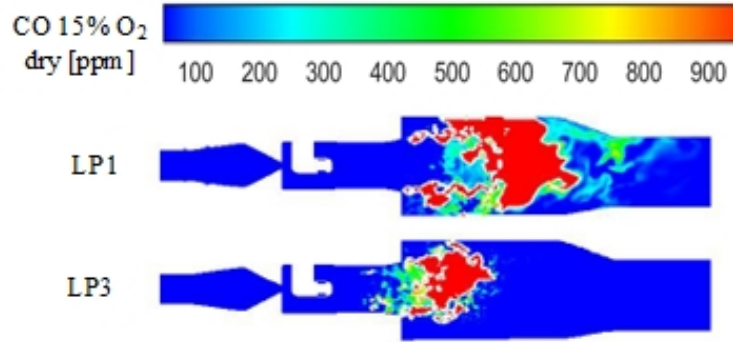


Figure 2.19: Snapshot of symmetry plane CO distribution at part loads increasing from LP1 to LP3. White isoline is the 200 ppm [69]

Schulz and Noiray studied a Jet In Cross Flow (JICF) configuration with partially and perfectly premixed  $\text{CH}_4/\text{air}$  as a simplified version of Ansaldo GT26 geometry [71]. They found that, after an initial autoignition in the recirculation zone, the flame can transition to premixed combustion, and move to the chamber inlet as shown in Figure 2.20. Autoignition kernels induce non-linear flame response to the inlet temperature forcing, and autoignition in the mixing stage can interact with the wall.

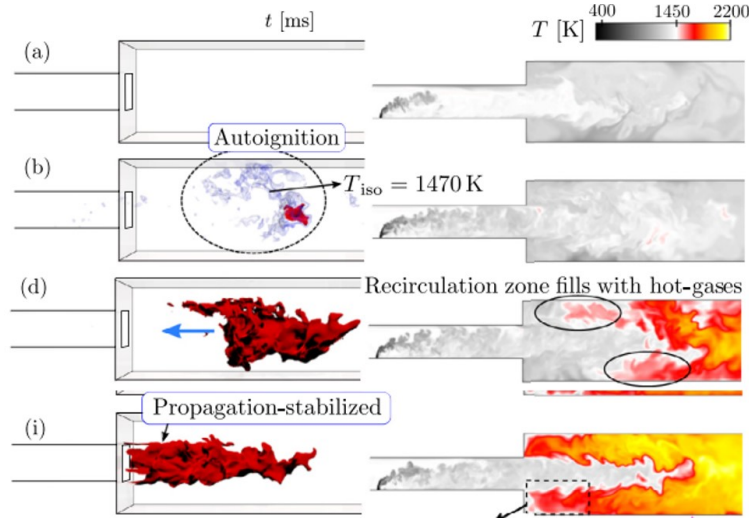


Figure 2.20: Mode-switching in a sequential combustor. The red contour on the left column is the iso-surface at 1500 K. Figure is adapted from [71]

Compared to RANS and LES, DNS can fully resolve the finest scales of the turbulence structures. Recently, Aditya et al. conducted 3D DNS on the simplified reheat combustor with  $H_2$  [70]. They reported that the thermal boundary layer near the sudden expansion corner cools the fuel down and leaves unburned fuel near the wall. These effects may promote FWI. Motion of autoignition into the mixing channel was observed, as shown in Figure 2.21, similar to Figure 2.20. In another study, DNS of turbulent boundary layer premixed combustion was conducted under auto-ignitive conditions [72]. It was shown that flame propagation is the dominant combustion mode near the wall. This study was conducted with  $H_2$  as the fuel, combustion of hydrocarbons and subsequent CO emissions have not yet been investigated in 3D DNS.

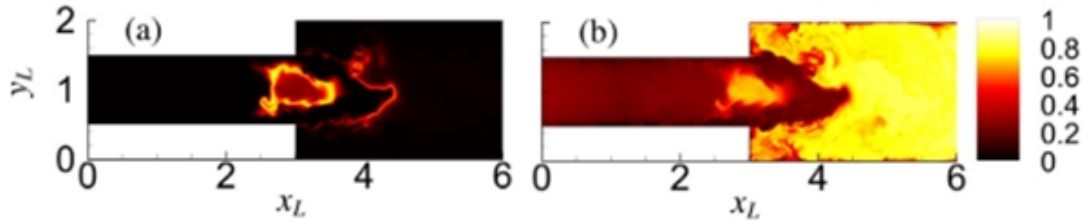


Figure 2.21: Instantaneous 2D iso-contours of normalized heat release rate (left) and temperature (right) at the midplane in the spanwise direction. Modified from [70]

As established, understanding CO requires high fidelity in both the flow and chemistry, which can be achieved in 3D DNS with detailed chemistry. However, due to

the computational costs involved, no 3D DNS has yet been conducted for diluted combustion of a methane/air flame for CO study, and especially not close to the wall, where grid resolution becomes prohibitive.

### 2.3.3 Exhaust CO Emissions

One of the major objectives of diluted combustion is reducing emissions. The goal of low  $\text{NO}_x$  is often achieved in laboratory MILD burners experimentally. However, CO has proven challenging to achieve consistently low values. Figure 2.22 is a summary of CO and  $\text{NO}_x$  emissions measurements in burners with hot combustion dilution. The results show that  $\text{NO}_x$  emissions are generally within 10 ppm, while CO can be two orders of magnitude higher for some burners and conditions. The following potential CO sources were cited: working conditions [69], dilution [73] and wall quenching [74].

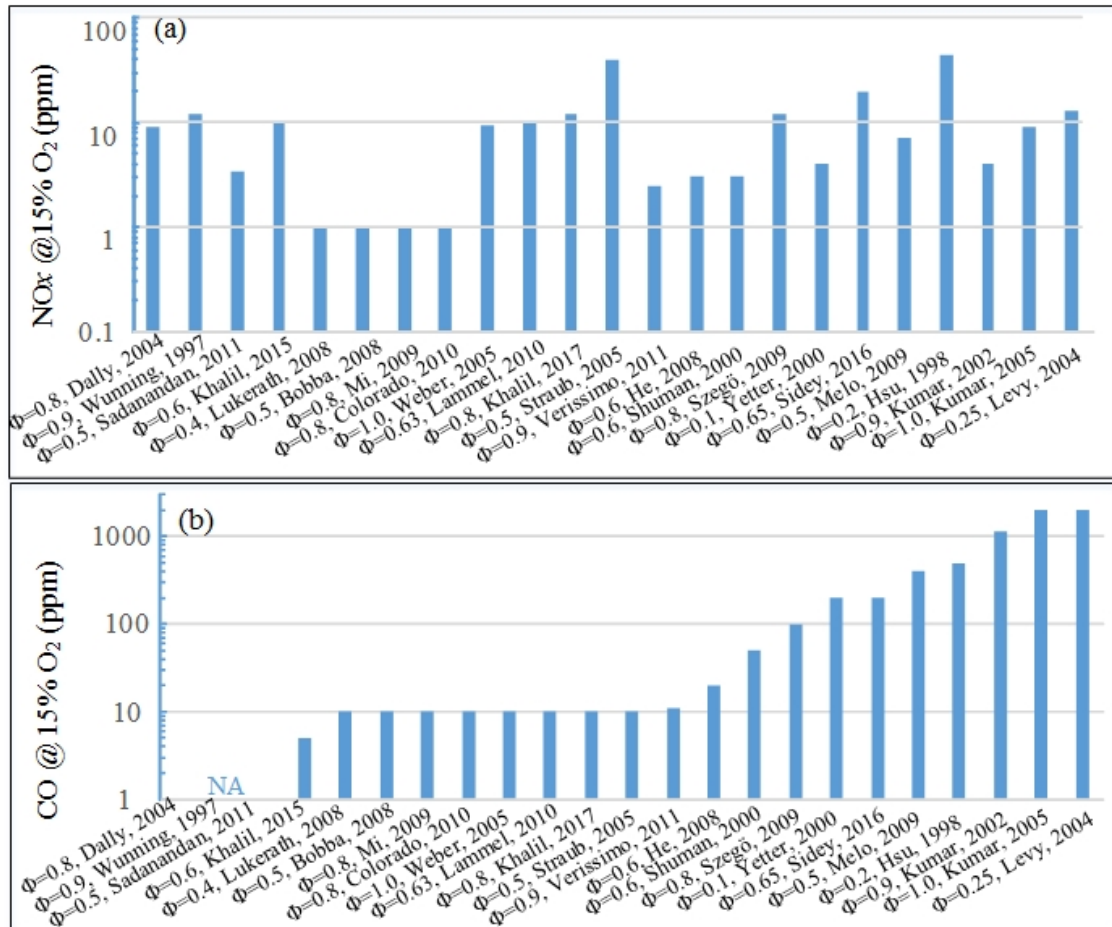


Figure 2.22: Measured  $\text{NO}_x$  (a) and CO (b) emissions in diluted combustors reported in literature. Modified from [7]

Systematic studies of full-combustor exhaust emissions are prohibitive, however simplified fully coupled approaches have enabled insight into the competing timescales. The impact of turndown for an axially-staged gas turbine on CO emissions was studied by Rivera et al. [75]. They conducted a chemical reactor network to simulate the exhaust CO. Figure 2.23 demonstrates the CO turndown effect as part-load conditions are used. The results showed that the exhaust CO increase was mainly dominated by the conditions and timescales in the secondary (diluted) combustor rather than the primary combustor or discharge nozzle.

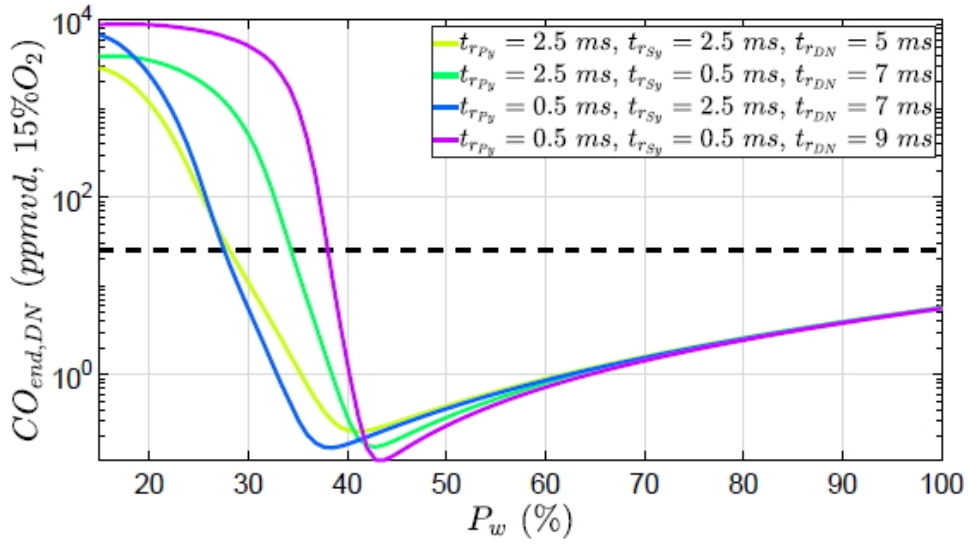


Figure 2.23: Exhaust CO at different arrangements of residence times in primary ( $\tau_{rPy}$ ) and secondary combustors ( $\tau_{rSy}$ ) and discharge nozzle ( $\tau_{rDN}$ ) [75].

As reviewed in Section 2.3.1, low  $O_2$ , and high  $H_2O$  and  $CO_2$  in hot combustion products as diluents decrease flame temperature and inhibits thermal  $NO_x$ . However, the major species have different or even opposing effects on the radical pool concentrations, which can influence CO formation and oxidation. Less  $O_2$  tends to reduce the OH and O, while high  $H_2O$  and  $CO_2$  could increase OH. CO emissions rely on these radicals pools.

Mardani et al. studied this CO behaviour for methane/air combustion with a 0D Well-Stirred Reactor (WSR) [76]. They claimed that the ethane oxidation pathway (i.e.,  $CH_3 \rightarrow C_2H_6 \rightarrow C_2H_5 \rightarrow C_2H_4 \rightarrow C_2H_3 \rightarrow C_2H_2 \rightarrow CO$ ) had a significant effect on the CO formation under MILD conditions. This pathway is an order magnitude smaller than the  $CH_3$  pathway at high temperatures, but becomes increasingly

relevant at low temperatures.

## 2.4 FWI for Flames Diluted by Hot Combustion Products

One of the CO emission sources in gas turbines is believed to be incomplete combustion induced by flame quenching [3]. There are three characteristics of EGR-type MILD combustion which promote FWI or quenching:

1. Internal recirculation is commonly used to dilute reactants in MILD gas turbines, which can increase the contact area and time between hot products and wall. Therefore, the CO burnout in the post flame may be affected by the cold wall.
2. The reaction zone is distributed, especially at low load conditions [69]. Therefore, the contact area between MILD combustion and wall can be increased, which may increase the probability of quenching.
3. Downsizing is a trend for gas turbines to achieve a high heat release intensity, and MILD combustion has an advantage to achieve this due to its high thermal efficiency. However, a small confinement further increases the possibility of FWI.

As an example, Figure 2.24 shows the temperature field of the secondary combustor of a staged gas turbine. It shows that the main reaction zone are adjacent to the wall. The authors discuss that the induced FWI could be a source for the higher CO at the exhaust as shown in Figure 2.25.



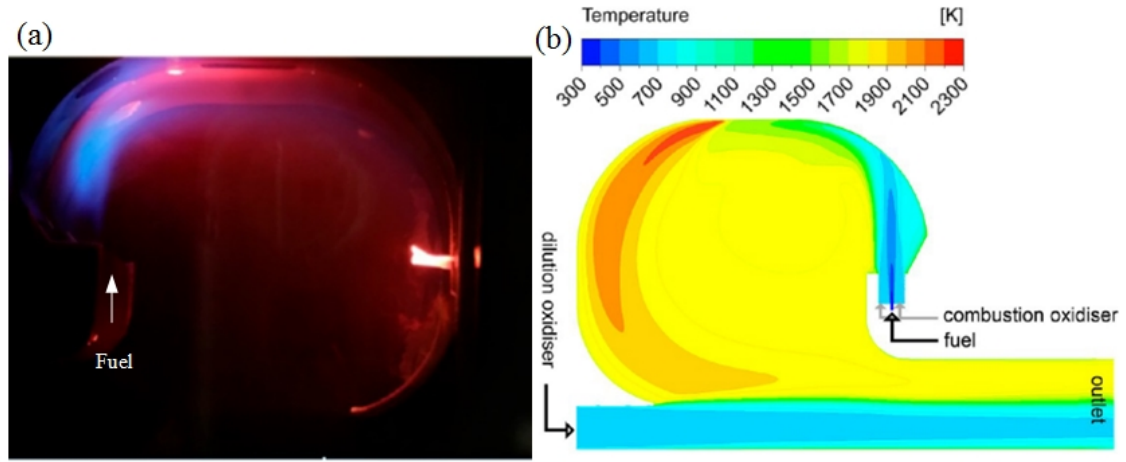


Figure 2.24: Experimental photograph (left) and numerical temperature field (right) of a secondary combustor in a staged gas turbine [77]

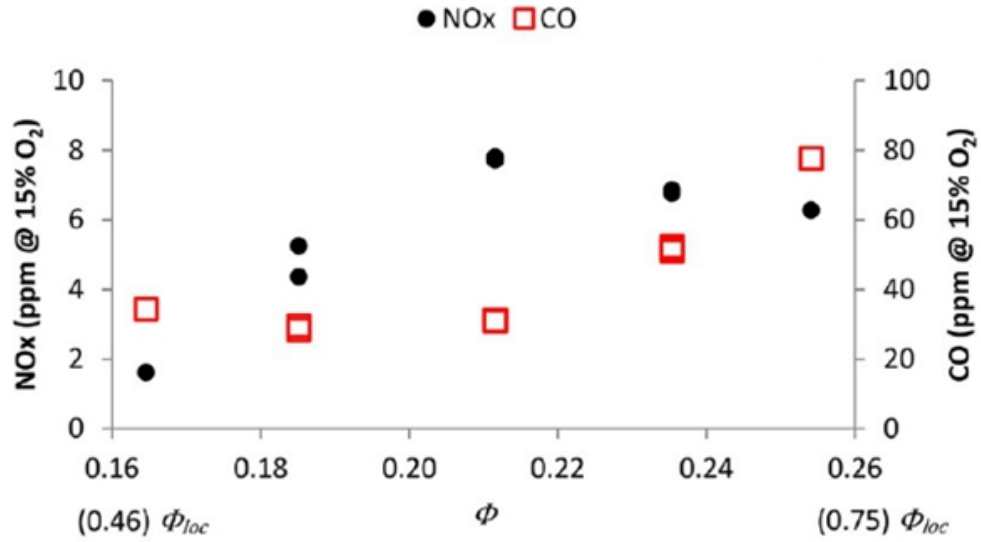


Figure 2.25: Measured CO and NO<sub>x</sub> emissions from the above secondary burner [77].

Only two studies have investigated diluted FWI, and only in a HOQ configuration. As an EGR-type HOQ, Yenerdag et al. investigated the effects of EGR ratio on wall heat flux with a 1D constant volume configuration [22]. They reported that the wall heat flux reduces with increasing dilution level as shown in Figure 2.26, since the flame temperature drops. Another potential reason is the reduced near-wall temperature gradient, as a high dilution level increases the flame thickness and the quenching distance.



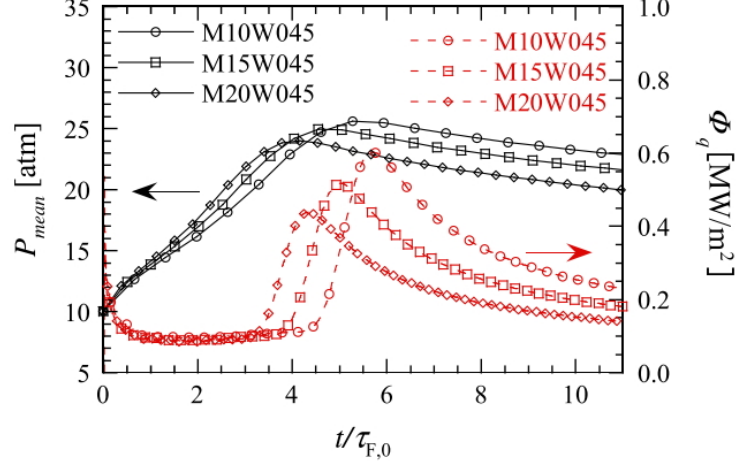


Figure 2.26: Temporal developments of mean pressure and wall heat flux of methane flames with different EGR ratio. (M10W045: methane/air flame with 10 % EGR ratio, 450 K wall temperature)[22]

Another diluted FWI was done by Owston et al. for inert  $N_2$  effects on FWI, although it is not EGR-type FWI [23]. As mentioned in Section 2.3.1.1, with adding  $N_2$  to reactants, both near-wall thermal conductivity and temperature gradient decrease, which reduces the wall heat flux. Similar to Yenedag et al., this study does not count all the species in combustion products and does not include autoignition [22].

It is clear from this that the influences of combustion product dilution have not been considered in the context of exhaust CO due to FWI. Given the motivation for attempting MILD or high dilution levels in GT combustors, this is an area that requires detailed investigation.

## 2.5 Summary and Research Aims

CO turndown limits the part-load operations of industrial gas turbines. The flame in the secondary stage is diluted by hot combustion products. This type of dilution can achieve MILD combustion at high dilution level and further reduce the emissions. However, the wall introduces heat loss and alters near-wall chemistry and flow fields. These can potentially inhibit MILD stabilisation, and increase emissions. This is one of potential sources for CO emission in diluted burners. It has been demonstrated in this review that this is an area that has not been addressed to date, and CO

turndown is a key design parameter for advanced industrial gas turbines, wall effects on flames diluted by hot combustion products will be investigated in this study.

Non-diluted FWI has been studied recently by many investigators, including the effects of pressure, wall temperature, quenching effects on CO, and wall heat flux. Further insight has been gained by examining the species transport mechanisms of CO. These approaches set a good reference for the study of CO under diluted FWI and will be used here to contrast the finding from this work.

The highest fidelity near the wall is required to resolve these phenomena. As such, detailed chemistry DNS of dilute methane/air combustion will be used to investigate CO formation and oxidation pathways near cool and hot walls in a variety of configurations.

The specific gaps are listed as follows:

1. FWI for flames diluted by major species in combustion products has only been studied in a 1D, constant volume configuration. Wall heat transfer was studied, while emissions were not reported. Turbulent DNS of FWI with methane/air flames diluted by hot combustion products has not yet been investigated.
2. A thermal boundary layer alters the wall heat transfer and wall-turbulence, and they can potentially affect near-wall CO chemistry. Effects of the thermal boundary layer on FWI have not been investigated, even for undiluted flames.
3. The combustion mode affects flame stabilisation, CO formation and oxidation rates. FWI effects on the combustion mode and subsequent non-adiabatic temperature-CO manifolds of diluted combustion have not been investigated.

To fill these gaps, 1D, 2D and 3D DNS will be used to study both the behaviour of flames diluted by combustion products near walls and their implication for near-wall CO modelling. More specifically, the following research questions will be considered:

1. **What are the effects of head-on quenching on the CO characteristics and combustion modes in 1D laminar flames diluted by hot combustion products?**

1D transient HOQ DNS will be used to conduct this study. Unsteady FWI effects on CO display significant differences in thermochemical states to steady FWI, as per [42]. These 1D studies mark the effects of different working parameters, including dilution level, inlet velocity (strain rate), ambient pressure and wall temperature, and set a reference for the 2D and 3D setups. They provide the data required for such approaches followed for undiluted flames by [37, 78].

**2. What are the effects of side-wall quenching on the CO characteristics and combustion modes in stationary and forced 2D laminar flames diluted by hot combustion products?**

The HOQ configuration cannot be used to investigate the effects of a velocity boundary layer. The use of a 2D channel flames enables a study of these effects. A forced inlet velocity allows the study of unsteady laminar FWI, which has been demonstrated to undergo a mix of HOQ, SWQ and premixed flame propagation in undiluted cases. The forcing introduces flame curvature and stretch effects, the study of which can aid the interrogation of 3D turbulent FWI results. The 2D flame also introduces tangential diffusion effects that can alter autoignition stability and chemistry

**3. What is the impact of 3D turbulent FWI on CO and flame behavior for flames diluted by hot combustion products?**

Near-wall turbulence can wrinkle the flames and introduce mixing between combustion products and reactants. These factors potentially affect near-wall CO transport. Heat loss inside the thermal boundary layer can inhibit autoignition and attenuate both the CO formation and oxidation rates. These effects will be investigated with 3D turbulent DNS with Analytically Reduced Chemical (ARC) kinetics. Both hot and cold walls will be investigated, to separate MILD autoignitive FWI from cold-wall quenching.

## 2.6 Publications

Appeared and submitted articles related to the contents of this thesis are listed below.

### Peer-Reviewed Papers

- Chapter 4 [Published]: Jiang, B., Gordon, R. L. and Talei, M. (2019). Head-on Quenching of Laminar Premixed Methane Flames Diluted with Hot Combustion Products. *Proceedings of the Combustion Institute*, 37(4), 5095–5103.

### Conference Proceedings

- Section 3.6.3.2 in Chapter 3 (Abstract accepted): Jiang, B., Brouzet, D., Talei, M., Gordon, R. L., Cazerres, Q., and Cuenot, B.. Developing Boundary Conditions for DNS of Diluted Flames in a Duct. (2020). *Proceedings of the 22th Australasian Fluid Mechanics Conference*.
- Jiang, B., Gordon, R. L. and Talei, M. (2017). Mode-switching behaviour of preheated and diluted flames in a stagnation burner. *Proceedings of the 11th Asia-Pacific Conference on Combustion*.
- Appendix: Jiang, B., Palulli, R., Rivera, J. E., Gordon, R. L. and Talei, M. (2016). CO Emission of Premixed and Diluted Flames in a 1-D Stagnation Burner. *Proceedings of the 20th Australasian Fluid Mechanics Conference*.
- Palulli, R. Jiang, B., , Rivera, J. E., Gordon, R. L. and Talei, M. (2016). Direct Numerical Simulation of Flame-Wall Interaction for a Forced Laminar Flame. *Proceedings of the 20th Australasian Fluid Mechanics Conference*.

# Chapter 3

## Numerical Methods

### 3.1 Introduction

Direct Numerical Simulation (DNS) was used to investigate Flame-Wall Interaction (FWI) for flames diluted by hot combustion products. This was systematically studied with 1D HOQ, 2D steady and forced V-flame and 3D turbulent configurations. 1D HOQ captures the transient FWI feature, while avoiding complex multi-dimensional transport. 2D V-flame configuration considers steady and forced laminar flames to study the impact of variation of the flow timescale on FWI behaviors. For both 1D and 2D simulations, detailed chemistry was used. Finally, a 3D turbulent flame in a channel was simulated with an Analytically Reduced Chemical (ARC) mechanism. With a brief description of the DNS code (NTMIX-CHEMKIN), the detailed setup of the above 1D, 2D and 3D cases will be described in this chapter.

### 3.2 Governing Equations

The numerical solver is known as NTMIX-CHEMKIN, which is a DNS solver, originally developed at CERFACS [13] and has been frequently used to simulate reacting and non-reacting flows [37, 79, 80]. The continuity, momentum, energy and species

equations are given in dimensional forms as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0 , \quad (3.2.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} , \quad (3.2.2)$$

$$\frac{\partial \rho e_t}{\partial t} + \frac{\partial (\rho e_t + p) u_j}{\partial x_j} = \frac{\partial (u_j \tau_{ij})}{\partial x_j} - \frac{\partial q_j}{\partial x_j} , \quad (3.2.3)$$

$$\frac{\partial \rho Y_\alpha}{\partial t} = \underbrace{-\frac{\partial \rho Y_\alpha u_j}{\partial x_j}}_{\text{mass convection (C)}} + \underbrace{-\frac{\partial \rho Y_\alpha V_{\alpha j}}{\partial x_j}}_{\text{molecular diffusion (D)}} + \underbrace{MW_\alpha \dot{\omega}_\alpha}_{\text{reaction source term (R)}} . \quad (3.2.4)$$

The variables  $x_j$  represent the  $j$ -th component of the spatial coordinate vector  $\mathbf{x} = [x, y, z]$  and  $t$  denotes time. The streamwise, transverse and spanwise directions are denoted by  $x$ ,  $y$  and  $z$ , respectively. In addition,  $\rho$  is the mixture density and  $u_j$  is the  $j$ -th component of the flow velocity vector  $\mathbf{u}$ . The pressure,  $p$ , is computed using the ideal gas law,

$$p = \rho \frac{R}{\overline{MW}} T , \quad (3.2.5)$$

where  $R$  is the ideal gas constant,  $T$  is the gas temperature and  $\overline{MW}$  is the mixture-averaged molecular weight defined as,

$$\overline{MW} = \left( \sum_{\alpha=1}^{N_s} \frac{Y_\alpha}{MW_\alpha} \right)^{-1} . \quad (3.2.6)$$

The expressions  $Y_\alpha$  and  $MW_\alpha$  refer to the mass fraction and molecular weight of species  $\alpha$ . The viscous stress tensor  $\tau$  in Equation 3.2.2 is defined assuming a Newtonian fluid, so that

$$\tau_{ij} = \bar{\mu} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) , \quad (3.2.7)$$

where  $\delta_{ij}$  is the Kronecker delta.  $\bar{\mu}$  refers to the mixture-averaged dynamic viscosity, which is calculated by using mixing rules with the pure species. The pure species

viscosity is computed based on polynomial fits by using the CHEMKIN transport package. The mixture-averaged dynamic viscosity is then calculated as:

$$\bar{\mu} = \frac{1}{2} \left( \sum_{\alpha=1}^{N_s} X_{\alpha} \mu_{\alpha} + \left( \sum_{\alpha=1}^{N_s} \frac{X_{\alpha}}{\mu_{\alpha}} \right)^{-1} \right) , \quad (3.2.8)$$

The gas total energy,  $e_t$ , which includes its kinetic energy and internal energy,  $e$ , is defined as follows:

$$e_t = \frac{1}{2} u_k^2 + e = \frac{1}{2} u_k^2 + \sum_{\alpha=1}^{N_s} h_{\alpha} Y_{\alpha} - \frac{p}{\rho} , \quad (3.2.9)$$

where  $h_{\alpha}$  represents the enthalpy of species  $\alpha$ , defined as,

$$h_{\alpha}(T) = \Delta h_{f\alpha}^0 + \int_{T_0}^T c_{p,\alpha}(T') dT' . \quad (3.2.10)$$

The expression  $\Delta h_{f\alpha}^0$  stands for the enthalpy of formation for species  $\alpha$  at standard condition  $T_0 = 298.15$  K and  $c_{p,\alpha}$  represents the specific heat of species  $\alpha$  at constant pressure. The heat flux in the  $j$ -th direction  $q_j$  in Equation 3.2.3 comprises of energy fluxes due to thermal conduction, species diffusion and species concentration gradients (Dufour effect):

$$q_j = \underbrace{-\bar{\lambda} \frac{\partial T}{\partial x_j}}_{\text{thermal conduction}} + \underbrace{\rho \sum_{\alpha=1}^{N_s} h_{\alpha} Y_{\alpha} V_{\alpha j}}_{\text{flux due to species diffusion}} - \underbrace{\frac{p}{\rho} \sum_{\alpha=1}^{N_s} \frac{D_{\alpha}^T}{MW_{\alpha} X_{\alpha}} \frac{\partial X_{\alpha}}{\partial x_j}}_{\text{Dufour effect}} . \quad (3.2.11)$$

Similar to the mixture-averaged viscosity, the mixture-averaged thermal conductivity,  $\bar{\lambda}$ , is computed based on a mixing rule [81].

$$\bar{\lambda} = \frac{1}{2} \left( \sum_{\alpha=1}^{N_s} X_{\alpha} \lambda_{\alpha} + \left( \sum_{\alpha=1}^{N_s} \frac{X_{\alpha}}{\lambda_{\alpha}} \right)^{-1} \right) , \quad (3.2.12)$$

The thermal diffusion coefficient is denoted by  $D_{\alpha}^T$  and  $X_{\alpha}$  presents the molar fraction of species  $\alpha$ . The Dufour term is established by neglecting the effect of pressure gradients.

Using a mixture-averaged formulation, the diffusion velocity,  $V_{\alpha j}$ , equal to,

$$V_{\alpha j} = \frac{D_{\alpha}}{X_{\alpha}} \frac{\partial X_{\alpha}}{\partial x_j} - D_{\alpha}^T \frac{\partial(\log(T))}{\partial x_j} , \quad (3.2.13)$$

where  $D_{\alpha}$  is the diffusion coefficient of species  $\alpha$  into the rest of the mixture.

$$D_{\alpha} = \frac{(1 - Y_{\alpha})}{\sum_{\beta=1; \beta \neq \alpha}^{N_s} \frac{X_{\beta}}{D_{\alpha\beta}}} , \quad (3.2.14)$$

where  $D_{\alpha\beta}$  denotes the binary diffusion coefficients derived from the kinetic theory of gases [82]. However, Equation 3.2.13 will not satisfy the mass conservation equation (Equation 3.2.1). A correction term is therefore added to the diffusion velocities so that the net diffusive flux is zero:

$$\sum_{\alpha=1}^{N_s} Y_{\alpha} V_{\alpha j} = 0 , \quad (3.2.15)$$

leading to the following formulation for the corrected diffusion velocity  $V_{\alpha j}$ ,

$$V_{\alpha j} = \frac{D_{\alpha}}{X_{\alpha}} \frac{\partial X_{\alpha}}{\partial x_j} + \sum_{\beta=1}^{N_s} Y_{\beta} \frac{D_{\beta}}{X_{\beta}} \frac{\partial X_{\beta}}{\partial x_j} - D_{\alpha}^T \frac{\partial(\log(T))}{\partial x_j} - \sum_{\beta=1}^{N_s} Y_{\beta} \frac{D_{\beta}^T}{X_{\beta}} \frac{\partial(\log(T))}{\partial x_j} . \quad (3.2.16)$$

The first two terms in Equation 3.2.16 describe the corrected species fluxes due to concentration gradients while the last two terms represent the corrected species fluxes resulting from the temperature gradient, also known as Soret effect.

Finally, the term,  $\dot{\omega}_{\alpha}$ , in Equation 3.2.4 represents the production rate of the species  $\alpha$ . The details of the chemical kinetics and the transport equations are described in [83].

### 3.3 Non-dimensionalisation

NTMIX-CHEMKIN uses the non-dimensional form of the governing equations. Two sets of reference values are defined to normalize the equations and denoted with subscript *ref* in the following description. One set of references is defined as user inputs, and the present study used the unburned gas properties outside the wall-



influenced region. It includes the speed of sound ( $c_{ref}$ ), density ( $\rho_{ref}$ ) and dynamic viscosity ( $\mu_{ref}$ ). The other set of reference values,  $T_{ref}$  and  $p_{ref}$  are obtained by using the following Equations 3.3.1.

$$T_{ref} = (\gamma_u - 1)T_u ; p_{ref} = \rho_{ref}c_{ref}^2 ; \cdot \quad (3.3.1)$$

where  $\gamma_u$  denotes the ratio of specific heat of the unburned gas, and  $T_u$  presents the unburned gas temperature. The acoustic Reynolds number,  $Re_{ac}$ , is defined as.

$$Re_{ac} = \frac{c_{ref}\rho_{ref}L_{ref}}{\mu_{ref}} \quad (3.3.2)$$

where  $L_{ref}$  presents the reference length with the half-channel width. A summary of the reference values is in Table 3.1

Table 3.1: Reference value in the 1D, 2D and 3D baseline simulations

| Quantity                 | 1D simulations        | 2D simulations        | 3D simulation         |
|--------------------------|-----------------------|-----------------------|-----------------------|
| $L_{ref} (mm)$           | 5                     | 5                     | 2.5                   |
| $c_{ref} (m.s^{-1})$     | $3.54 \times 10^2$    | $7.59 \times 10^2$    | $8.02 \times 10^2$    |
| $\rho_{ref} (kg.m^{-3})$ | $1.12 \times 10^{-1}$ | $2.23 \times 10^{-1}$ | $3.95 \times 10^{-1}$ |
| $T_{ref} (K)$            | 114                   | 399                   | 518                   |

After substituting the reference quantities into the governing equation in Section 3.2, the governing equations can be recast into the non-dimensional form as following Equations 3.3.3 ~ 3.3.6, which is used in NTMIX-CHEMKIN calculation:

$$\frac{\partial \rho^*}{\partial t^*} + \frac{\partial \rho^* u_j^*}{\partial x_j^*} = 0 , \quad (3.3.3)$$

$$\frac{\partial \rho^* u_i^*}{\partial t^*} + \frac{\partial \rho^* u_i^* u_j^*}{\partial x_j^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{1}{Re_{ac}} \frac{\partial \tau_{ij}^*}{\partial x_j^*} , \quad (3.3.4)$$

$$\frac{\partial \rho^* e_t^*}{\partial t^*} + \frac{\partial (\rho^* e_t^* + p^*) u_j^*}{\partial x_j^*} = \frac{1}{Re_{ac}} \frac{\partial (u_j^* \tau_{ij}^*)}{\partial x_j^*} - \frac{1}{Re_{ac}} \frac{\partial q_j^*}{\partial x_j^*} , \quad (3.3.5)$$

$$\frac{\partial \rho^* Y_\alpha^*}{\partial t^*} + \frac{\partial \rho^* Y_\alpha^* u_j^*}{\partial x_j^*} = -\frac{1}{c_{ref}} \frac{\partial \rho^* Y_\alpha^* V_{\alpha j}^*}{\partial x_j^*} + \frac{t_{ref}}{\rho_{ref}} MW_\alpha \hat{\omega}_\alpha . \quad (3.3.6)$$

### 3.4 Numerical Solver and Stability

NTMIX-CHEMKIN features an 8<sup>th</sup>-order central finite difference scheme for spatial derivatives and a 3<sup>rd</sup>-order Runge–Kutta time integrator. The time step is limited using a combination of Courant–Friedrichs–Lewy (*CFL*) number, Fourier number (*Fo*) and a chemical number, presenting the convection, diffusion and reaction transports.  $Re_{ac}$  in Equation (3.4.2) is to dimensionalize the  $\nu$ ,  $t$  and  $h$ , and thus eliminate the effects of user-defined references. The definitions of the first two numbers are:

$$CFL = (Max.[|u + c|, |u - c|]) \frac{\Delta t}{\Delta x} , \quad (3.4.1)$$

$$Fo = Max.(\bar{\nu} \frac{\Delta t}{\Delta h^2} \frac{1}{Re_{ac}}) , \quad (3.4.2)$$

where  $u$ ,  $c$ ,  $\Delta x$  and  $\bar{\nu}$  are the local streamwise velocity, speed of sound, grid size and mixture-averaged kinematic viscosity;  $\Delta h$  is the minimum grid size in the domain. Although the  $u$  is only in streamwise direction, it is evaluated in the whole domain. The chemical number is the maximal allowed rate of changes for all the species mass fraction. In this study,  $CFL = 0.6$ ,  $Fo = 0.1$  and chemical number = 0.001.

A 10<sup>th</sup>-order explicit filter was also used to eliminate numerical errors due to the high order of finite difference scheme, similar to the reference [84] used.

### 3.5 Dilution Method

This thesis considers adiabatic mixing to generate the diluted reactants. The homogeneous mixtures with different levels of dilution were prepared in the same manner as Sidey et al. [57]. Hot products of premixed methane/air were produced with the FPF of CHEMKIN [85] at 298 K inlet temperature and stoichiometric conditions with GRI 3.0 chemical mechanism. The domain length was large enough (100 mm)

such that at the outlet the hot products of the premixed burner are in chemical equilibrium at the adiabatic flame temperature. Also, a long domain ensures the zero gradient on both sides as required for the convergence of 1D FPF. These hot products were then mixed with cold reactants. The degree of mixing is given by the dilution level ( $\zeta$ ), which is the ratio of hot products mass flow rate and the fresh mixture as described in Sidey et al. [57]. Undiluted cold reactants are defined as  $\zeta = 0$ , which is conventional premixed stoichiometric combustion, while pure hot products at the adiabatic flame temperature correspond to  $\zeta = 1.0$ . As a result of this mixing, enthalpy of the final mixture remains the same for different values of  $\zeta$ . The final mixture temperature was then calculated using the mixture enthalpy. The mixture temperature and oxygen concentration are shown in Figure 3.1. With an increase in the dilution level, the mixture temperature increases while the oxygen mole fraction decreases.

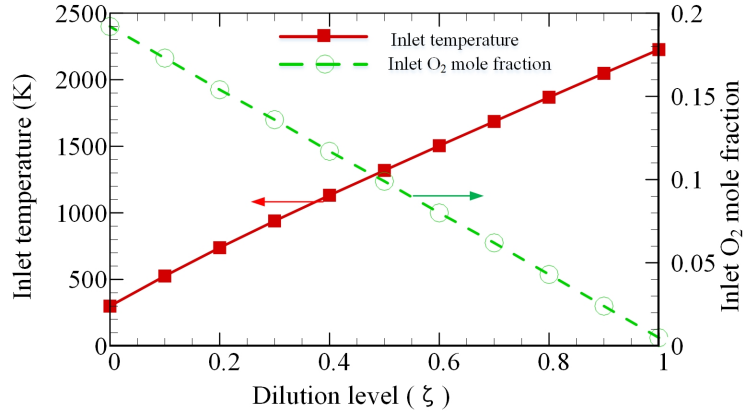


Figure 3.1: Mixture temperature and O<sub>2</sub> mole fraction profiles under different dilution levels at atmospheric pressure.

The dilution levels for the 1D simulations were  $\zeta = 0, 0.4$  and  $0.6$ , presenting the non-diluted condition, diluted condition with premixed flame propagation, and diluted condition with autoignition, respectively at 1 atm. The combustion mode switches to autoignition at  $\zeta = 0.4$  at 15 atm.

In the 2D simulation,  $\zeta = 0.5, 0.6$  and  $0.7$  at 1 atm are simulated to vary the combustion mode from premixed flame to autoignition, without changing the domain length and inlet velocity.

In the 3D simulation,  $\zeta = 0.7$  at 2 atm was chosen. This higher pressure than

1 atm ensures that autoignition can be captured using a shorter domain length, thereby reducing the computational cost. Table 3.2 shows that the required length for autoignition inside the 3D domain is  $7.5H$  ( $H$  is the half channel width, 2.5 mm) at 2 atm pressure, and it is 3 times shorter than the case at 1 atm. Increasing pressure reduces the kinematic viscosity, and thus decreases the centreline velocity at a fixed Reynolds number  $\approx 3200$ , defined with the the maximum inlet velocity and half-channel width. A lower centreline velocity further reduces the domain length. The inlet maximum velocity is  $187 \text{ m.s}^{-1}$  at 2 atm with 0.23 Mach number. The doubling of the ambient pressure also increases the relevance of the results to the industrial application.

Table 3.2: Required length ( $L_{required, domain}$ ) for autoignition occurrence with Reynolds number = 3200 at the inlet center plane.  $L_{required, domain} = U_{CL} \cdot \tau_{AI}$ , where  $U_{CL}$  is the centre-line streamwise velocity, and  $\tau_{AI}$  is the autoignition delay time from PFR.

| $p$ (atm) | $Viscosity$ ( $\text{m}^2.\text{s}^{-1}$ ) | $U_{CL}$ ( $\text{m.s}^{-1}$ ) | $\tau_{AI}$ (ms) | $Required\ length(H)$ |
|-----------|--------------------------------------------|--------------------------------|------------------|-----------------------|
| 1         | 2.86e-4                                    | 374                            | 0.15             | 23H                   |
| 2         | 1.43e-4                                    | 187                            | 0.10             | 7.5H                  |
| 3         | 9.50e-5                                    | 124                            | 0.08             | 4H                    |
| 5         | 5.75e-5                                    | 75                             | 0.06             | 2H                    |

The reactant composition was set to  $\zeta = 0.7$  at 2 atm , and the ignition delay and composition at  $\zeta = 0.7$  are shown in Table 3.3. The reactant temperature is higher than the autoignition temperature, and  $\text{O}_2$  mass (molar) fraction is 7% (6%), satisfying the MILD or flameless condition [5, 86]. At 2 atm, autoignition can be captured using a shorter domain, thereby reducing the computational cost. The reactant temperature of 1705 K allows an upper bound investigation of the high temperature autoignition effects and a contrast through the thermal boundary layer with intermediate and frozen chemistry.

Table 3.3: Ignition delay and reactants compositions at  $\zeta = 0.7$  at 2 atm.

| Temperature (K) | $\tau_{AI}$ (ms) | $Y_{CH_4}$ | $Y_{O_2}$ | $Y_{H_2O}$ | $Y_{CO_2}$ | $Y_{CO}$ |
|-----------------|------------------|------------|-----------|------------|------------|----------|
| 1705            | 0.103            | 0.016      | 0.070     | 0.100      | 0.085      | 0.005    |

## 3.6 Computational Setup

Three different configurations were considered, including 1D HOQ, 2D acoustically forced, laminar flame interacting with a relatively cold wall and a 3D flame interacting with walls at relatively high and low temperatures. In this section, the computational setup of each configuration is discussed.

### 3.6.1 1D Head-On Quenching Simulations

#### 3.6.1.1 Computational Domain and Flow Parameters

Figure 3.2 shows a schematic of the 1D HOQ case. The domain length  $L$  varies from  $4 L_{ref}$  at  $\zeta = 0$  to  $12 L_{ref}$  at  $\zeta = 0.6$  with the grid resolution being discussed in Section 3.7. A wall boundary condition was used on the LHS, and a non-reflecting boundary condition was considered on the RHS. Near the wall, a thermal boundary layer (BL) was initialised. The initialisation also allows a flame to propagate from the right side towards the wall.

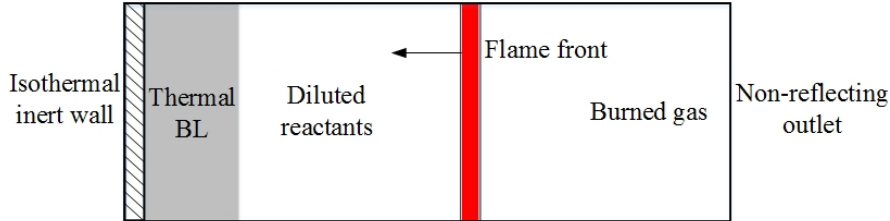


Figure 3.2: Schematic of the 1D HOQ case.

Non-diluted and two diluted cases were tested. A diluted case at  $\zeta = 0.4$  presents diluted premixed flame without autoignition at atmospheric pressure, while  $\zeta = 0.6$  has autoignition during the initial flame approaching the wall. Table 3.4 shows the initial thermal boundary layer thickness for all cases considered.

Table 3.4: Initial thermal boundary layer thickness (mm) at test conditions

| $\zeta$ | $T_{wall} = 300 \text{ K}$<br>$p = 1 \text{ atm}$ | $T_{wall} = 600 \text{ K}$<br>$p = 1 \text{ atm}$ | $T_{wall} = 300 \text{ K}$<br>$p = 15 \text{ atm}$ |
|---------|---------------------------------------------------|---------------------------------------------------|----------------------------------------------------|
| 0.0     | —                                                 | 0.45                                              | —                                                  |
| 0.4     | 0.85                                              | 0.80                                              | 0.20                                               |
| 0.6     | 1.01                                              | 0.90                                              | 0.26                                               |

### 3.6.1.2 Initial and Boundary Conditions

Figure 3.3 shows the initial conditions of the HOQ case by taking an example at  $\zeta = 0.6$ ,  $T_{wall} = 300$  K,  $p = 1$  atm. The initial conditions consist of three regions: region A with a thermal boundary layer; region B with the unburned premixed reactants, and region C with a premixed flame.

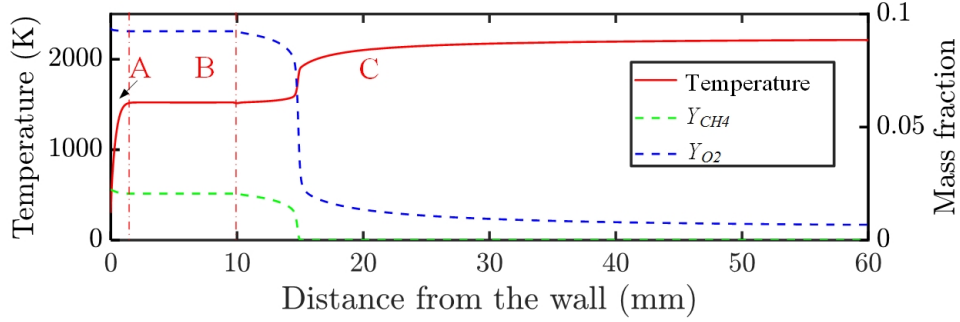


Figure 3.3: Initial domain of 1D HOQ.

Region A: The thermal boundary layer was created with a non-reacting stagnation flow model in CHEMKIN [85] with a 10 mm domain, and 10 m.s<sup>-1</sup> inlet velocity towards the wall. In all cases, the flame was initialised sufficiently far from the wall such that the thermal boundary layer relaxes to a quasi-steady state prior to the FWI event.

Region B: The composition and the temperature of the premixture were used to initialise the region between the thermal boundary layer and the flame.

Region C: The flame profile was extracted from a CHEMKIN premixed flame model[85]. For initialisation of the cases at low dilution levels, a freely propagating flame was used. At high dilution levels, a burner-stabilised premixed flame model was used. After the initialisation, the flame propagates at a constant speed for some time, achieving a quasi-steady state [87].

The wall boundary condition for all configurations (1D, 2D and 3D) was set to an inert isothermal, non-slip wall. The convection and diffusion velocities were set to zero at the wall. At the outflow boundary of all configurations, the Navier-Stokes Characteristic Boundary Condition (NSCBC) was used [83, 88]. A partially reflecting outflow boundary condition [89] was used, as a perfectly non-reflecting

outflow boundary condition can lead to mean pressure drifting. A factor,  $K$ , was used to control the reflection wave amplitude,  $L_1$ ,

$$L_1 = K(p - p_\infty) , \quad (3.6.1)$$

where  $p_\infty$  denotes the ambient mean pressure;  $K$  is a constant calculated using the following equation,

$$K = \frac{\delta(1 - Ma^2)c}{L} . \quad (3.6.2)$$

The variable,  $Ma$  is the local Mach number,  $L$  is the characteristic size of the domain, and  $\delta$  is a constant, and usually takes around 0.2 [89].

### 3.6.2 2D Laminar Flame Simulation

#### 3.6.2.1 Computational Domain and Flow Parameters

Figure 3.4 shows a schematic of the computational domain. The domain size are  $L_x = 30$  mm and  $L_y = 5$  mm, where  $x$  and  $y$  represent the streamwise and wall-normal directions, respectively. A mixture of reactants diluted by hot combustion products enters the domain from the LHS boundary. A temperature profile was imposed such that the flame is anchored at the inlet, and a thermal boundary layer presents near the top wall. A non-reflecting boundary condition was imposed at the RHS boundary. A symmetric boundary condition was imposed on the bottom side.

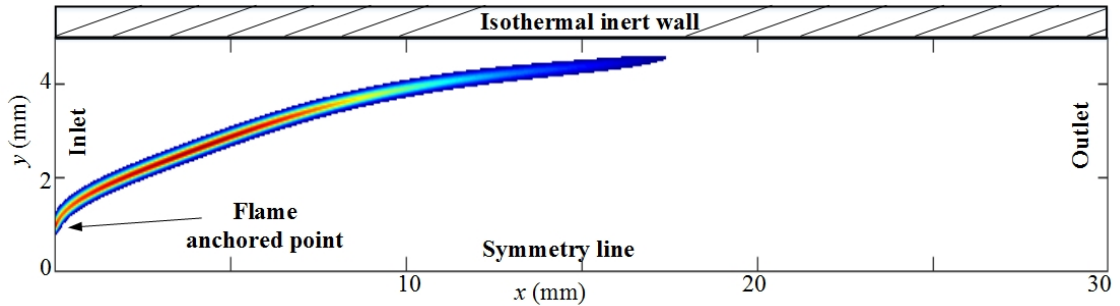


Figure 3.4: Schematic of 2D laminar simulation presented with HRR contours around the main reaction zone at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K.

Three dilution levels  $\zeta = 0.5$ ,  $0.6$  and  $0.7$  were considered. Each dilution level was tested at various wall temperatures and forcing frequencies, or Strouhal numbers as

shown in Table 3.5. The highest  $T_{wall}$  was set to be the diluted reactant temperature ( $T_{reactants}$ ) at each  $\zeta$ , i.e. 1319 K, 1504 K and 1686 K at  $\zeta = 0.5$ , 0.6 and 0.7, respectively.

Table 3.5: 2D test conditions with different dilution levels, wall temperatures and Strouhal numbers.

| Dilution level ( $\zeta$ ) | Wall temperature (K) | Strouhal number |
|----------------------------|----------------------|-----------------|
| 0.5                        | 300                  | 0               |
|                            | 600                  | 0               |
|                            | 1319                 | 0               |
| 0.6                        | 300                  | 0, 0.25         |
|                            | 600                  | 0, 0.25, 1, 2   |
|                            | 1504                 | 0, 0.25         |
| 0.7                        | 300                  | 0, 0.25         |
|                            | 600                  | 0               |
|                            | 1686                 | 0               |

### 3.6.2.2 Initial and Boundary Conditions

The inlet boundary conditions of the 2D flames were imposed using the temperature, velocity and species mass fraction profiles. These profiles are shown in Figure 3.5. Two main regions exist as described below:

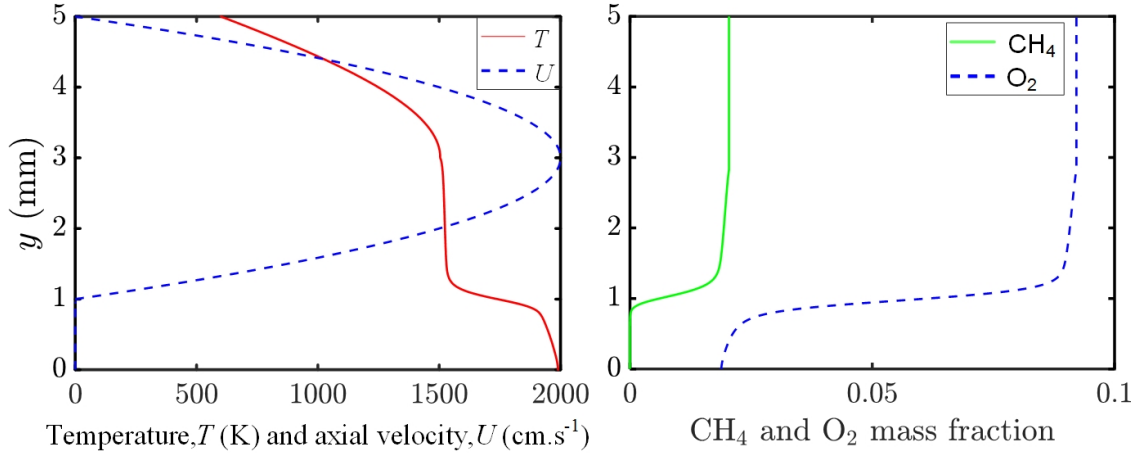


Figure 3.5: 2D inlet boundary conditions. Left:  $T$  and  $U$  profiles. Right: representative species profiles.

Region (1): From  $y = 0$  mm to 3 mm, the flame profile was extracted from a CHEMKIN premixed flame model [85]. The flame profiles, including the species composition and temperature, were used to anchor the 2D flame by setting the



maximum heat release rate at  $y = 1$  mm (the anchoring point). The streamwise velocity from  $y = 0$  mm to 1 mm is zero, and from  $y = 1$  mm to 3 mm was imposed using the analytical solution of a fully-developed laminar channel.

Region (2): From  $y = 3$  mm to 5 mm, the thermal boundary layer was created with a non-reacting channel flow model in CHEMKIN [85] with a 2 mm half-domain width, where the compressible gas was modelled in the thermal BL region, i.e. the density changes with the temperature. The domain length was long enough to fully develop the thermal boundary layer, such that the thermal and velocity boundary layers are coupled. The results for the velocity and temperature profiles are shown in Figure 3.6. The species concentrations are the same as at  $y = 3$  mm inside the thermal boundary layer.

The maximum inlet velocity was set to  $20 \text{ m.s}^{-1}$  at  $y = 3$  mm to achieve a Reynolds number of around 450. The transverse velocity at the inlet was set to zero.

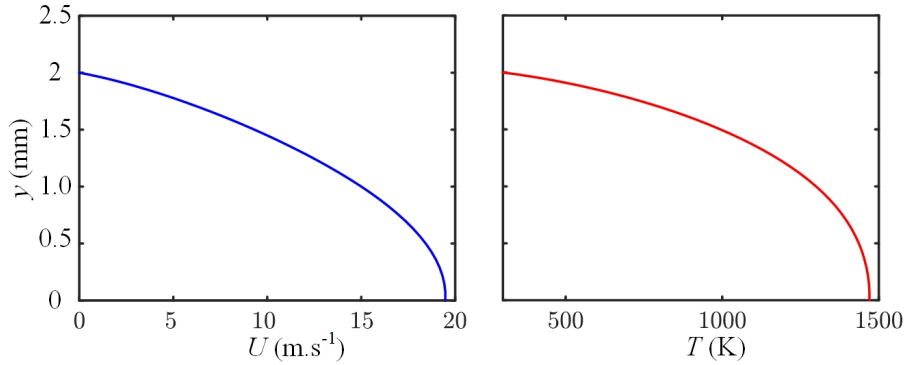


Figure 3.6: Velocity and temperature profiles in a laminar, fully-developed channel with CHEMKIN channel flow solutions [85].

$$U(y) = U_{in} \left( 1 - \frac{(y-3)^2}{4} \right) \quad (3.6.3)$$

where  $U_{in}$  is the inlet velocity at  $y = 3$  mm.

Velocity perturbations were then added to the inlet velocity for several cases (see Table 3.5) using a sine function with the amplitude at 0.25 of maximum inlet velocity. After initialisation with the inlet boundary conditions, the simulations were first run for at least 4 flow through times without adding perturbations. These solutions were

then used as the initial conditions of the forced cases, and the simulations were run for at least 3 forcing cycles to obtain a periodic flow with the repeatable outflow characteristics in one cycle.

### 3.6.3 3D Turbulent Flame Simulation

#### 3.6.3.1 Computational Domain and Flow Parameters

Figure 3.7 shows the 3D domain with an iso-surface of the instantaneous flame front marked by the progress variable of  $c_{CH_4} = 0.94$ . The fresh reactants diluted by hot combustion products enter the domain from the LHS boundary. A cylindrical hot patch was imposed at  $y/H = 0$  and  $x/H = 1$ . It extends throughout the whole spanwise direction, where periodic boundary condition was imposed. This hot patch ignites the reactants and forms two flame branches. The hot patch was created with a Gaussian temperature and species mass fraction profiles varying from the state of the inlet mixture to the burned state, similar to [24]. The velocity was not imposed in this hot patch, and is calculated by solving the governing equations at every timestep. The radius of the hot patch is 1.5% of the half channel width, and small enough to eliminate the non-physical disturbances created by the hot patch to the flow field. Further downstream, the two flame branches interact with the top-hot wall and bottom-cold wall separately. The outlet is on the RHS featuring a non-reflecting boundary condition. The details of the computational domain and the flow parameters are shown in Table 3.6. In this table, Reynolds number is defined with the inlet velocity and gas viscosity at  $y = 0$  and channel half-width.

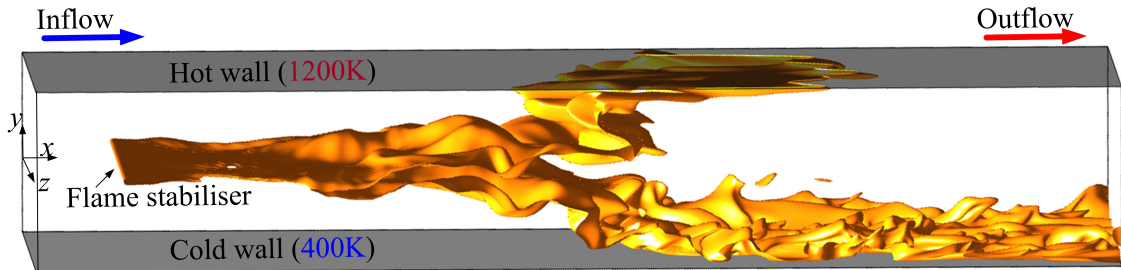


Figure 3.7: Schematic of the 3D DNS domain. The hot-wall temperature is 1200 K and the cold-wall temperature is 400 K. The flame is anchored at  $x/H = 1$  ( $H$  is half channel width, 2.5 mm) and  $y/H = 0$  with  $0.015 H$  radius. The domain size is  $12 H$ ,  $2 H$  and  $3 H$  in the streamwise, transverse and spanwise directions, respectively.

Table 3.6: Configuration setup of the 3D reacting simulation.

| Variables                                                                          | Value                              |
|------------------------------------------------------------------------------------|------------------------------------|
| Reynolds number at the inlet centre plane                                          | $\sim 3200$                        |
| Friction Reynolds number ( $Re_\tau$ )                                             | 576 (cold wall)<br>214 (hot wall)  |
| Reactant temperature at the inlet centre plane (K)                                 | 1705                               |
| Wall temperature (K)                                                               | 400 (cold wall)<br>1200 (hot wall) |
| Domain size ( $L_x \times L_y \times L_z$ )                                        | $12H \times 2H \times 3H$          |
| Kolmogorov length at the inlet ( $\mu\text{m}$ )                                   | 6.0 (cold wall)<br>16.0 (hot wall) |
| Minimum grid size ( $\Delta x \times \Delta y \times \Delta z$ ) ( $\mu\text{m}$ ) | $30 \times 5 \times 30$            |
| Maximum grid size ( $\Delta x \times \Delta y \times \Delta z$ ) ( $\mu\text{m}$ ) | $30 \times 30 \times 30$           |
| Time step in non-reacting and reacting simulations ( $\Delta t$ ) (ns)             | 4                                  |

### 3.6.3.2 3D Inlet Turbulence Generation

The inlet turbulence was generated with an auxiliary non-reacting simulation. Figure 3.8 shows a schematic representation of the non-reacting and reacting cases used. The non-reacting simulation results were collected at the plane,  $x/H = 4$ , and then were fed into the reacting flow simulation at the inlet boundary. This turbulence generation allows coupling of the velocity and temperature fluctuations at the inlet. The sampling data is from a fixed streamwise position of the non-reacting simulation with  $2 \times 10^{-8}$  s sampling frequency, every 5 time steps.

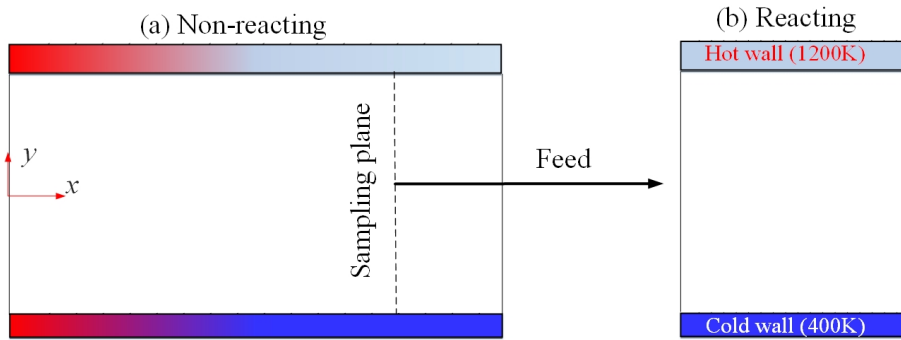


Figure 3.8: Schematic of the reacting and non-reacting cases. Streamwise location ( $x$ ) normalised by the half-channel width ( $H$ , 2.5 mm), and  $y$  is the wall-normal distance. Configuration (a) presents a non-reacting auxiliary simulation. Configuration (b) shows the reacting simulation with the inlet boundary condition generated from the auxiliary simulation. The hot and cold walls are at 1200 K and 400 K, respectively. The sampling plane is at  $x/H = 4$  (dashed line in Figure (a)).

Using the Passot-Pouquet spectrum for the turbulent kinetic energy, velocity fluc-

tuations were first produced. The inlet turbulence for the non-reacting simulation was then generated by re-scaling these fluctuations with the Root Mean Square (RMS) profiles of a fully developed channel flow at the Reynolds number of 3200 [90, 91]. Next this was fed into the domain with a convection velocity 0.75 times the mean inlet velocity at the centreline. This accounts for a correction to the Taylor’s hypothesis due to the high near-wall shear stress [92]. Non-reflecting Navier-Stokes Characteristic Boundary Condition (NSCBC) was used for the outlet boundary, and a periodic boundary condition was used in the  $z$  direction. The hot and cold walls were inert and non-slip, with the temperature imposed using Equation (3.6.4):

$$T_{wall} = 0.5(T_{in} + T_{target}) - 0.5(T_{in} - T_{target}) \tanh[3(x/H - 1)], \quad (3.6.4)$$

where  $T_{in}$  is the mixture temperature at the inlet and  $T_{target}$  is the target temperature for each wall. These profiles, shown in Figure 3.9, allow for a gradual transition from the inlet temperature to the target temperature at the walls. Periodic boundary conditions were imposed in the spanwise direction.

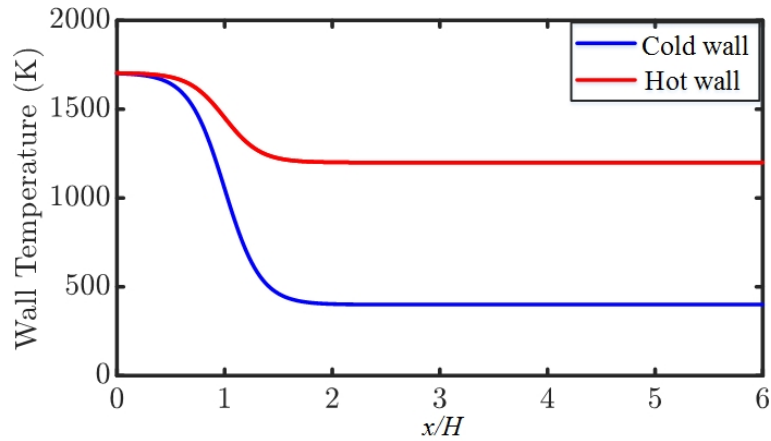


Figure 3.9: Wall temperature for the non-reacting, auxiliary simulation (hot wall temperature = 1200 K, cold wall temperature = 400 K).

The fresh reactants are from a stoichiometric methane/air mixture at 298 K and 2 atm pressure. They are adiabatically mixed with hot products of the same stoichiometric mixture such that the dilution level  $\zeta = 0.7$ . The mixture temperature

at the inlet is  $T_{in} = 1705$  K. Two different wall target temperatures of 400 K and 1200 K were chosen for the cold and hot walls, respectively. This setup permits the examination of different regimes of FWI in one configuration.

Figure 3.10 shows the instantaneous temperature,  $T$ , streamwise velocity,  $U$  and magnitude of vorticity contours in the  $x - y$  plane at  $z/H = 1.5$ . High velocity fluctuations can be observed particularly within  $0.5 H$  wall distance on both sides, where the vorticity magnitude is also high. The growth of the thermal boundary layer is noticeable from about  $x/H = 2$  on both sides, and the vorticity field starts becoming more non-uniform. As expected, the wall-affected temperature field near the hot wall is quite thin. The temperature fluctuations on the cold wall seem higher compared with the top-hot wall. However, there is no clear difference in terms of the level of velocity fluctuations between two sides. These features will be examined in more detail using the velocity and temperature statistics.

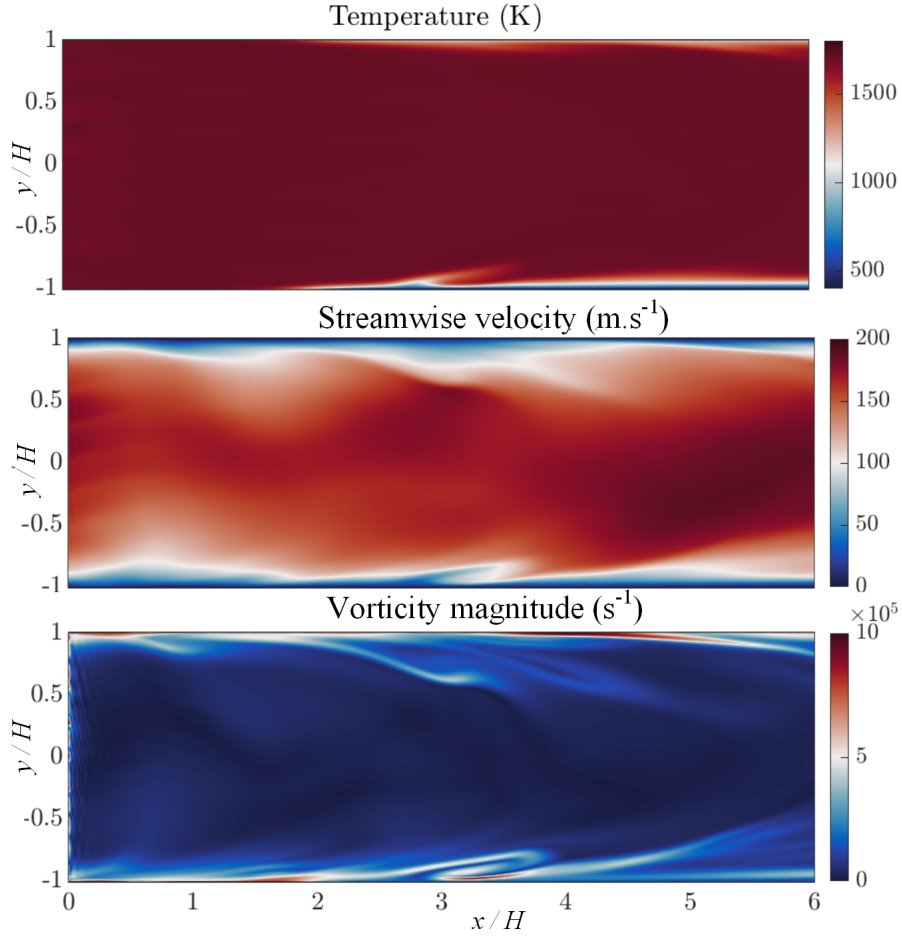


Figure 3.10: Instantaneous temperature (top), streamwise velocity (middle) and vorticity (bottom) contours in the  $x - y$  plane at  $z/H = 1.5$ .

The results of the non-reacting simulation were sampled over 5 jet flow-through times. The mean and RMS of velocity at four streamwise locations  $x/H = 0$  (inlet), 2, 4, 6 (outlet) are shown in Figure 3.11. The level of velocity fluctuations in the near-wall region initially decreases from the inlet to  $x/H = 2$ . Once the flow experiences the near-wall temperature gradient, these fluctuations increase. Temperature fluctuations increase rapidly from the inlet to  $x/H = 4$ , then increase slowly from  $x/H = 4$  to 6, especially near the hot wall. The data is therefore sampled at  $x/H = 4$ . The choice of sampling position leads to an initial thermal boundary layer thickness of  $0.16 H$  and  $0.2 H$  on the hot and cold-wall sides, respectively. Such thin thermal boundary layers are not fully developed. However, the smaller developing thermal boundary layer avoids an upstream interaction between the thermal boundary layer and main reaction around the hot patch. Given the nature of the developing boundary layer, the approach was chosen to ensure coupled temperature-velocity fluctuations from the inlet plane. The Kolmogorov length scale,  $\eta_k$ , at  $x/H = 4$  is presented in Figure 3.12, and it varies from  $6 \mu\text{m}$  to  $82 \mu\text{m}$ .

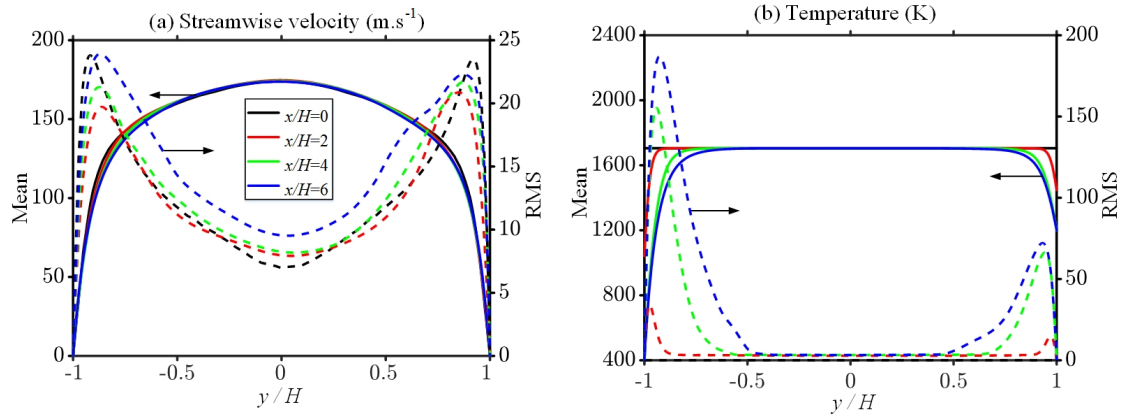


Figure 3.11: Streamwise velocity (a) and temperature (b) profiles at  $x/H = 0$  (inlet), 2, 4, 6 (outlet) averaged over 5 flow-through time ( $\tau_f$ ) and whole span ( $z$ ). Solid lines marks the mean profiles and the dashed lines for the RMS profiles.

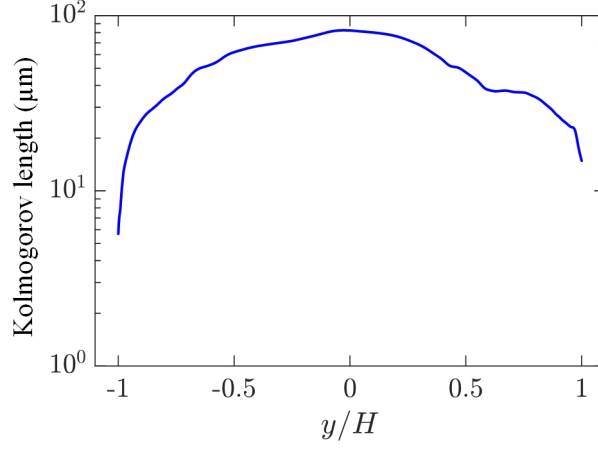


Figure 3.12: Kolmogorov scale at the sampling plane.

Figure 3.13 shows the mean streamwise velocity in a log scale. The mean velocity is normalized by the friction velocity and  $y$  is in wall units. The results show a good match with the Log-law and the linear regions. The log region has the same Von Karman constant with 4 with literature [91], although the intercept with 6 is slightly above 5.5 and was also observed as per [91] with a slight offset the friction velocity. The linear region starts to deviate from the mean profile after  $Y^+ = 4$  as expected. This validates the resolution of the non-reacting case.

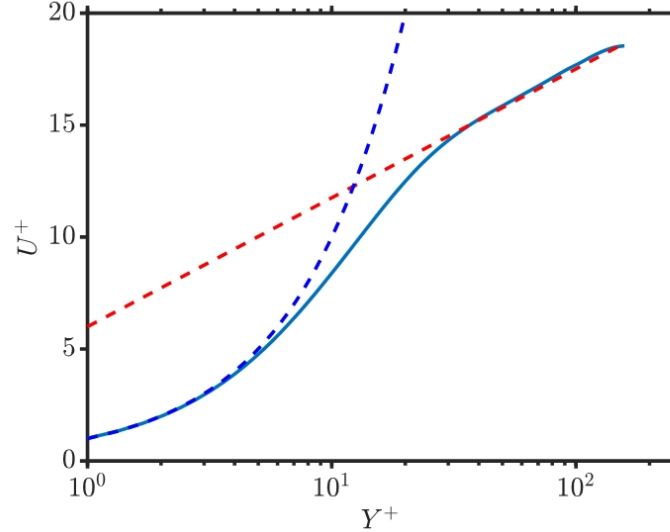


Figure 3.13: Mean streamwise velocity at the inlet of the non-reacting simulation in log scale. The red dashed line follows the Log law with  $U^+ = 2.5\ln(Y^+) + 6$ , and the blue dashed line presents the linear region with  $U^+ = Y^+$ .

The feeding process is verified by comparing the data sampled in the non-reacting case and that at the inlet of the reacting case. Ideally, the sampling and feeding

data are exactly the same. However, numerical artifacts such as errors due to interpolation of the data for time steps, smaller than the sampling time-step, can lead to differences between the sampling and feeding data.

Figure 3.14 shows the absolute and relative differences between these data-sets in terms of the instantaneous results. The maximum difference in the streamwise velocity is  $0.03 \text{ m.s}^{-1}$  in magnitude and  $0.4\%$  relative to the local  $U$ . The maximum difference in the temperature is  $0.06 \text{ K}$  in magnitude and  $0.006\%$  relative to the local  $T$ . The maximum difference appears to be in the near-wall region.

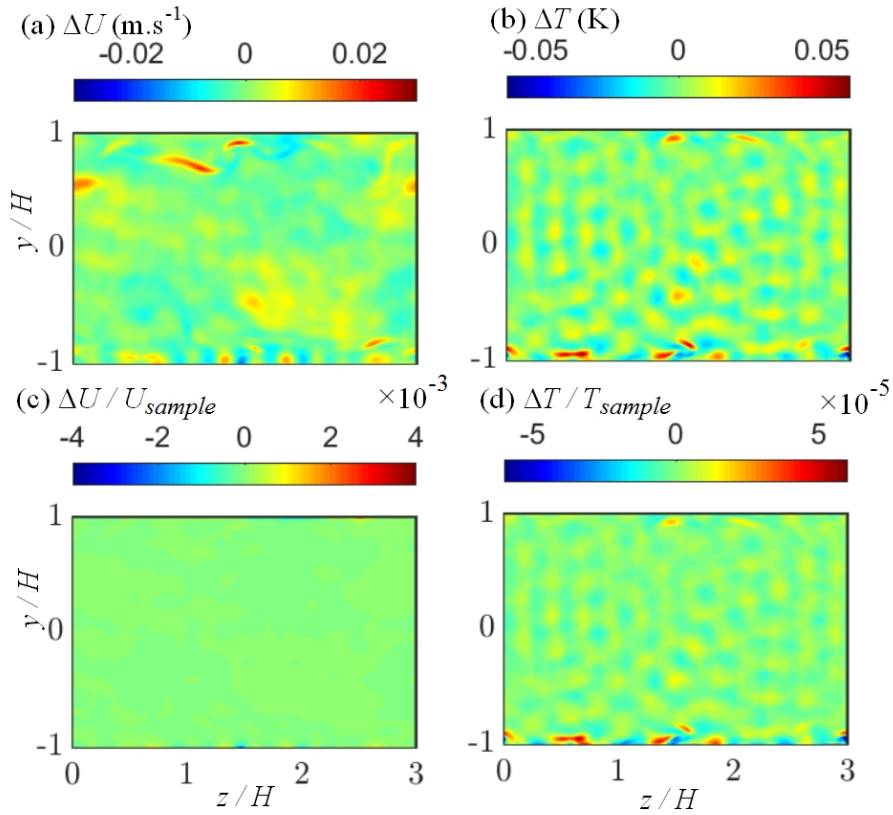


Figure 3.14: Verification of the inlet turbulence generation based on the absolute(a,b) and relative (c,d) difference of the instantaneous streamwise velocity (a,c) and temperature (b,d) between sampling and feeding planes.

Figure 3.15 compares the mean and RMS of velocity and temperature between the two datasets over 0.5 flow through time. The asymmetry of the streamwise RMS velocity may be due to the reduced sampling dataset as well as the asymmetric wall temperature distribution. However, the purpose here is to validate the feeding process. The maximum difference in the mean streamwise velocity is  $0.8 \text{ m.s}^{-1}$  at  $y/H = -0.85$ , and  $0.7\%$  relative to the mean  $U$ . The maximum difference in the



RMS of streamwise velocity is  $0.3 \text{ m.s}^{-1}$  at  $y/H = -0.4$  around 4% of the local RMS value, while this difference is only about 0.2% for the mean velocity at the same  $y/H$ . A maximum difference of about 2 K is observed for both the mean and RMS of temperature with 0.2% and 1.6% relative to the local  $T$ , respectively. This 1.6% difference in RMS is only about 0.15% of the mean at the same  $y/H$ . These results show that the proposed methodology can be used to generate fully coupled velocity-temperature profiles for confined diluted flames by hot products.

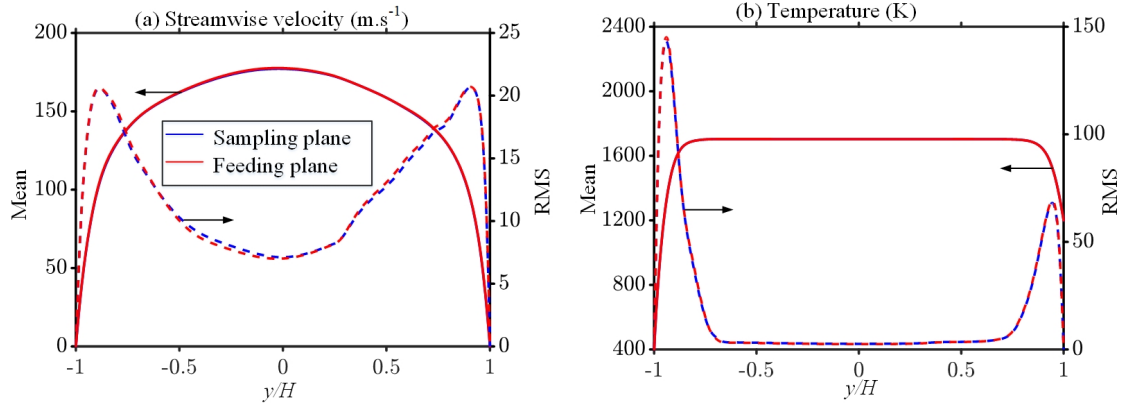


Figure 3.15: Verification of the present inlet turbulence generation based on difference of mean and RMS streamwise velocity (left) and temperature (right) between sampling (blue) and feeding (red)  $y - z$  planes. Profiles are attained from the averaged data over  $0.5 \tau_f$  and whole span ( $z$ ). Solid line is the mean profile and the dashed line is the RMS profile.

After initialisation, the reacting simulations were run for 2 flow-through times on the coarse grid, and then 3 flow-through times on the fine grid. The total computational cost for non-reacting sampling and reacting simulations are about 15,000 CPU-h and 500,000 CPU-h, respectively, running on Intel Xeon E5-2690V3 ‘Haswell’ processors.

## 3.7 Grid Resolution

### 3.7.1 1D HOQ Simulations

Grid independence tests were conducted for both non-diluted and diluted cases at different wall temperatures and pressures. Figure 3.16 shows variation of CO mass fraction at the wall for the cases with  $T_{wall} = 300 \text{ K}$  at  $\zeta = 0$  and 0.6 at 1 atm.

With a  $4\ \mu\text{m}$  grid size, the peak CO is almost identical as that for a  $3\ \mu\text{m}$  grid size. After quenching, a 20% difference between the resolutions is observed. For  $\zeta = 0.6$ , the agreement for two resolutions is even better. At 15 atm,  $\zeta = 0.6$ , the  $1\ \mu\text{m}$  grid size resolved the CO with 10 % difference from the case with  $0.5\ \mu\text{m}$  grid size next to the wall over 2 ms. Based on the result of the grid independence study, the grid size was set to  $4\ \mu\text{m}$  for cases at 1 atm, and  $1\ \mu\text{m}$  for cases at 15 atm pressure.

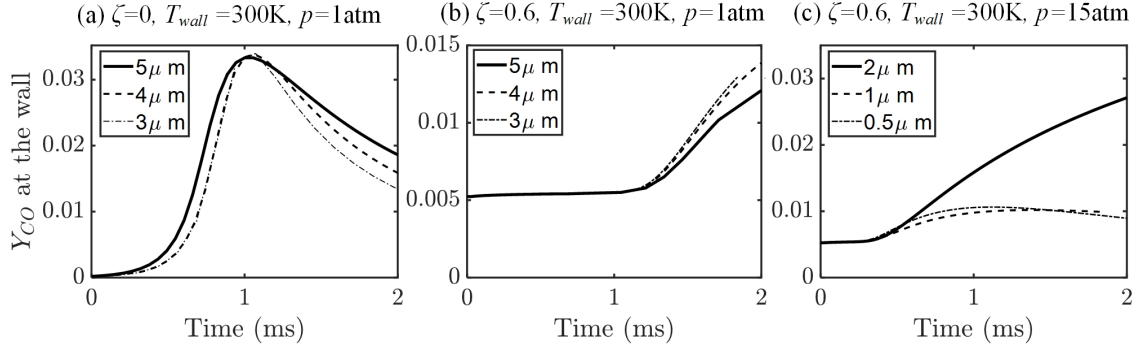


Figure 3.16: 1D grid independence for the dilution level, (a)  $\zeta = 0$  and (b)  $\zeta = 0.6$ ,  $T_{wall} = 300\text{ K}$ , pressure = 1 atm; (c)  $\zeta = 0.6$ ,  $T_{wall} = 300\text{ K}$ , pressure = 15 atm.

### 3.7.2 2D Laminar Flame Simulations

A 2D computational domain as shown in Figure 3.4 was used with  $20\ \mu\text{m}$  uniform grid size in the streamwise direction, and ensures about 20 grid points within the flame thickness at  $\zeta = 0.5$  in the adiabatic region. In the wall-normal direction, the grid size is stretched from  $10\ \mu\text{m}$  at the wall to the  $20\ \mu\text{m}$  at the centreline. A grid independence study was conducted to choose the minimum grid size next to the wall. Three grid sizes were tested, including  $5\ \mu\text{m}$ ,  $10\ \mu\text{m}$  and  $15\ \mu\text{m}$ . The 600 K wall temperature case was chosen as the flame is supposed to be closer to the wall than the 300 K case, and thus requires finer resolution for the near-wall region. CO mass fraction and HRR at the wall are chosen in this examination, since these two parameters are relevant to the following study in Chapter 5. Figure 3.17 shows that CO mass fraction at the wall has less than 5% maximum difference between the  $5\ \mu\text{m}$  and  $10\ \mu\text{m}$ , while the maximum difference increases to about 15% between the  $5\ \mu\text{m}$  and  $15\ \mu\text{m}$  grid sizes. The maximum difference of HRR at the wall is less than 2% between the  $5\ \mu\text{m}$  and  $10\ \mu\text{m}$  grid sizes, and less than 5% between the  $5\ \mu\text{m}$  and  $15\ \mu\text{m}$  grid sizes. Therefore, the  $10\ \mu\text{m}$  grid size next to the wall was used

in the 2D simulation.

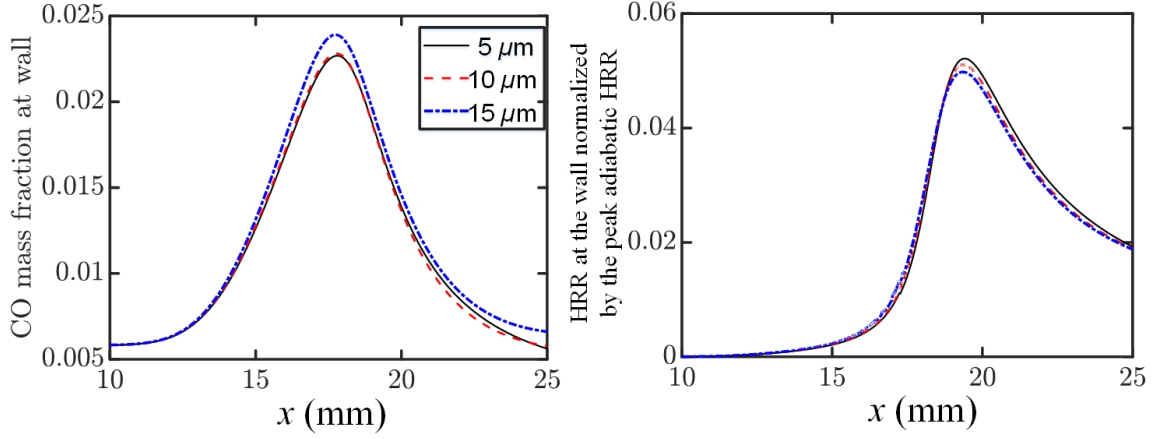


Figure 3.17: CO mass fraction at the wall (left) and HRR at the wall normalized by the peak adiabatic HRR (right) with three different wall-normal grid sizes next to the wall, including 5  $\mu\text{m}$ , 10  $\mu\text{m}$  and 15  $\mu\text{m}$ , at  $\zeta = 0.6$ ,  $T_{\text{wall}} = 600$  K

Figure 3.18 shows the near-wall CO and HRR contours with 5  $\mu\text{m}$ , 10  $\mu\text{m}$  and 15  $\mu\text{m}$  minimum grid sizes. The near-wall HRR and CO mass fraction are visually identical for the 5  $\mu\text{m}$  and 10  $\mu\text{m}$  cases. However, the near-wall HRR around the flame tip is distorted for the 15  $\mu\text{m}$  case. The near-wall CO appears to be higher for the 15  $\mu\text{m}$  case than the other two cases, and this is consistent with the profiles in Figure 3.17. The spurious region in HRR contour for the 15  $\mu\text{m}$  case is likely from the large mesh aspect ratio of  $y$  to  $x$ , which reaches about 40 in that region. This further confirms that the 10  $\mu\text{m}$  grid size next to the wall can resolve the near-wall CO chemistry.

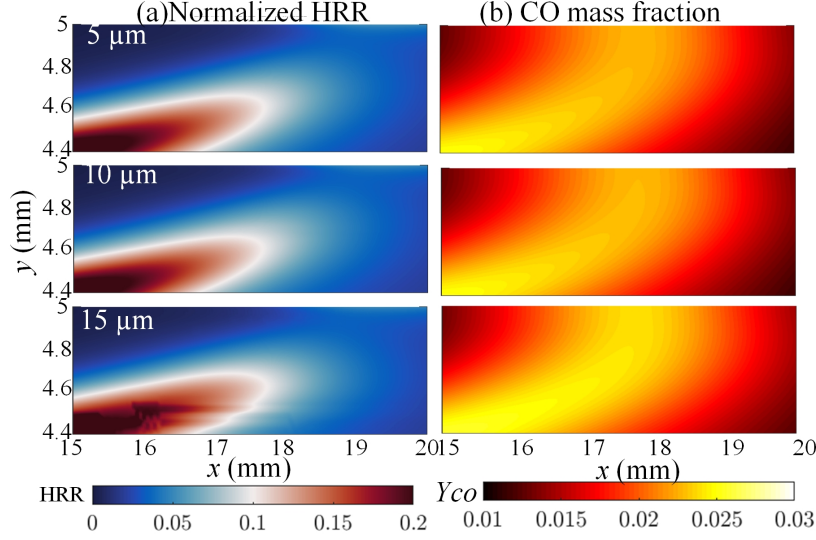


Figure 3.18: Contours of near-wall HRR normalized by the peak adiabatic HRR (a) and CO mass fraction (b) with different grid sizes at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K

### 3.7.3 3D Turbulent Flame Simulation

There are several criteria for grid resolution in the 3D case:

- 1) There should be at least one grid point within the wall unit,  $Y^+ = yu_\tau/\nu$ , where the  $y$  is the wall distance and  $u_\tau$  and  $\nu$  are the friction velocity and gas viscosity at the wall, respectively [24]. A  $5 \mu m$   $y$ -grid size next to the wall satisfies this constraint for both cold and hot wall.
- 2) The mean grid size, defined as  $(\Delta x \Delta y \Delta z)^{1/3}$ , should be less than 1.4 times Kolmogorov length scale ( $\eta_k$ ) [93]. This results in a  $30 \mu m$  uniform  $x$  and  $z$  grid size. The grid size in the  $y$  direction was stretched from  $5 \mu m$  at the wall to  $30 \mu m$  at the centreline, and the near-wall grid size in  $y$  direction is dominated by the  $Y^+$  criterion [24].
- 3) The premixed flame or the main reaction zone of auto-ignition needs to be fully resolved, as both combustion modes co-exist in this case. 3D results showed that the premixed flame structures are generally thinner than the autoignitive flames. Based on this observation, 1D FPFs at different reactant temperatures were simulated with CHEMKIN [85]. The thermal flame thickness is the thinnest ( $\approx 0.77$  mm) at 1100 K reactant temperature. With the chosen grid size discussed earlier, there are around

20 grid points inside the thermal flame thickness at 1100 K.

### 3.8 Chemical Mechanisms

In the 1D and 2D simulations, GRI 3.0 chemical mechanism [44], which includes 53 species and 325 reactions was used to calculate the chemical source terms. In the 3D case, a reduced chemical mechanism was required to reduce the computational cost. A reduced chemical mechanism was developed using Analytically Reduced Chemistry (ARC) [94]. This was undertaken using GRI 3.0 as the reference mechanism with the flame speed, autoignition delay time and CO chosen as target parameters. The final results had less than 5% difference between GRI 3.0 and the ARC chemical mechanism for the maximum and endpoint values. The reduced mechanism has 23 transported species, 12 Quasi-Steady State (QSS) species, and 205 reactions. 0D homogeneous autoignition and 1D HOQ at 400 K and 1200 K wall temperatures and 2 atm pressure have been tested as shown in Figure 3.19 and 3.20. In the 0D model, the difference between temperature profiles is less than 5%. In the HOQ case, the CO mass fraction at the wall has a difference of less than 1% with the reference mechanism.

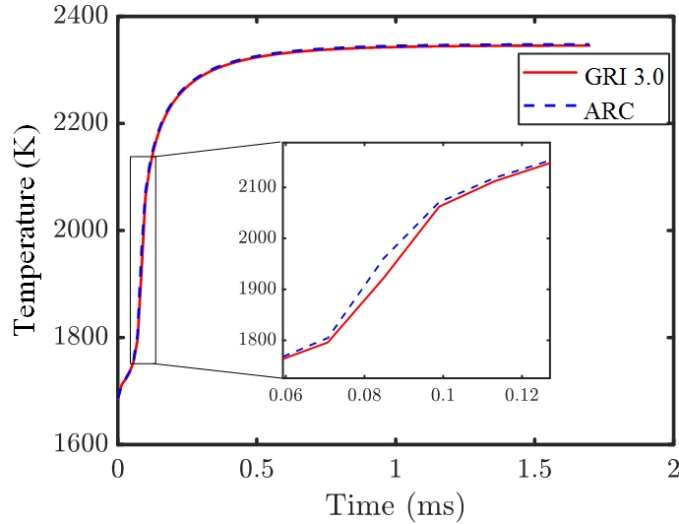


Figure 3.19: Comparison of temporal temperature with ARC and GRI 3.0 chemical mechanism in a 0D homogeneous model at  $\zeta = 0.7$ , 2 atm

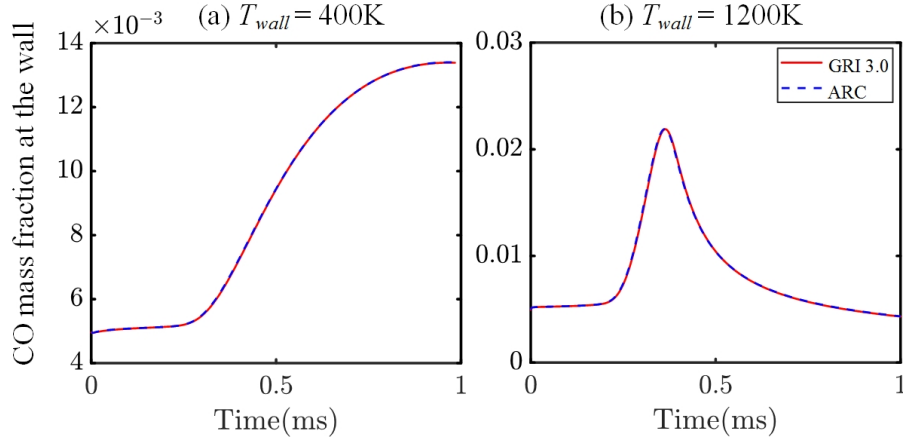


Figure 3.20: Comparison of temporal CO mass fraction at the wall with ARC and GRI 3.0 chemical mechanism in a 1D HOQ at  $\zeta = 0.7$ , 2 atm. (a): 400 K wall temperature; (b): 1200 K wall temperature.

## 3.9 Flame Front Markers

### 3.9.1 1D and 2D Simulations

In 1D and 2D cases, the peak  $\text{CH}_4$  production rate,  $\dot{\omega}_{\text{CH}_4}$ , was used to mark the flame. Figure 3.21 shows the time-distance contour of HRR with the chosen flame marker overlaid. Due to radical recombination, a region of high HRR is observed at the wall during quenching, as also reported in [95]. As a result, the chosen marker is close to the location of the peak HRR up to a distance from the wall but shows the expected behaviour which is the main flame being retracted due to quenching.

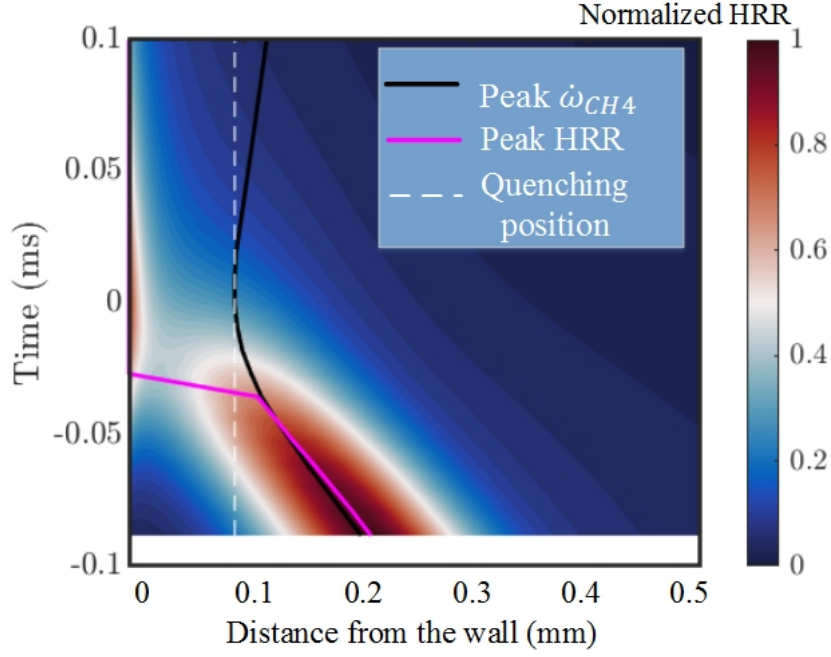


Figure 3.21: Time and distance contour of HRR normalized by peak adiabatic HRR around the quenching instant, and over-plotted with flame front marked by the peak HRR and peak  $\text{CH}_4$  consumption rate ( $\dot{\omega}_{\text{CH}_4}$ ) at  $\zeta = 0.0$ ,  $T_{\text{wall}} = 600$  K.

Figure 3.22 shows how the chosen flame marker performs for the 2D cases at  $\zeta = 0.6$ . The two approaches are closely co-located. The flame tip is identified as the location where the flame-front  $\dot{\omega}_{\text{CH}_4}$  drops below 5 % of the maximum flame-front  $\dot{\omega}_{\text{CH}_4}$ . This threshold is chosen to exclude the post-flame near-wall  $\text{CH}_4$  reactions from being classified as a flame tip. This definition of flame tip also is closely co-located with the definition based on flame-front HRR dropping below 10 % of the maximum flame-front HRR.

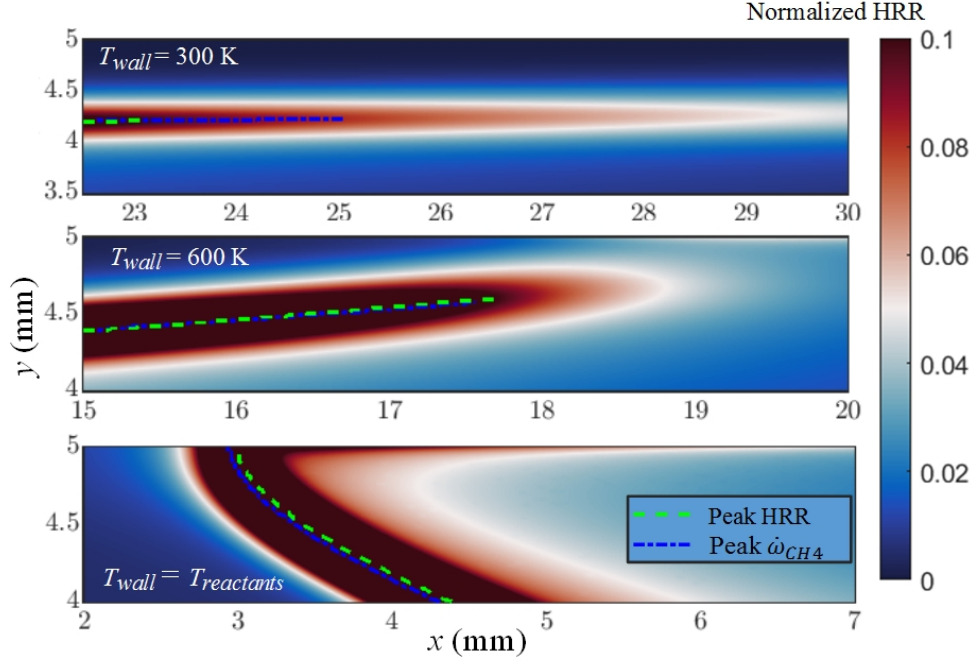


Figure 3.22: Zoomed-in HRR contour normalized by peak HRR around the flame tip and over-plotted with flame front marked by the peak HRR and peak  $\text{CH}_4$  consumption rate ( $\dot{\omega}_{\text{CH}_4}$ ) at  $\zeta = 0.6$ ,  $T_{\text{wall}} = 300$  K, 600 K and  $T_{\text{reactants}}$ .

### 3.9.2 3D Simulation

Unlike the 1D and 2D configurations, the highly wrinkled flame surface in the 3D case makes it difficult to find a peak value to mark the flame front. A progress variable-based flame marker can be used to make the flame in this configuration [24, 96]. The progress variable in this study is calculated as,

$$c_\alpha = \frac{Y_\alpha - Y_{\alpha, \text{unburned}}}{Y_{\alpha, \text{burned}} - Y_{\alpha, \text{unburned}}}. \quad (3.9.1)$$

To find a suitable progress variable, 1D flames were tested to guide the choice of the 3D progress variable. Table 3.7 shows the progress variable values at the peak HRR for different definitions of the progress variable at varied reactants temperatures. The reactant temperature of 900 K is at the flammability limit of the composition used for the 3D case. The reactant temperature of 1700 K is close to the maximum reactant temperature (1705 K) in the 3D case. For the reactant temperature of 900 K and 1100 K, the FPF model was used while for the reactant temperatures of



1600 K and 1700 K featuring auto-ignition, the PFR models with a similar residence time to the 3D case had to be used. The results show that the  $\text{CH}_4$ -based progress variable gives the smallest variation over [900 1700]K reactant temperatures.

Table 3.7: Progress variable values at the peak HRR for 1D flames at different inlet temperature ( $T_{in}$ ) with the composition of  $\zeta = 0.7$ .

| $T_{in}$ (K)                | 900   | 1100  | 1600  | 1700  | max. $\Delta c$ |
|-----------------------------|-------|-------|-------|-------|-----------------|
| $c_{\text{CH}_4}$           | 0.984 | 0.950 | 0.942 | 0.930 | 0.054           |
| $c_{\text{CO}+\text{CO}_2}$ | 0.857 | 0.708 | 0.676 | 0.645 | 0.212           |
| $c_{\text{O}_2}$            | 0.876 | 0.747 | 0.654 | 0.640 | 0.236           |
| $c_T$                       | 0.856 | 0.71  | 0.612 | 0.540 | 0.316           |
| $c_{\text{CO}_2}$           | 0.756 | 0.463 | 0.118 | 0.117 | 0.639           |

To determine a unique value for the  $\text{CH}_4$ -based progress variable, 3D flame fronts with different values of the progress variable are shown at a representative instant in Figure 3.23. The results show that the progress variable at 0.94 marks the overall peak HRR, including the autoignition and near-wall isolated flame fronts inside the reactants or the products. Other species were tested, and the performance is ordered as  $\text{CH}_4 > \text{CO}_2+\text{CO} > \text{O}_2 > \text{CO}_2 > T$ , and consistent with the 1D test shown in Table 3.7.

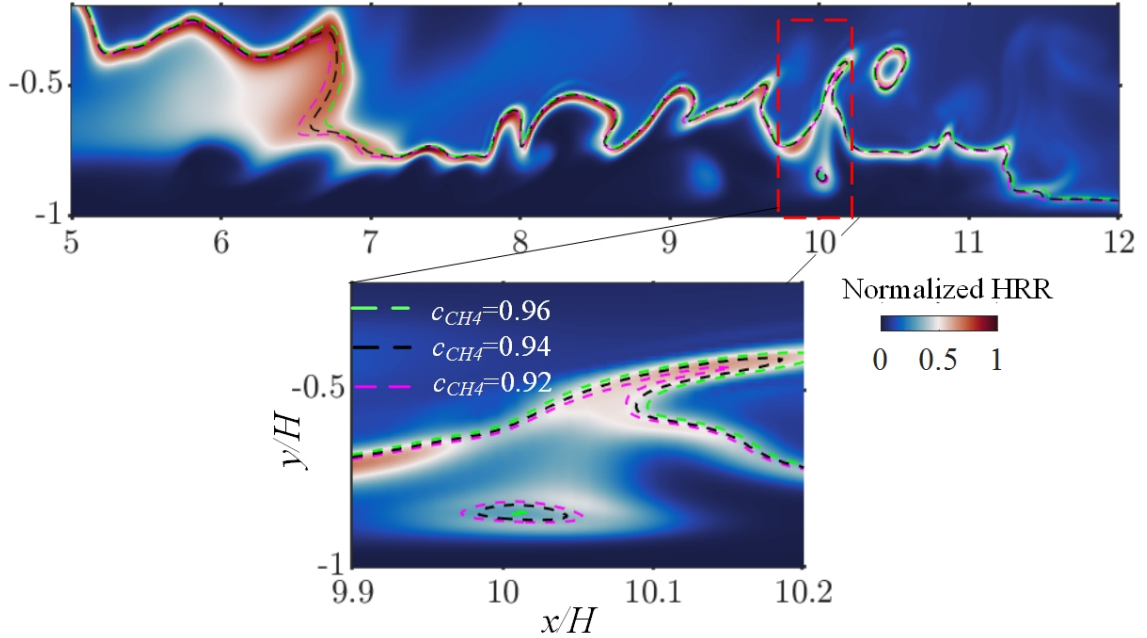


Figure 3.23: Zoom-in HRR contour normalized by peak HRR near the cold wall. The dashed lines are the iso-line of  $\text{CH}_4$  progress variable at different levels.

## 3.10 Conclusions

This chapter presented the numerical methods used to simulate three different configurations in this thesis. Premixed flame and autoignition diluted by combustion products were simulated using DNS with the code known as NTMIX-CHEMKIN. Three configurations in 1D, 2D and 3D were set up to study the interaction of these flames with walls at different temperatures. The first configuration was a 1D Head-On Quenching of flames with different dilution levels in the presence of an inert wall. The second configuration featured a 2D laminar V-flame inside a duct perturbed with velocity perturbations at the inflow. Finally, in the last configuration, a 3D V-flame stabilized inside a duct using a hot spot interacted with the top and bottom walls at relatively high and low temperatures.

The details of the numerical solver was first presented. This is followed by the description of dilution method and each configuration including the computational domain, flow parameters and boundary and initial conditions. The chosen grid resolution with the obtained level of accuracy was then discussed. In the next section, the chemical mechanism used for each configuration was presented. Finally, the parameters used to mark the flame in each configuration were presented and their performance to identify the flame front was assessed.

# Chapter 4

## 1D Diluted HOQ

### 4.1 Introduction

The CO emissions of a head-on quenching Flame-Wall Interaction for flames diluted by hot combustion products is investigated with 1D laminar fully resolved simulations with detailed chemistry. Palulli et al. simulated 1D HOQ without dilution with the fresh reactant mixture and the wall at 800 K [37]. They reported that peak CO mass fraction is around 0.06. The CO mass fraction at the wall changes non-monotonically during the quenching process, and flame deceleration was observed prior to the quenching instant.

Effects of dilution levels, wall temperature and pressure on CO within the quenching region are examined in a constant pressure HOQ configuration. Dilution level stratification is also investigated, and temperature, CO, OH and NO are reported. Following the approach of Ganter et al., the CO species transport budgets are evaluated during HOQ [45]. Approximation of near-wall CO is then considered under these conditions. This study has been published in Jiang et al. [80].

### 4.2 Simulation Parameters

One undiluted and two diluted cases were tested. The  $\zeta = 0.4$  case represents a diluted premixed flame without autoignition, while  $\zeta = 0.6$  has autoignition during

the initial flame approach to the wall. Table 4.1 shows the mixture initial temperature ( $T_{ini}$ ), mass fractions of CH<sub>4</sub>, O<sub>2</sub>, H<sub>2</sub>O, CO<sub>2</sub>, CO, laminar flame speed ( $s_L$ ), ignition delay ( $\tau_{AI}$ ) at these three dilution levels at 1 atm. All combustion products and minor species are retained in the mixture, but the concentrations of minor species are not shown for brevity.

Table 4.1: Initial conditions and properties of reactants.

| $\zeta$ | $T_{ini}$ (K) | $Y_{CH_4}$ | $Y_{O_2}$ | $Y_{H_2O}$ | $Y_{CO_2}$ | $Y_{CO}$ | $s_L$ (m.s <sup>-1</sup> ) | $\tau_{AI}$ (ms) |
|---------|---------------|------------|-----------|------------|------------|----------|----------------------------|------------------|
| 0.0     | 300           | 0.055      | 0.220     | –          | –          | –        | 0.37                       | –                |
| 0.4     | 1132          | 0.034      | 0.136     | 0.048      | 0.053      | 0.003    | 2.60                       | 107.8            |
| 0.6     | 1504          | 0.023      | 0.093     | 0.072      | 0.080      | 0.005    | –                          | 0.69             |

Table 4.2: Quenching distance (mm) at test conditions

| $\zeta$ | $T_{wall} = 300$ K<br>$p = 1$ atm | $T_{wall} = 600$ K<br>$p = 1$ atm | $T_{wall} = 300$ K<br>$p = 15$ atm |
|---------|-----------------------------------|-----------------------------------|------------------------------------|
| 0.0     | 0.220                             | 0.100                             | 0.058                              |
| 0.4     | 0.408                             | 0.246                             | 0.185                              |
| 0.6     | 0.502                             | 0.332                             | 0.147                              |

### 4.3 Results

The results for temperature and CO concentration are presented on distance in mm-time in ms ( $x - t$ ) contour plots (Figures 4.1-4.3). The figures are composites of the 1D domain plotted at each point in time, proceeding from bottom to top and with the wall at  $x = 0$  mm. The quenching distance,  $\delta_Q$ , and quenching time,  $t_Q$ , are determined by the closest flame position to the wall. A vertical dashed line is overlaid at the quenching position ( $x = \delta_Q$ ). The flame position is defined at the maximum CH<sub>4</sub> consumption rate as verified in Section 3.9.1.

The quenching time is set as a reference between cases such that  $t_Q = 0$  ms. From the temperature contours, the flame propagation and the reaction zone retreat after quenching can be observed. The gradient of the isothermal contour at 0.9 temperature-based progress variable,  $c_T$ , as per [13] represents the flame speed at  $\zeta = 0$  and the reaction speed for autoignition cases.

The near-wall temperature gradient is proportional to the wall heat flux. A test of the effects of composition on the thermal conductivity was conducted at the wall temperature. It is found that the thermal conductivity only varies 10% from unburned gas to the products composition at 300 K and 3% at 600 K. Changing pressure from 1 atm to 15 atm does not change the thermal conductivity. The gradients of the CO  $x - t$  contours represent the rate of change of CO.

### 4.3.1 Effects of Dilution Level, $\zeta$

Figure 4.1 shows the  $x - t$  contour plots for changes in the dilution level at 1 atm and  $T_{wall} = 300$  K. As shown in Table 4.2, the quenching distance increases from 0.22 mm at  $\zeta = 0$  to 0.5 mm at  $\zeta = 0.6$ . The 0.22 mm quenching distance at  $\zeta = 0$  and  $T_{wall} = 300$  K is close to the experimental value of 0.17 mm from Mann et al. [42].

The CO at the wall lasts longer at a higher  $\zeta$ , although the peak near-wall CO is lower. For instance, at 2 ms after quenching time, CO mass fraction at the wall at  $\zeta = 0.6$  is about 2 times greater than at  $\zeta = 0$ , although the near-wall peak CO at  $\zeta = 0.6$  is around half the value at  $\zeta = 0$ . This peak CO behavior is consistent with the results in a stagnation configuration as per [97].

Due to the sudden expansion from the autoignition, the premixed flame is pushed away from the wall, which can be seen in the temperature contour plot, marked as “AI-PF interaction”. Quantitatively, tracking the isothermal line at 2100 K with  $0.9 c_T$ , the premixed flame is pushed from  $x = 11$  mm to 14 mm. At the quenching time, the flame after autoignition at  $\zeta = 0.6$  propagates more slowly towards the wall, compared to the case at  $\zeta = 0$ . With the definition of the flame front at  $0.9 c_T$ , the flame propagation speed is around 5 times slower during quenching than the initial adiabatic propagation speed at  $\zeta = 0.6$ . However, the propagating speed at  $\zeta = 0$  is around 10 times faster during quenching than the adiabatic flame speed, consistent with the observation in Wichman and Bruneaux [98].

The near-wall temperature gradient is around half as steep for  $\zeta = 0.6$ , which reduces heat transfer to the wall. Near-wall OH within the quenching layer is almost zero, and its distribution follows the temperature distribution. OH concentration

decreases with increasing dilution level. The NO concentration reduces towards the wall inside the quenching region, yet the near-wall NO increases after quenching. NO increases with increasing dilution level, and is about 100 to 200 ppm near the quenching position at  $\zeta = 0.6$ .

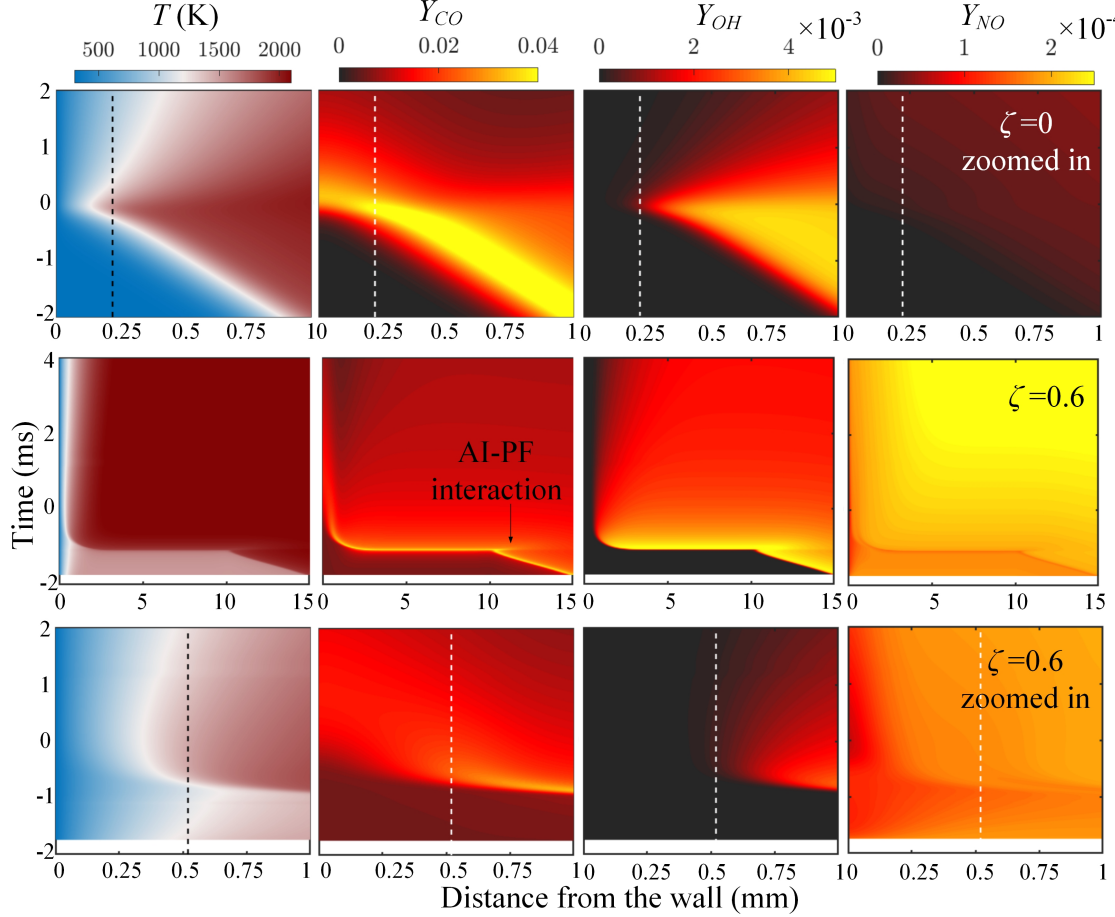


Figure 4.1:  $x - t$  contour plots of temperature (K) and CO, OH, NO mass fraction for  $\zeta = 0.0$  (top) and 0.6 (middle, bottom).  $p = 1$  atm,  $T_{wall} = 300$  K. The bottom row is zoomed into the closest 1 mm to wall for  $\zeta = 0.6$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

### 4.3.2 Effects of Wall Temperature

The isothermal, inert wall temperature was doubled to 600 K to study the effect of wall temperature. Table 4.2 shows that the quenching distance decreases for both cases with increasing wall temperature, consistent with Yenerdag et al. and Westbrook and Dryer [22, 87]. The  $\zeta = 0.0$  case now has a thermal boundary layer (negative gradient) of 0.45 mm, and the initial thermal boundary layer at  $\zeta = 0.6$  has

decreased from 1.0 mm to 0.9 mm. The decrease of quenching distance and thermal boundary layer thickness from 300 K to 600 K increase the near-wall temperature gradient by around 2 times.

Figure 4.2 shows that, compared with the 300 K wall temperature case, the near-wall CO decreases significantly faster at a 600 K wall temperature. The reactions for CO oxidation at the wall was examined at the quenching instant. Increasing wall temperature from 300K to 600K, CO production rates from these four reactions in Table 4.3 changes from zero to the positive contribution on CO oxidation, and these increases are more obvious at  $\zeta = 0$  than  $\zeta = 0.6$ . The increase of reaction rate for  $(CO + O + M = CO_2 + M, \text{Reaction 2.2.7})$  is consistent with Popp and Baum [41], although it is still negligible at  $\zeta = 0.6$ , likely due to the larger quenching distance and the dilution effects.

The increased wall temperature affects the near-wall temperature gradient, the near-wall reactant temperature, and increases the equilibrium CO as per Ganter et al. and Rivera et al. [45, 55]. Near-wall OH increases with increasing the wall temperature from 300 K to 600 K and becomes non-zero at the wall at 600 K wall temperature. Near-wall NO increases with increasing wall temperature.

Table 4.3: Reactions CO oxidation at  $T_{wall}=600\text{K}$ ,  $p = 1$  atm at the quenching instant at the wall.

| Reactions                                                                     | Rate of production<br>at $\zeta = 0$ ( $\text{kg.m}^{-3}.\text{s}^{-1}$ ) | Rate of production<br>at $\zeta = 0.6$ ( $\text{kg.m}^{-3}.\text{s}^{-1}$ ) |
|-------------------------------------------------------------------------------|---------------------------------------------------------------------------|-----------------------------------------------------------------------------|
| $\text{CO} + \text{OH} = \text{CO}_2 + \text{H}$                              | 58                                                                        | 1.5                                                                         |
| $\text{H} + \text{CO} + \text{H}_2\text{O} = \text{HCO} + \text{H}_2\text{O}$ | 1.6                                                                       | 0.02                                                                        |
| $\text{H} + \text{CO} + \text{M} = \text{HCO} + \text{M}$                     | 1.0                                                                       | 0.01                                                                        |
| $\text{O} + \text{CO} + \text{M} = \text{CO}_2 + \text{M}$                    | 0.2                                                                       | 0                                                                           |

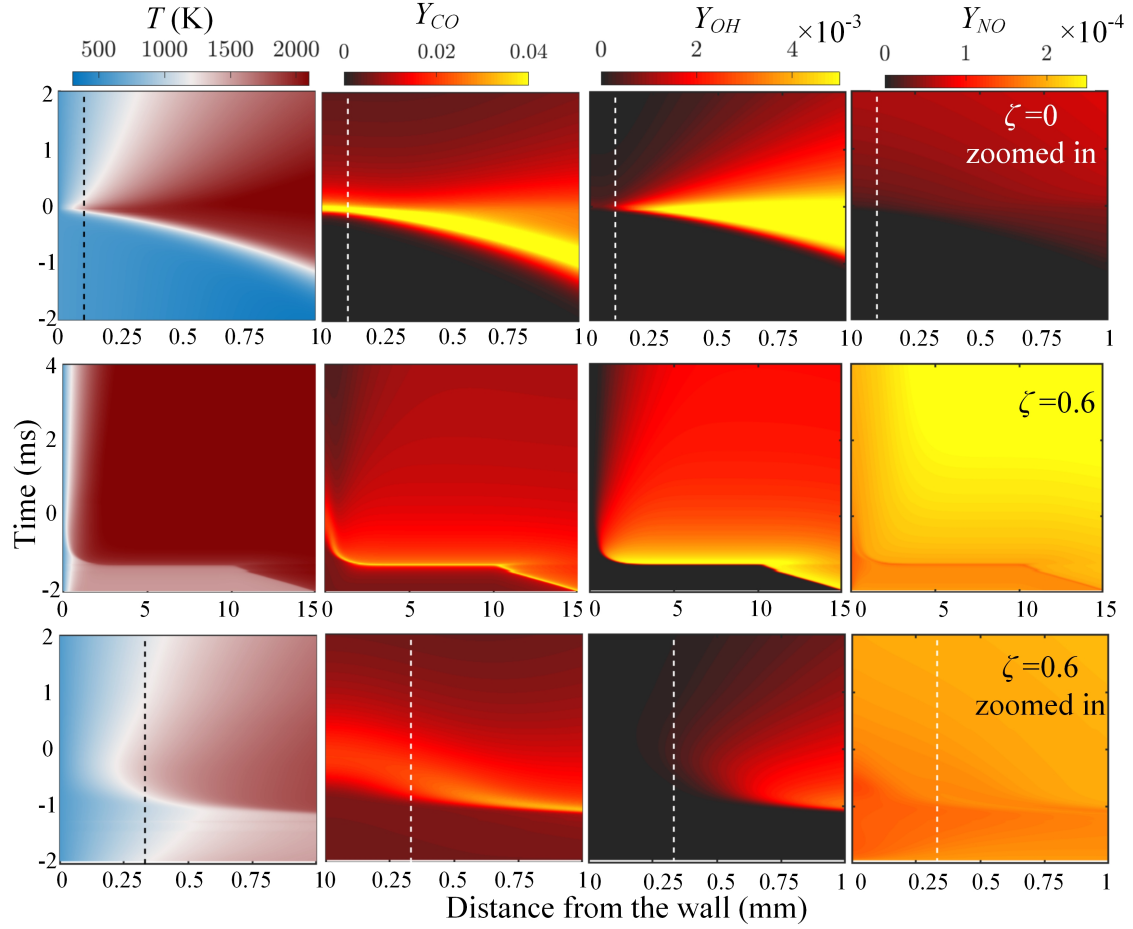


Figure 4.2:  $x - t$  contour plots of temperature (K) and CO , OH, NO mass fraction for  $\zeta = 0.0$  (top) and 0.6 (middle, bottom).  $p = 1$  atm,  $T_{wall} = 600$  K. The bottom row is zoomed into the closest 1 mm to wall for  $\zeta = 0.6$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

### 4.3.3 Effects of Pressure

The effect of pressure is investigated through comparing cases at 15 atm, 300 K  $T_{wall}$  as shown in Figure 4.3. The  $\zeta = 0.6$  case displays autoignition at 15 atm, but the small timescale of the ignition delay makes comparison with the  $\zeta = 0$  case challenging as shown in Figure 4.4.  $\zeta = 0.4$  at 15 atm also displays autoignition, so is used to compare with  $\zeta = 0$ . At higher pressure, the quenching distance decreases as shown in Table 4.2, consistent with literature [87]. The quenching distance is 4 times larger than the empirical formula in Equation 2.2.6 as per [87] at  $\zeta = 0$ .

The peak CO at the wall is about half that of the 1 atm results. A 1D FPF flame



at  $\zeta = 0$  shows that the peak CO oxidation rate of the reaction 4.3.1



is  $180 \text{ kg.m}^{-3}.\text{s}^{-1}$ , which is about 7 % of the peak net CO oxidation rate ( $2500 \text{ kg.m}^{-3}.\text{s}^{-1}$ ) at 15 atm, while this reaction is negligible at 1 atm. This is consistent with literature [99, 100]. NO mass fraction within the quenching layer decreases to zero with increasing the pressure from 1 atm to 15 atm, while the adiabatic post-flame NO increases. OH decreases with increasing the pressure as per [100].

For the  $\zeta = 0.4$  case at higher pressure, the decrease of initial thermal boundary layer from 0.8 mm to 0.2 mm and quenching distance from 0.4 mm to 0.19 mm nearly doubles the near-wall temperature gradient.

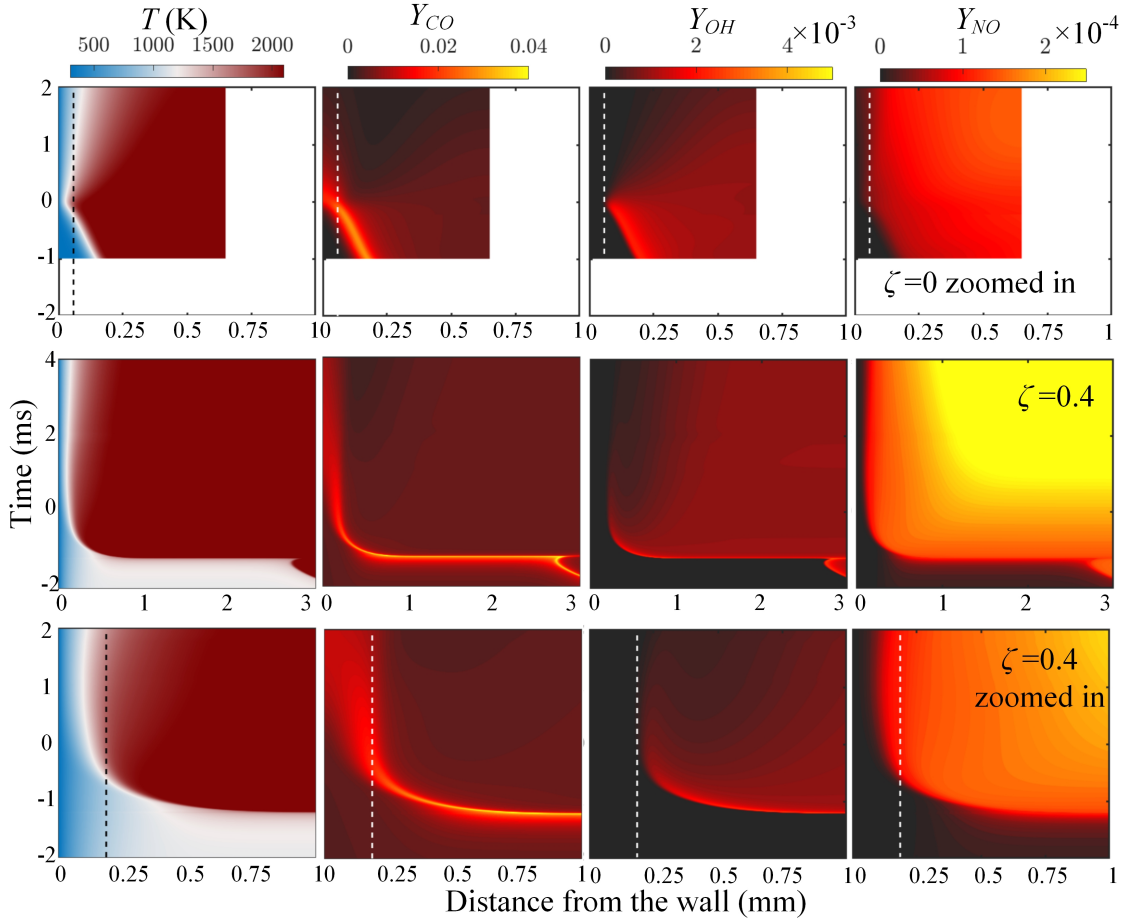


Figure 4.3:  $x - t$  contour plots of temperature (K) and CO, OH, NO mass fraction for  $\zeta = 0.0$  (top) and 0.4 (middle, bottom).  $p = 15 \text{ atm}$ ,  $T_{wall} = 300 \text{ K}$ . The bottom row is zoomed into the closest 1 mm to wall for  $\zeta = 0.4$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

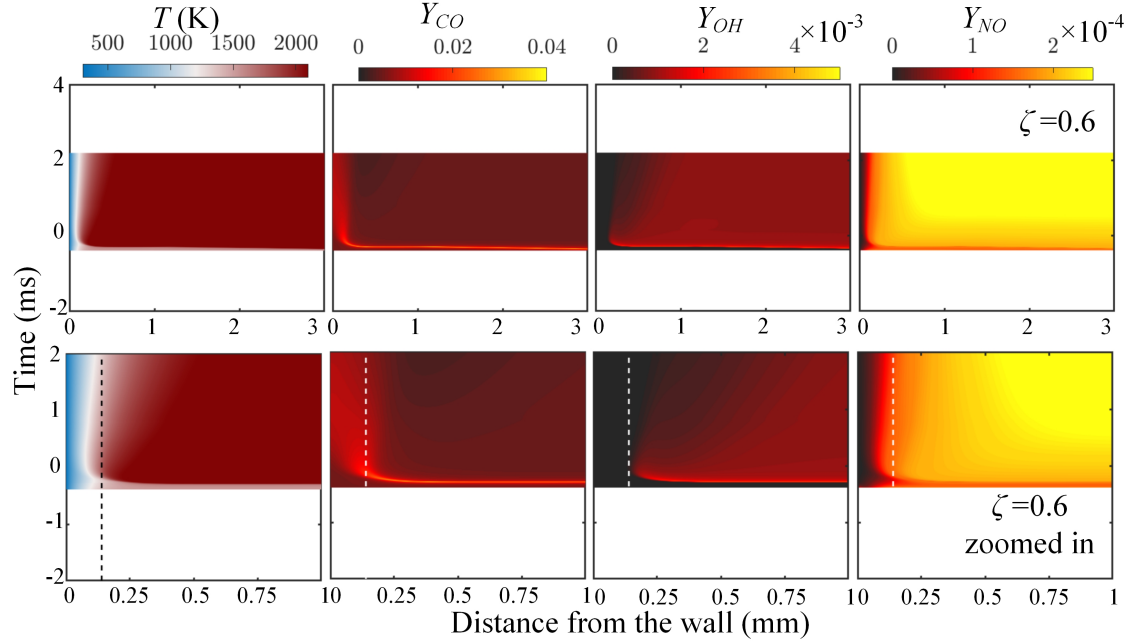


Figure 4.4:  $x - t$  contour plots of temperature (K) and CO, OH, NO mass fraction for  $\zeta = 0.6$  (middle, bottom).  $p = 15$  atm,  $T_{wall} = 300$  K. The bottom row is zoomed into the closest 1 mm to wall for  $\zeta = 0.6$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

#### 4.3.4 Effects of Stratified Dilution Level

It is possible in the HOQ configuration for there to be a stratification of dilution near the wall. This could either take the form of cold reactants near the wall mixing with free-stream combustion products or hot combustion products trapped near the wall and mixing with free-stream cold reactants. To consider such inhomogeneous mixing, a gradient in  $\zeta$  was tested for these two configurations.

The first case, referred to as the negative  $\zeta$  gradient case ( $d\zeta/dx < 0$ ), has products ( $\zeta = 1$ ) next to the wall, with a linear transition over 5 mm to non-diluted reactants ( $\zeta = 0$ ) away from the wall. The second case, referred to as the positive  $\zeta$  gradient case ( $d\zeta/dx > 0$ ), has non-diluted reactants at  $\zeta = 0$  next to the wall, with a linear transition over 5 mm to hot combustion products at  $\zeta = 1$ . The initial temperature and  $O_2$  mass fraction profiles for both cases are shown in Figure 4.5. A premixed flame front was initialized at  $x = 5$  mm for both cases. The wall temperature is 300 K. As a consequence, the negative gradient case has an initial thermal boundary layer of 0.4 mm initialised between the wall and hot combustion products.

Figure 4.6 shows the  $x - t$  contour plots for these cases. For the negative  $\zeta$  gradient case, the near-wall reaction zone moves away from the wall, and leaves combustion products next to the wall. Near-wall CO within this region decreases over time towards equilibrium, and the low CO region follows the thermal boundary layer thickness. The near-wall NO decreases over time. There is effectively no FWI in this case, as the main reaction zones are pushed away from the wall by the expansion of the product gases.

For the positive  $\zeta$  gradient case, the main reaction zone moves towards the wall and quenches at a similar position to the  $\zeta = 0$  case at around 0.22 mm. The reaction zone moves faster towards the wall at a higher  $\zeta$  due to the higher local temperature and intermediate species. Peak CO mass fraction is lower at the higher dilution levels. Near-wall species show almost the same features with the  $\zeta = 0$  case. This identifies that the dilution gradient, or simulated mixing of reactants and diluent, has little effect on the FWI and subsequent post-quench CO where the reactants are close to the wall.

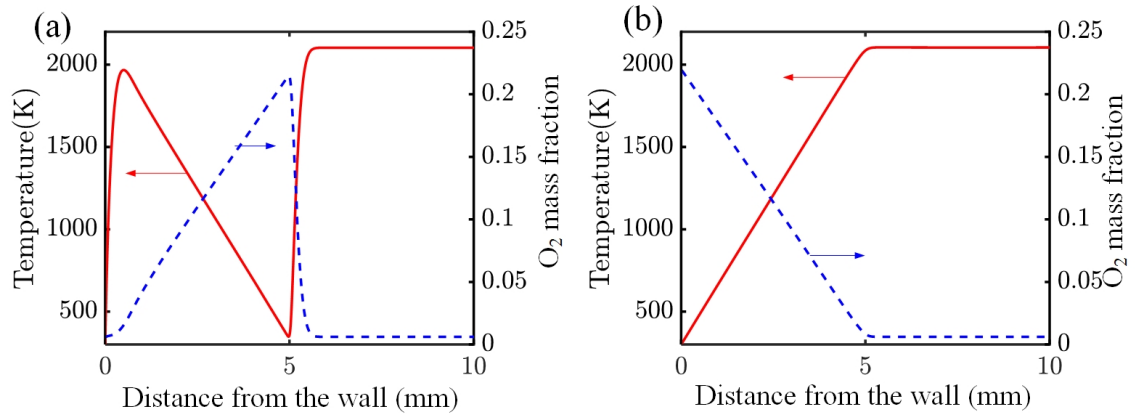


Figure 4.5: Initial temperature and  $O_2$  mass fraction profile at the stratified  $\zeta$  configurations. Left:  $\zeta$  transits from 1 to 0 as further away from the wall (i.e.  $d\zeta/dx < 0$ ). Right:  $\zeta$  transits from 0 to 1 as further away from the wall (i.e.  $d\zeta/dx > 0$ ).

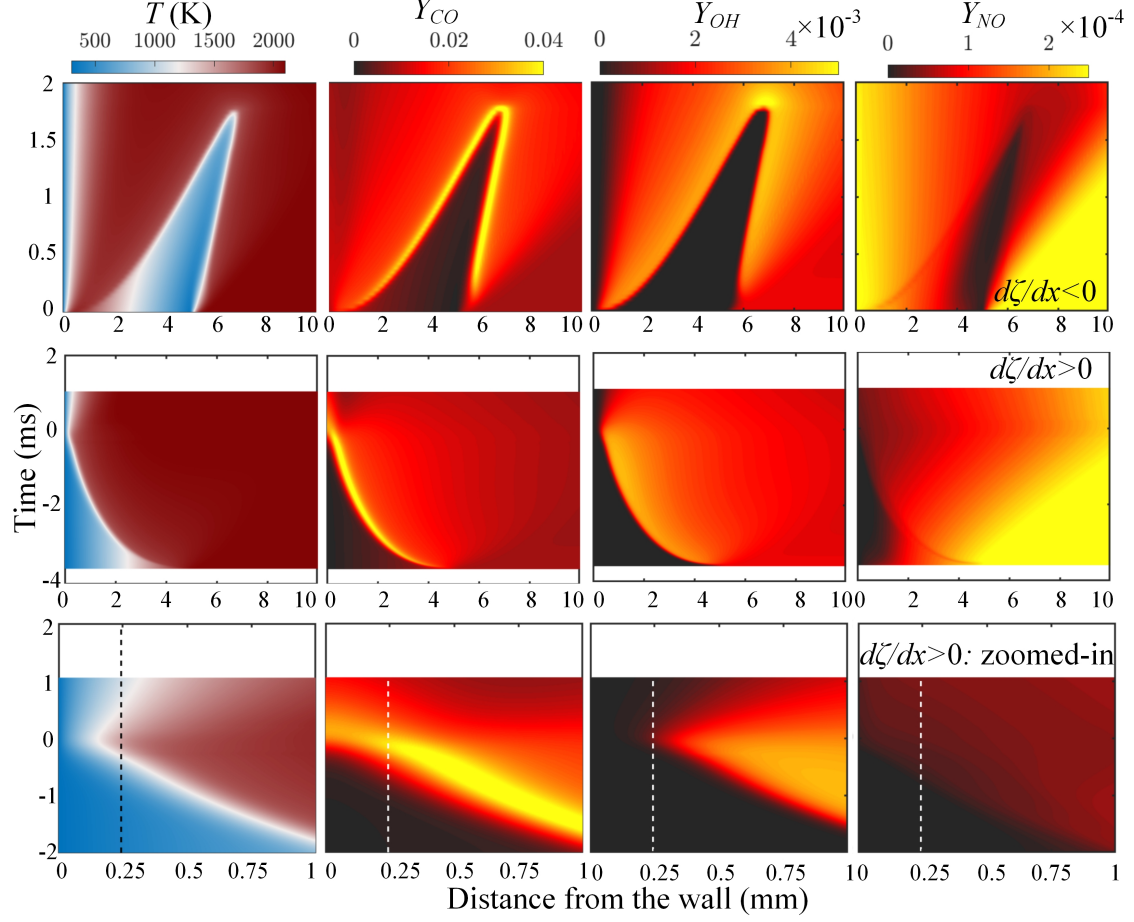


Figure 4.6:  $x - t$  contour plots of temperature (K) and CO, OH, NO mass fraction for  $d\zeta/dx < 0$  (top) and  $d\zeta/dx > 0$  (middle, bottom).  $p = 1$  atm,  $T_{wall} = 300$  K. The bottom row is zoomed into the closest 1 mm to wall for  $d\zeta/dx > 0$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

## 4.4 Discussion

Increasing the dilution level from 0.0 to 0.6 halves the peak CO at the wall, and near-wall CO reduces approximately half as slowly after quenching. However, increasing the wall temperature from 300 K to 600 K increases the wall CO reduction rate by an order of magnitude. The spatially-averaged near-wall CO within the quenching distance is now further characterized to determine under what conditions the results can be modelled simply.

#### 4.4.1 Spatially Averaged CO within the Quenching Distance

The average CO mass fraction within the quenching distance was calculated from the beginning of the simulation for each case. The average CO mass fraction,  $\tilde{Y}_{co}$ , is determined within one quenching distance, and is defined as Equation 4.4.1. The averaged CO is normalized to a dry, 15% O<sub>2</sub> basis (see Equation 4.4.2) according to established industrial practice (e.g. [3]).

$$\tilde{Y}_{co} = \frac{\int_0^{\delta_Q} \rho Y_{co} dx}{\int_0^{\delta_Q} \rho dx} \quad (4.4.1)$$

$$CO(ppmvd, 15\%O_2) = 1 \times 10^6 \frac{0.059 X_{CO}}{0.209(1 - X_{H_2O}) - X_{O_2}} \quad (4.4.2)$$

Figure 4.7 plots  $\tilde{Y}_{co}$  from 2 ms prior to quenching to 2 ms after quenching for  $\zeta = 0, 0.4$  and  $0.6$  for different  $T_{wall}$  and  $p$ . Figure 4.7(a) shows that at a higher dilution level, the average CO has a lower peak but lasts longer, indicated by the average CO at 2 ms reducing from  $4.5 \times 10^4$  at  $\zeta = 0.0$  to  $3.5 \times 10^4$  at  $\zeta = 0.4$  and  $3.0 \times 10^4$  at  $\zeta = 0.6$ .

Comparison of Figures 4.7(a) and 4.7(b) shows that the peak average CO increases at 600 K wall temperature by a factor of 1.2 for all dilution levels. Comparison of Figures 4.7(a) and 4.7(c) shows that the CO peak decreases at a 15 atm by a factor of 0.46, 0.47 and 0.33 for  $\zeta = 0.0, 0.4$  and  $0.6$ , respectively. Analysis of the gradients of the curves shows that the reduction rate of average CO is lower at higher pressure and higher at higher  $T_{wall}$  as shown in Figure 4.8. These results are consistent with those presented in Figures 4.1 - 4.3.

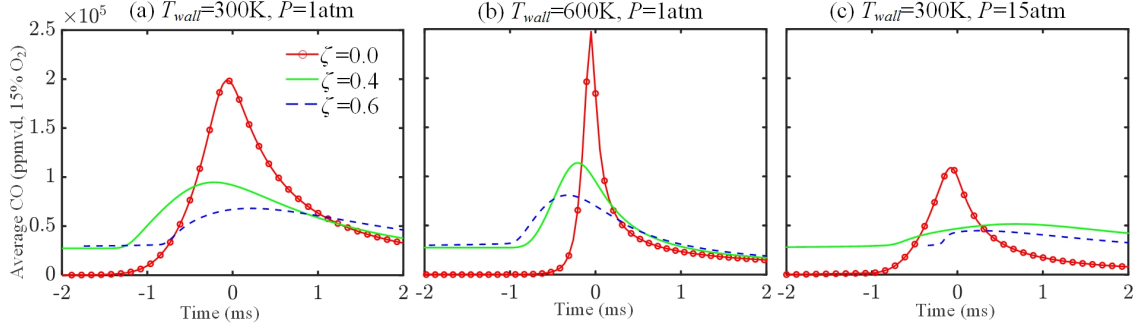


Figure 4.7: Average near-wall CO over time within the quenching distance.

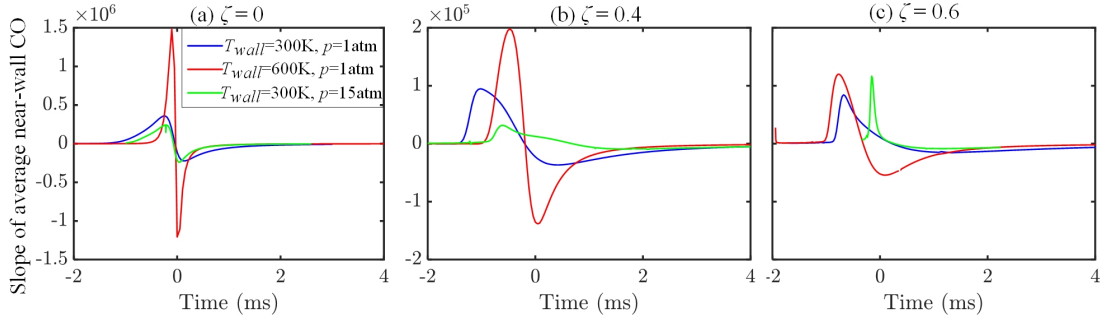


Figure 4.8: Gradient of average near-wall CO profiles in Figure 4.7.

The results at  $\zeta = 0.4$  used a 5 mm initial flame-wall distance ( $\delta_{ini,fw}$ ), while  $\zeta = 0.6$  used 15 mm  $\delta_{ini,fw}$ . The main reason for this is the elimination of the initial premixed flame effects on FWI, due to the increased propagation speed of the hotter  $\zeta = 0.6$  case. To determine if changing  $\delta_{ini,fw}$  affects the results, a later test was conducted with 15 mm  $\delta_{ini,fw}$  at  $\zeta = 0.4$  as shown in Figure 4.9. Both cases with 5 mm and 15 mm  $\delta_{ini,fw}$  at  $\zeta = 0.4$  have a higher gradient of average CO and higher peak CO than at  $\zeta = 0.6$ . However, the 15 mm  $\delta_{ini,fw}$  has a smaller gradient of average CO than the 5 mm  $\delta_{ini,fw}$  case, and the thermal BL prior to the FWI becomes thicker, increasing the quenching distance.

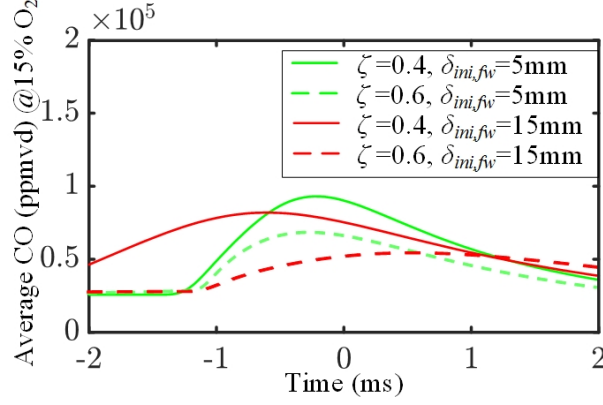


Figure 4.9: Average near-wall CO for the case initialised with 5 mm and 15 mm initial flame-wall distance at dilution level,  $\zeta = 0.4$  and 0.6.

The effect of the initial thermal BL thickness was examined as well. Figure 4.10 shows two cases at  $\zeta = 0.6$  with different initial thermal BL thicknesses but the same initial flame-wall distance. The results show that, compared with the case with 1mm initial thermal BL, the quenching distance is about 20% larger with 3mm initial thermal BL, resulting in about 20% smaller peak CO at the wall and a slower decrease. This is similar to the effect of initial flame-wall distance. However, one should note that the definition of thermal BL after quenching is different from traditional non-reacting thermal BL, because of the reaction and species diffusion inside this layer.

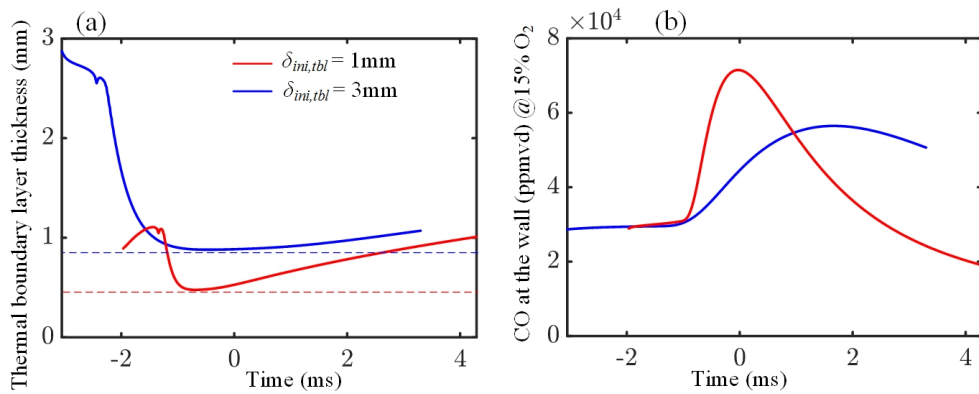


Figure 4.10: Evolution of (a) the thermal BL thickness defined with  $0.99 \times T_{reactants}$  (1504 K) and (b) CO at the wall at  $\zeta = 0.6$ ,  $T_{wall} = 300$  K,  $p = 1$  atm with 1mm and 3mm initial thermal BL thickness. (Dashed lines mark the quenching distances.)

## 4.4.2 CO Species Transport Budgets

The species transport budget shown in Equation 3.2.4 can be used to analyze the CO transport near the wall, which gives the contribution of each term to the CO concentration as per [45].

### 4.4.2.1 Dilution Level Effects

Figure 4.11 shows the CO species transport budget for  $\zeta = 0$  and 0.6,  $T_{wall} = 300$  K and 1 atm, at three time instants: 0.5 ms before quenching; the moment of quenching; and 0.5 ms after quenching ( $t = -0.5, 0, 0.5$  ms). At the quenching time, the near-wall CO transport is dominated by diffusion and reaction, while the convection term is relatively small. The peak convection term inside the quenching layer is less than a quarter of  $D$  or  $R$  and almost zero at  $\zeta = 0.6$  case.

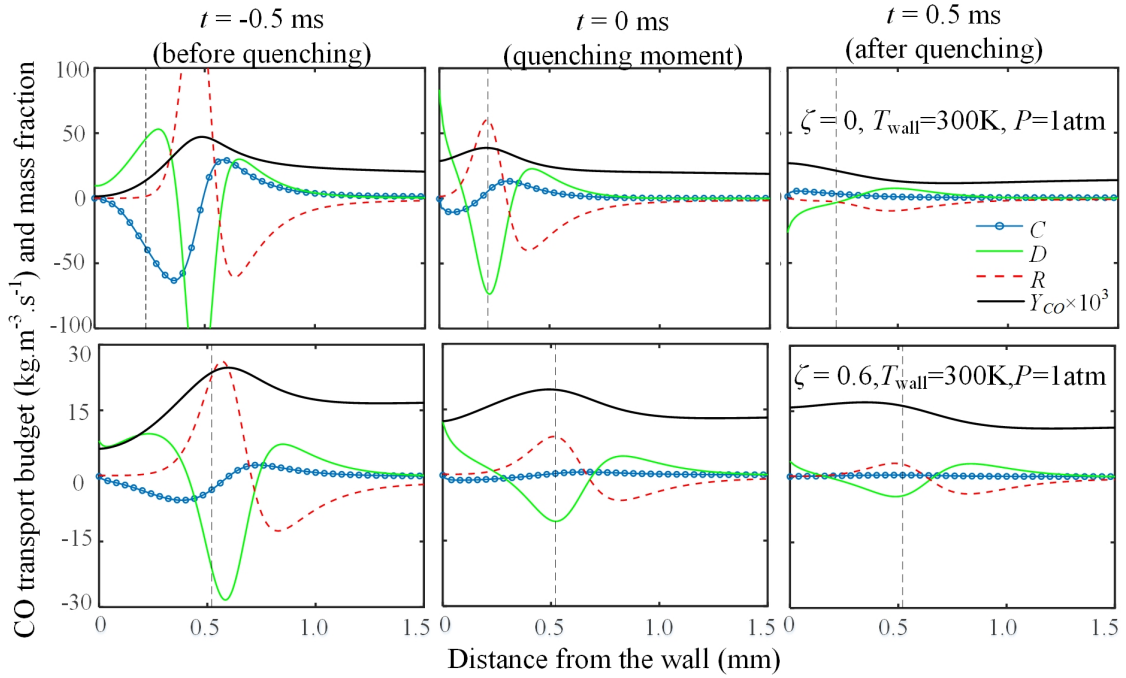


Figure 4.11: Species transport budgets and CO mass fraction for  $\zeta = 0.0$  (top) and 0.6 (bottom) 0.5 ms before, during, and 0.5 ms after quenching.  $p = 15$  atm,  $T_{wall} = 300$  K. The bottom row is zoomed into the closest 1 mm to wall for  $\zeta = 0.6$  case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

The contribution of these terms is indicated by the sign of terms in the corresponding region. For  $\zeta = 0$ , the region with positive  $R$  is identified as the premixed flame



reaction zone. Before quenching ( $t = -0.5$  ms),  $R > 0$  and  $D < 0$  in the reaction zone, which indicates that CO generated in the flame is diffused out of the reaction zone. The effect is enhanced as the flame gets closer to the wall, and at the quenching time all the contributions increase the near-wall CO. After quenching ( $t = 0.5$  ms), the diffusion and reaction terms decrease the near-wall CO, and diffusion again has the dominant role. For the  $\zeta = 0.6$  case, all three terms are an order of magnitude lower compared to the  $\zeta = 0$  case, while the reaction and convection terms are almost zero near the wall. CO transport is then mainly driven by diffusion. At all these times, the diffusion term makes positive contributions to near-wall CO.

#### 4.4.2.2 Wall Temperature and Pressure Effects

Figure 4.12 and Figure 4.13 show the  $C - D - R$  budgets at  $\zeta = 0$  and  $0.6$  at different wall temperatures and pressures. Increasing the wall temperature results in increased diffusion and reaction terms before and after quenching. At quenching, the diffusion and reaction terms are all negative, indicating a decrease of the near-wall CO, which is opposite to the low wall temperature cases.

Increasing the pressure increases both the diffusion and reaction terms before and after quenching by 1 and 2 orders of magnitude for  $\zeta = 0$  and  $\zeta = 0.6$ , respectively. Higher pressure increases the diffusion term, due to the decreased flame thickness which increases the mass fraction gradient. The reaction term also increases at higher pressure, because of the increased reactant density. Like the  $\zeta = 0.6$ ,  $p = 1$  atm case, at  $p = 15$  atm, the near-wall diffusion term after quenching is still positive, so the near-wall CO increases after quenching, as shown in the average CO profile in Figure 4.7.

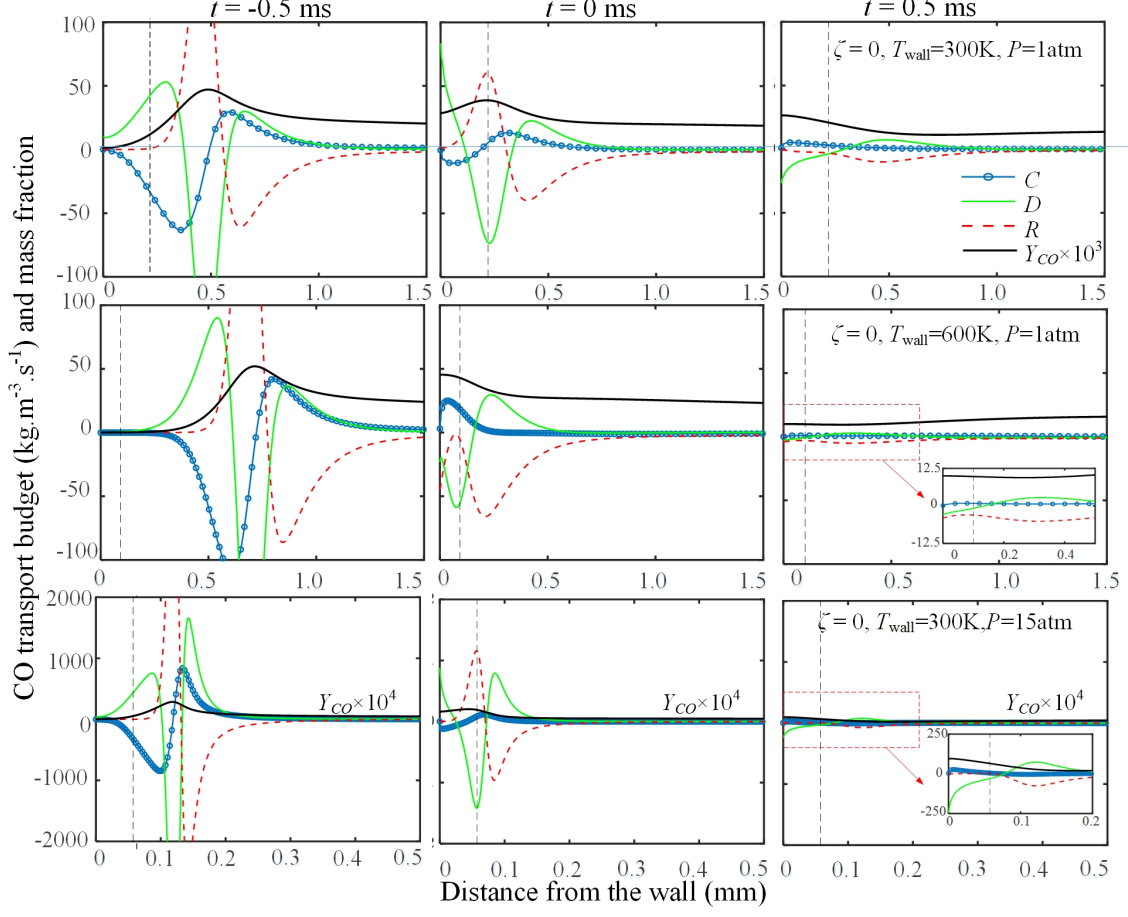


Figure 4.12: Species transport budgets and CO mass fraction for  $T_{wall} = 300$  K,  $p = 1$  atm (top row),  $T_{wall} = 600$  K,  $p = 1$  atm (middle row) and  $T_{wall} = 300$  K,  $p = 15$  atm (bottom row) at  $\zeta = 0.0$ , 0.5 ms before, during, and 0.5 ms after quenching. The  $Y_{CO}$  in bottom row is 10 times higher than the top and middle rows, and is zoomed into the closest 0.2 mm to wall for comparison for  $p = 15$  atm case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

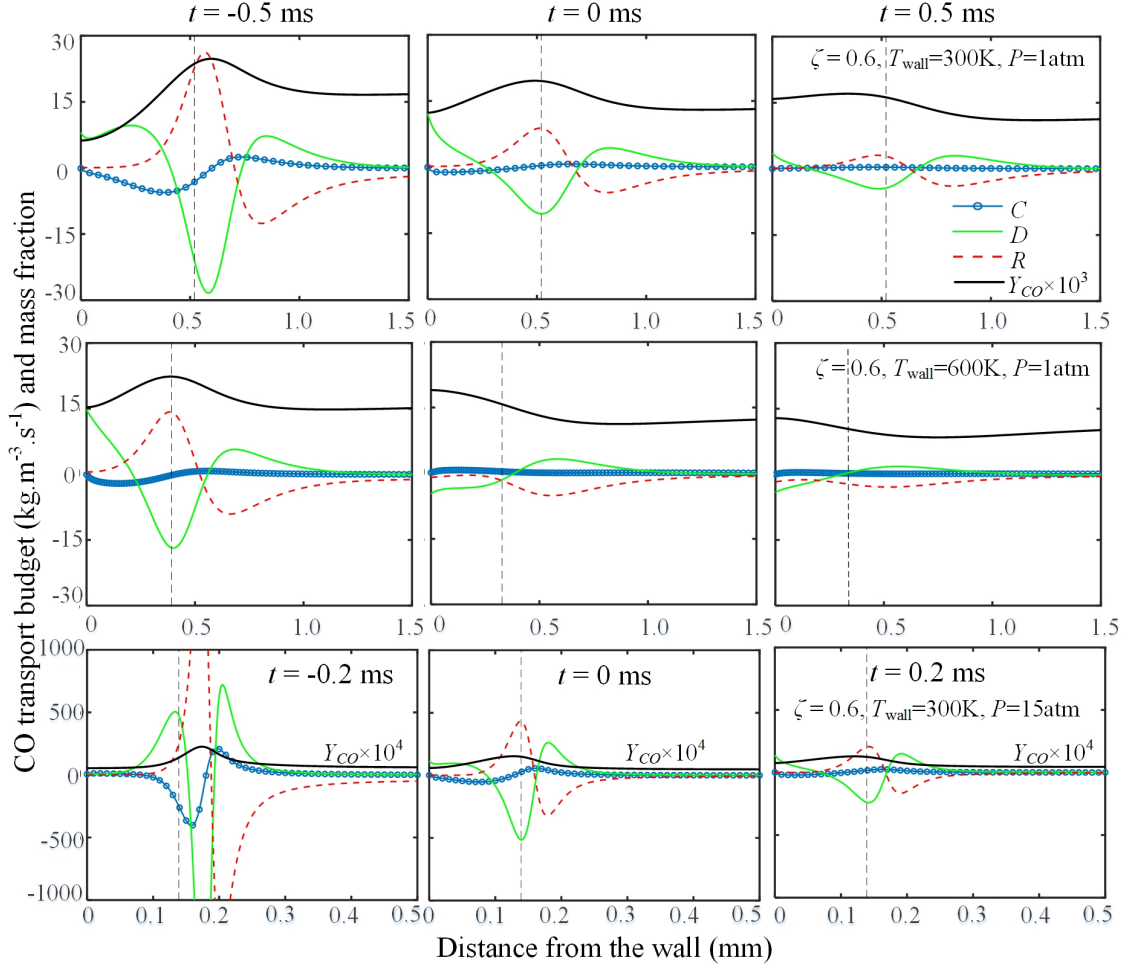


Figure 4.13: Species transport budgets and CO mass fraction for  $T_{wall} = 300$  K,  $p = 1$  atm (top row),  $T_{wall} = 600$  K,  $p = 1$  atm (middle row) and  $T_{wall} = 300$  K,  $p = 15$  atm (bottom row) at  $\zeta = 0.6$ , 0.5 ms before, during, and 0.5 ms after quenching. The  $Y_{CO}$  in bottom row is magnified 10 times for comparison for  $p = 15$  atm case. The vertical dashed line indicates quenching distance,  $\delta_Q$ .

#### 4.4.3 Approximation for Near-wall CO Modelling

It has been indicated in recent work by Ganter et al. that for some premixed, atmospheric, undiluted flames the integral of the diffusion term can largely predict the observed near-wall CO for a SWQ configuration [45]. A similar approach may be sufficient to predict near-wall CO within certain distances and times of quenching for the head-on quenching configuration, and the influence of dilution, pressure and wall temperature on this approach should be tested. It is confirmed that the reaction term decreases within the quenching distance  $\delta_Q$ , especially closer to the wall or during the reaction zone's retreat after quenching as shown in Figure 4.11. To

evaluate the relative importance of the diffusion to the other two terms, the spatial mean of the absolute of the terms are calculated as:

$$\frac{1}{n} \sum_{i=1}^n |G|_i \quad (4.4.3)$$

where  $G$  represents any one of the  $C - D - R$  transport terms.  $n$  is the total number of grid points in a sample region;  $i$  denotes the  $i^{th}$  grid point from the wall. The sample regions used in this analysis are  $0.5 \delta_Q$ ,  $0.75 \delta_Q$  and  $1 \delta_Q$ .

Figure 4.14 shows the average CO mass fraction from Equation 4.4.1, and average CO calculated from the integral of  $D$  at  $\zeta = 0.0$  and  $0.4$ . This is calculated as:

$$\tilde{Y}_{CO,D} = \frac{\int_0^{\delta_Q} D dt dx}{\int_0^{\delta_Q} \rho dx} \quad (4.4.4)$$

$\tilde{Y}_{CO,D}$  enables the evaluation of to what extent  $Y_{CO}$  can be determined from the diffusion term alone. These are compared to profiles of the mean absolute diffusion,  $|D|_{mean}$ , and the mean of the absolute convection and reaction terms,  $|C + R|_{mean}$ . The modelled  $\tilde{Y}_{CO,D}$  for the  $\zeta = 0$  case is only qualitatively captured when the integral is started from  $t = -2$  ms, whereas the modelled  $\tilde{Y}_{CO,D}$  for the  $\zeta = 0.4$  case matches  $\tilde{Y}_{CO}$  with less than 5 % error. The ratio of peak  $|C + R|_{mean}$  to  $|D|_{mean}$  is tested to determine whether the relative contributions of the transport terms can provide an indicator for the success of this approach. For  $\zeta = 0$  and  $0.4$  these ratios are 0.57 and 0.43, respectively.

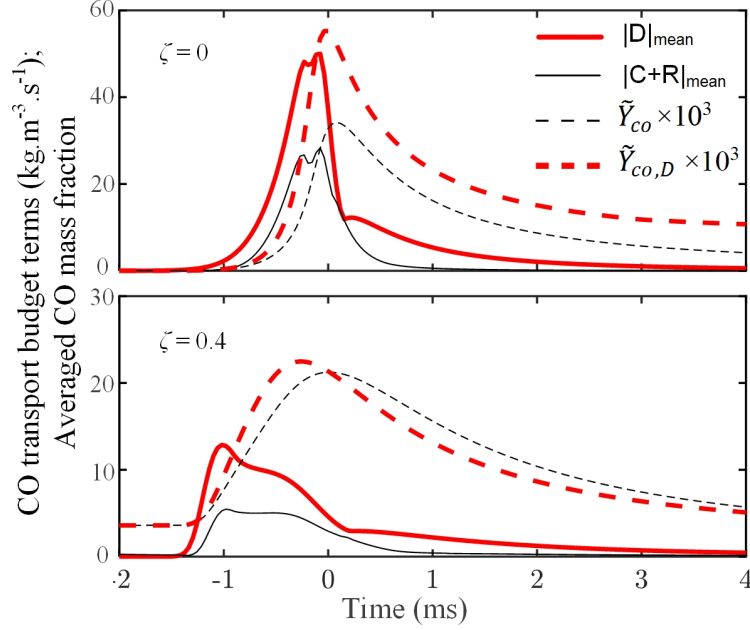


Figure 4.14: Solid lines: Mean absolute of  $D$  (thick red) and  $(C + R)$  (thin black) for CO. Dashed lines: Average CO mass fraction from DNS data (thin black) and from the integral of the CO diffusion species transport term (thick red) for  $\zeta = 0$  (top) and  $\zeta = 0.4$  (bottom).  $p = 1$  atm,  $T_{wall} = 300$  K.

For  $\tilde{Y}_{CO,D}$  to effectively model near-wall  $\tilde{Y}_{CO}$ , the diffusion term must be dominant in a certain spatial region. The previous analysis suggests a value of 0.5 or less for the ratio of peak  $|C + R|_{mean}$  to  $|D|_{mean}$  could be an indicator of such conditions. Table 4.4 presents this ratio evaluated for all cases for  $0.5 \delta_Q$ ,  $0.75 \delta_Q$  and  $1 \delta_Q$ . For cases where autoignition occurs, this ratio is only evaluated from after the autoignition event. The cases that meet the criterion are marked in bold face in the table. Generally, the ratio decreases for narrower spatial regions. The diluted cases that are not auto-igniting meet the 0.5 criterion over wider spatial regions than the undiluted cases. Higher pressure reduces the spatial regions where the ratio is less than 0.5. To further illustrate the effects of dilution level and pressure on the modelling with only considering the diffusion term, a spatial contour of the local  $|C + R|/|D|$  was shown in Figure 4.15 at different dilution levels and pressures. This ratio is different from the ratio of the peak  $|C + R|_{mean}$  to the peak  $|D|_{mean}$  in Table 4.4, because these two peaks in the latter ratio are spatially averaged qualities within quenching distance in the whole time period. Figure 4.15 shows that the general trend of the spatial region with  $|C + R|/|D| < 0.5$  increases with the increase of the

dilution levels but decreases with increasing pressure.

This approximation was evaluated by comparing the average near-wall CO at the peak and endpoint (at the last instant) as shown in Figure 4.16. In the peak CO plot, higher dilution levels or wall temperature show a better performance, while a higher pressure enlarges the difference between the DNS data and modelled near-wall CO, except for the  $\zeta = 0.6$  at  $T_{wall} = 600$  K case. This overall trend follows the ratio criterion in Table 4.4. Cases where the peak CO is modelled to within  $\pm 20\%$  are marked in Table 4.4 with an asterisk (\*). False-positive identification occurs for  $\zeta = 0$ ,  $T_{wall} = 300$  K at 1 atm and 15 atm close to the wall. False-negative identification occurs for  $\zeta = 0.4$ , 15 atm. Overall, 14 of the 20 cases identified by the ratio have good modelling of the peak CO, and only 4 have well modelled peak CO and are not identified by the ratio.

Table 4.4: Ratio of peak  $|C + R|_{mean}$  to  $|D|_{mean}$  at different  $\zeta$ ,  $p$  (atm),  $T_{wall}$  (K) within different distances from the wall. Bold indicates ratio  $\leq 0.5$ . \* indicates well-modelled peak CO. ° indicates well-modelled endpoint CO.

| $\zeta/p/T_{wall}$ | $1.0\delta_Q$ | $0.75\delta_Q$ | $0.5\delta_Q$ |
|--------------------|---------------|----------------|---------------|
| 0.0/1/300          | 0.57          | <b>0.50</b>    | <b>0.40</b>   |
| 0.4/1/300          | <b>0.43*</b>  | <b>0.42*</b>   | <b>0.35*</b>  |
| 0.6/1/300          | <b>0.38*</b>  | <b>0.24*°</b>  | <b>0.24*°</b> |
| 0.0/1/600          | <b>0.42*</b>  | <b>0.32*</b>   | <b>0.28*</b>  |
| 0.4/1/600          | <b>0.30*</b>  | <b>0.23*</b>   | <b>0.18*</b>  |
| 0.6/1/600          | <b>0.26</b>   | <b>0.18</b>    | <b>0.14</b>   |
| 0.0/15/300         | 0.82          | 0.61           | <b>0.48</b>   |
| 0.4/15/300         | 0.83*         | 0.57*°         | 0.56*         |
| 0.6/15/300         | 0.64*         | <b>0.29*°</b>  | <b>0.30*°</b> |

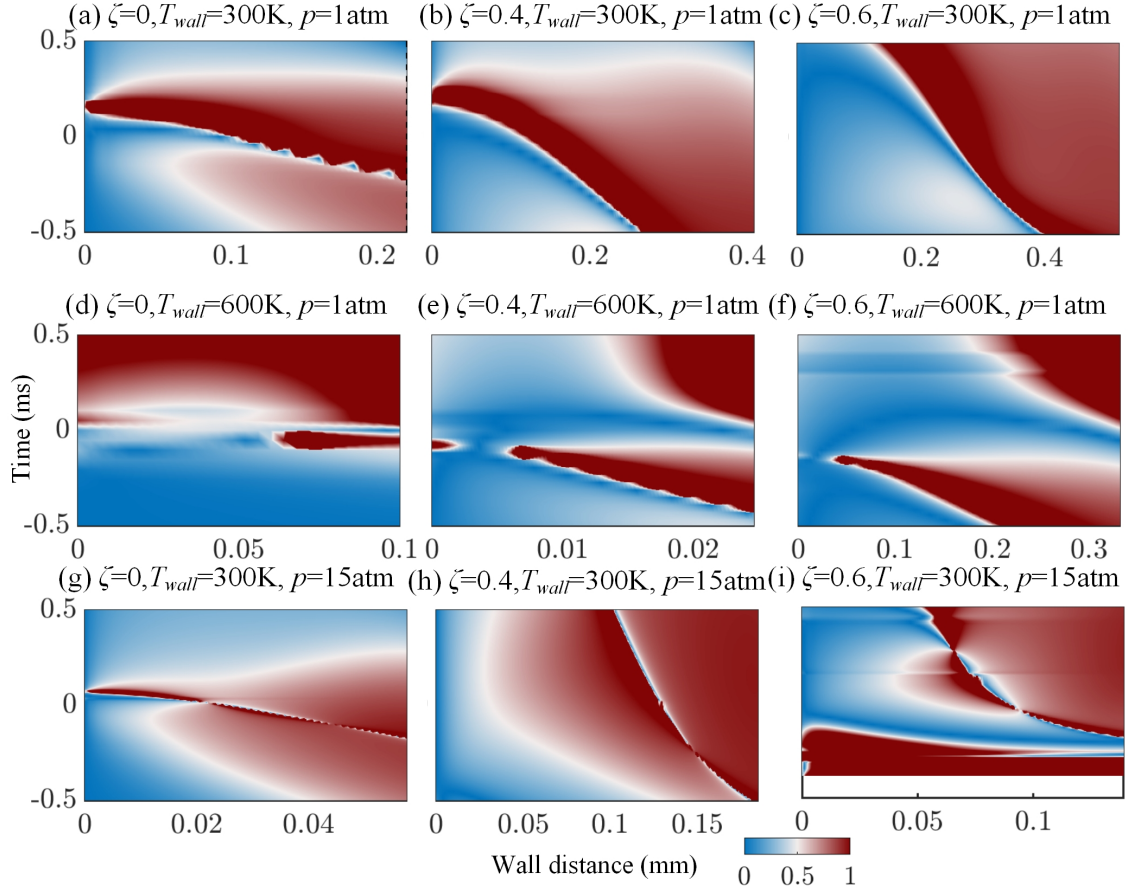


Figure 4.15:  $x - t$  contour plots of  $|C + R|/|D|$  at  $\zeta = 0, 0.4$  and  $0.6$  at  $T_{wall} = 300$  K,  $p = 1$  atm (a – c) at  $T_{wall} = 600$  K,  $p = 1$  atm (d – f) and at  $T_{wall} = 300$  K,  $p = 15$  atm (g – i) within one quenching distance.

Cases where the endpoint CO is modelled to within  $\pm 20\%$  are marked in Table 4.4 with a circle ( $\circ$ ). Most of the  $T_{wall} = 600$  K cases deviate from the DNS data, generally over-estimating the endpoint CO. One of the potential reasons is that the ratio is based on the peak  $|C + R|_{mean}$  and  $|D|_{mean}$ , which may not predict the CO oxidation well, especially in the presence of a non-negligible reaction term at higher wall temperatures. As the endpoint CO concentrations are also typically low, any propagated discrepancy from the peak CO will fall outside the  $\pm 20\%$  cutoff, even if the post-flame CO oxidation rate is well-captured by this integration. An example of this occurring can be observed in Figure 4.14 for the  $\zeta = 0.0$  case.

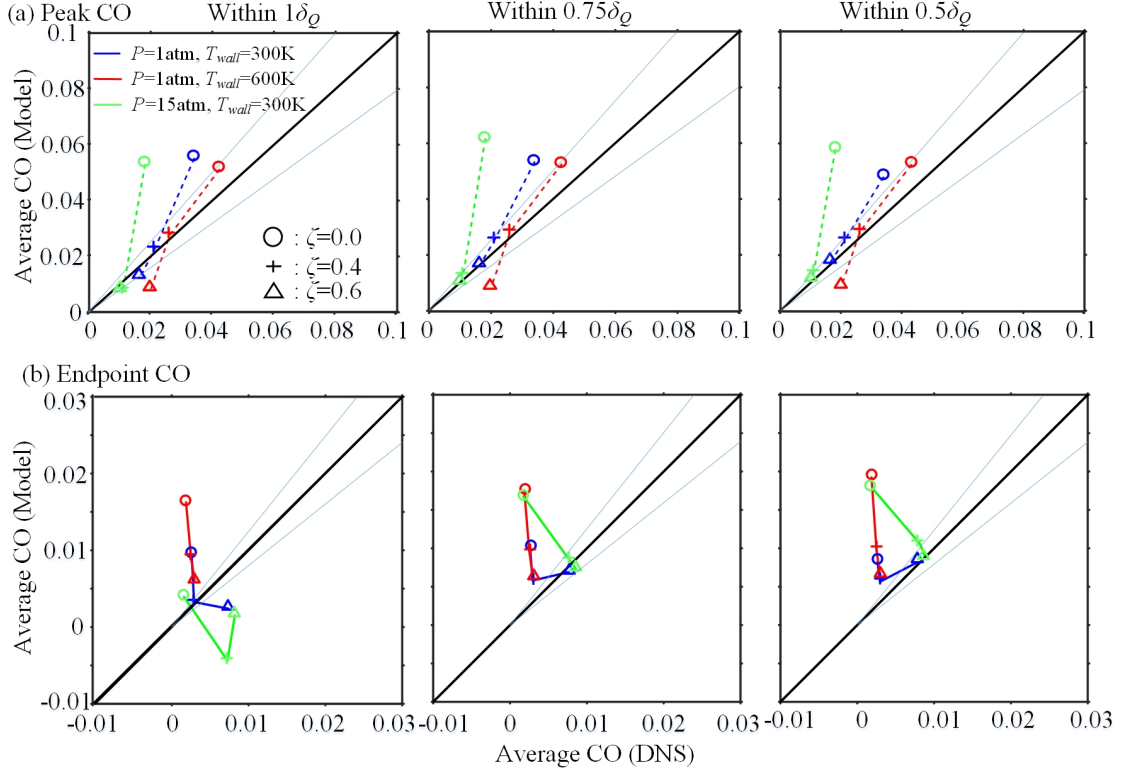


Figure 4.16: Peak CO (top row) and endpoint CO (bottom row) for the modelled CO based on integrated  $D$  versus  $\tilde{Y}_{CO}$  from the DNS. Light blue lines mark the  $\pm 20\%$  cutoff.

While the 0.5 ratio criterion may not a perfect marker for near-wall CO approximation with integrated  $D$ , it highlights the role of diffusion in near-wall CO estimation, and that increased dilution and wall temperatures magnify this role. This also highlights the need to fully resolve the influences on the formation and reduction of CO before a comprehensive model can be proposed. These simulations are laminar, 1D flames. It is acknowledged that multi-dimensional effects, turbulence and other quenching modes (e.g. SWQ) may have different behaviours.

## 4.5 Conclusions

1D fully resolved simulations with detailed chemistry and transport properties were used to simulate a constant pressure, laminar head-on quenching configuration with  $\text{CH}_4/\text{air}$  mixture diluted by hot combustion products. The effects of dilution levels, wall temperature and pressure on near-wall CO and species transport budgets were



studied.

The results show that increasing dilution level and pressure can create an autoignition between the propagating flame and the wall. Further:

1. At higher dilution levels and for higher pressure, the peak of averaged near-wall CO decreases, and the rate of near-wall CO reduction also decreases. However, increasing wall temperature increases the peak average near-wall CO and the near-wall CO reduction rate.
2. Initial flame-wall distance affects the thermal boundary layer evolution prior to the FWI, while the CO reduction rate has the same trend with the above conclusion.
3. Near-wall OH distribution follows the thermal boundary layer evolution. Near-wall NO increases with increasing dilution level.
4. Stratification of the dilution level near the wall can present a strong flame deceleration when the fresh gases are near the wall, however the near-wall CO behaviour is very similar to that of the  $\zeta = 0$  case. When initialising hot products next to the wall, the main reaction zone moves away from the wall and no FWI occurs. In light of this, it appears preferable to design for the diluent gases to shield the reaction zone from the wall.
5. The near-wall CO may be modelled using only the integrated species transport diffusion term within certain spatial regions where the diffusion is dominant. Dilution increases the spatial region where diffusion is dominant for atmospheric conditions, whereas increasing pressure reduces this region.

# Chapter 5

## 2D Laminar Diluted FWI

### 5.1 Introduction

The results of 2D simulations of laminar flames interacting with a wall are presented in this chapter. Both steady flames and unsteady flames are considered. Unsteadiness is simulated using acoustic forcing at the inflow for a range of frequencies. Both flame dynamics and CO mass fraction distribution are examined. The impact of different wall temperatures, dilution levels and forcing frequencies are investigated. Finally, the transport species budget for CO and OH are used to explain the transport mechanisms for these two species throughout the domain. The species transport budgets of OH are also used to investigate the effects of the thermal boundary layer on combustion mode.

### 5.2 Simulation Parameters

The details of the computational setup was discussed in Chapter 3. The cases considered are presented in Table 3.5. One of the important parameters which is needed for further discussion is the temperature at the flammability limit of the cases considered. It is defined as the adiabatic, unstrained flame speed at  $0.1 \text{ m.s}^{-1}$  [101]. Figure 5.1 shows the variation of this temperature as a function of dilution level. This increase has a similar gradient to that of the reactants temperature. Table 5.1 reports the values for the dilution levels studied in this chapter. For  $\zeta = 0.5$ , the

cases with  $T_{wall} = 600$  K still feature flammable mixture at the wall while for cases with  $\zeta = 0.6$  and  $0.7$ , the mixture at the wall is not flammable.

Another set of parameters reported in Table 5.1 includes the flame speed and the ignition delay at different  $\zeta$ . For  $\zeta = 0.5$ , both propagating flame and autoignition solutions could be found. However, due to the high reactivity of the mixtures with  $\zeta = 0.6$  and  $0.7$ , only autoignition solutions could be found for these cases.

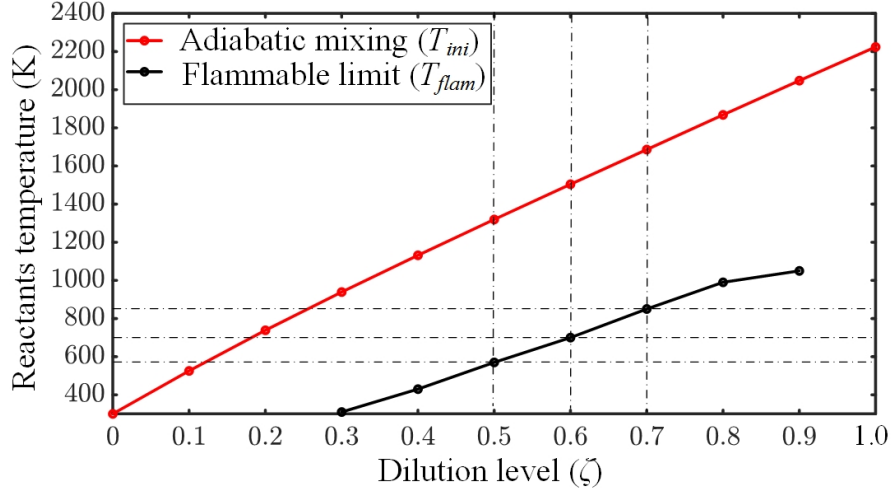


Figure 5.1: Diluted reactant temperature with adiabatic mixing between the fresh reactants and hot products and the flammability-limited temperature at different dilution level,  $\zeta$ .

Table 5.1: Initial conditions and properties of reactants for each case.  $\tau_{AI}$  denotes the ignition delay at  $T_{ini}$ .  $T_{flam}$  denotes the flammability-limited temperature (K)

| $\zeta$ | $T_{ini}$ (K) | $Y_{CH_4}$ | $Y_{O_2}$ | $Y_{H_2O}$ | $Y_{CO_2}$ | $Y_{CO}$ | $s_L$ (m.s <sup>-1</sup> ) | $\tau_{AI}$ (ms) | $T_{flam}$ (K) |
|---------|---------------|------------|-----------|------------|------------|----------|----------------------------|------------------|----------------|
| 0.5     | 1319          | 0.028      | 0.115     | 0.060      | 0.067      | 0.004    | 1.80                       | 6.8              | 570            |
| 0.6     | 1504          | 0.023      | 0.093     | 0.072      | 0.080      | 0.005    | —                          | 0.69             | 700            |
| 0.7     | 1686          | 0.017      | 0.072     | 0.084      | 0.094      | 0.006    | —                          | 0.15             | 850            |

## 5.3 Results and Discussion

### 5.3.1 Steady Flames

In this section, the temperature and CO mass fraction fields are examined by considering two groups of cases: those with different dilution levels at a given temperature and another group with different wall temperatures at a given dilution level. The case with  $\zeta = 0.6$  and  $T_{wall} = 600$  K was chosen as the baseline case.

Figure 5.2 shows the temperature and CO mass fraction contours of the unforced cases at  $T_{wall} = 600$  K and varying  $\zeta$  from 0.5 to 0.7. The dashed line is the iso-line at  $0.99\times$  the diluted reactant temperature at the inlet ( $y = 3$  mm) (i.e. 1319 K, 1504 K and 1686 K at  $\zeta = 0.5, 0.6$  and  $0.7$ , respectively). The dashed line upstream of the flame presents the edge of the thermal boundary layer. The solid line is the flame front. The flame length decreases with increasing  $\zeta$ , which is likely induced by the increase of the flame speed or decrease of the autoignition delay time at a higher  $\zeta$  as shown in Table 5.1. At  $\zeta = 0.5$  and  $0.6$ , the flame expansion compresses the thermal boundary layer edge within  $y = [3\ 5]$  mm. At  $\zeta = 0.7$ , the flame front enters the thermal boundary layer. A possible reason for this is that, as  $\zeta$  increases, the flame power is reduced and the wall heat flux plays a stronger role due to a higher temperature difference between the wall and reactants. It is therefore expected that the flame has a weaker impact on the thermal boundary layer in particular in the near-wall region.

The peak CO mass fraction inside the thermal boundary layer decreases with increasing  $\zeta$ , and is consistent with 1D HOQ as shown in Figure 4.7. The flame length has an important effect here. The shorter flame in the case with higher  $\zeta$  allows for more residence time to be available for oxidation. The lower near wall CO and a shorter flame for  $\zeta = 0.7$  minimises the impact of this region on the exhaust CO.

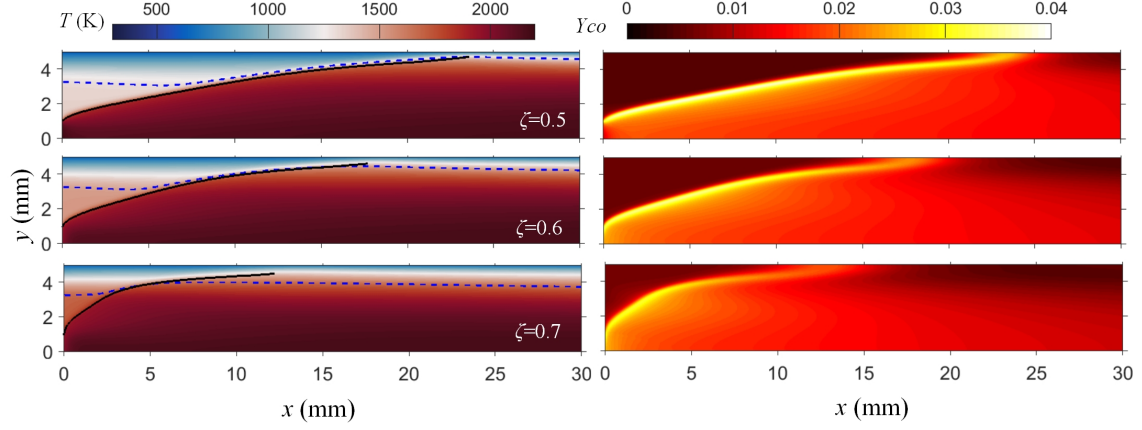


Figure 5.2: Temperature (left column) and CO mass fraction (right column) contours of unforced cases at  $\zeta = 0.5, 0.6, 0.7$  at  $T_{wall} = 600$  K. Solid line marks the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$  at the inlet ( $y = 3$  mm).

The wall temperature effects are now investigated using the  $\zeta = 0.6$  case as the baseline case (see Figure 5.3). The wall temperature is varied from 300 K to inlet reactants temperature under the adiabatic mixing. As the wall temperature increases, the near-wall mixture transitions from an inflammable mixture to a flammable mixture. The next transition is from a mixture that can support a premixed flame to a mixture under auto-ignition conditions. The ignition delay time of this mixture will be further reduced as the wall temperature approaches that of the reactants. The decrease of the flame length by increasing the wall temperature is therefore expected. At  $T_{wall} = 300$  K, the flame tip becomes parallel to the wall and follows the edge of the thermal boundary layer. This behavior can also be related to the flammability limit for this case. At  $T_{wall} = T_{reactants}$ , there is no inlet thermal boundary layer, and the flame tip is curved towards the inlet due to the autoignition.

With increasing  $T_{wall}$ , the peak near-wall CO increases monotonically. However, there is a competing effect which is related to the variation of the flame length as a result of changing the wall temperature. The longer flame for  $T_{wall} = 300$  K seems to have a strong dominating impact on the contribution of the near-wall CO on the exhaust CO emissions.

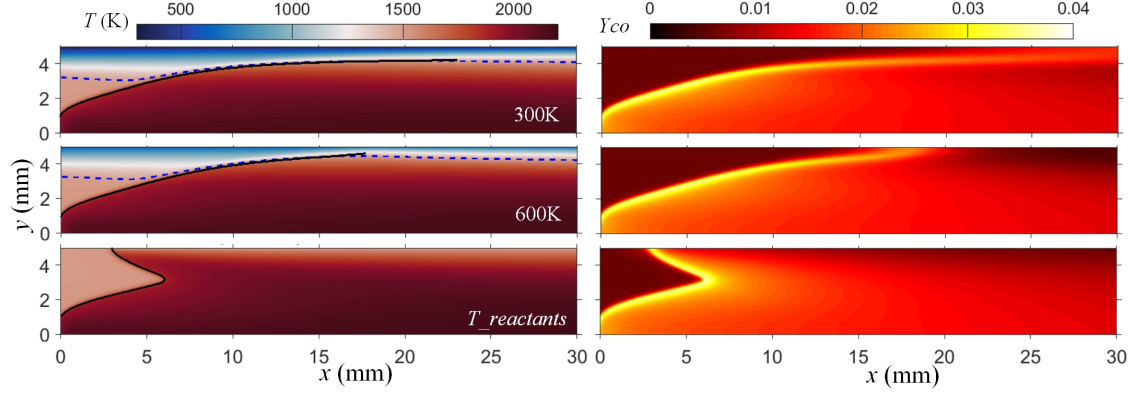


Figure 5.3: Temperature (left column) and CO mass fraction (right column) contours of unforced cases at  $\zeta = 0.6$  and  $T_{wall} = 300$  K, 600 K and  $T_{reactant}$ , 1504 K. Solid line marks the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$  at the inlet ( $y = 3$  mm).

### 5.3.2 Unsteady Flames

The effect of forcing frequency on the flame dynamics and CO distribution is now examined for the baseline case ( $\zeta = 0.6$ ,  $T_{wall} = 600$  K). Here, a Damköhler number is also defined as [102],

$$Da_f = \frac{1}{\tau_{F,0} f} \quad (5.3.1)$$

where  $\tau_{F,0}$  is the flame time as shown in Equation 2.2.3 and  $f$  is the forcing frequency.

Given that the unburned gas temperature varies from the reactant temperature to the wall temperature,  $\tau_{F,0}$  can be obtained using different temperatures. Two limiting cases are therefore considered here. When the temperature is the same with the adiabatic reactants temperature (1504 K), the autoignition delay time for this case can be used to calculate  $Da_f$ , which is equal to 0.6, 1.2 and 4.8 for  $St = 2$ , 1 and 0.25, respectively. When the mixture is at the flammability limit, the temperature is 700 K (see Table 5.1). Under this condition, the flame time defined in Equation (2.2.3) can be obtained using the FPF solution. Decreasing forcing frequency increases  $Da_f$  as shown in Equation (5.3.1). The values of  $Da_f$  are therefore 0.022, 0.045 and 0.18 for  $St = 2$ , 1 and 0.25, respectively, and summarized

in Table 5.2. These values will be used in the later discussion to explain the observed flame dynamics for different forcing frequencies. Decreasing the forcing frequency decreases the convective wave number, as such the flame front is expected to be less wrinkled outside the thermal BL. Inside the thermal BL, the flame time increases beyond the forcing timescale. As a result, the forcing response present by the flame wrinkling is weakened.

Table 5.2: Damköhler number ( $Da_f$ ) at different forcing frequencies.

| Temperature (K) | $St = 2$ | $St = 1$ | $St = 0.25$ |
|-----------------|----------|----------|-------------|
| 1504            | 0.6      | 1.2      | 4.8         |
| 700             | 0.022    | 0.045    | 0.18        |

Figure 5.4 shows five snapshots of temperature and CO mass fraction contours of the baseline case at  $St = 2$ . Although a strongly wrinkled flame is observed close to the inlet, the flame is almost parallel to the wall close to the tip. Also, the tip streamwise location is almost constant during forcing. As a result of this, there is an insignificant variation of the CO distribution in the near-wall region and close to the outlet. Now considering the values of  $Da_f$  for this case, one can note that  $Da_f \ll 1$  in the near-wall region. Therefore, the reduced amount of wrinkling is expected close to the tip.

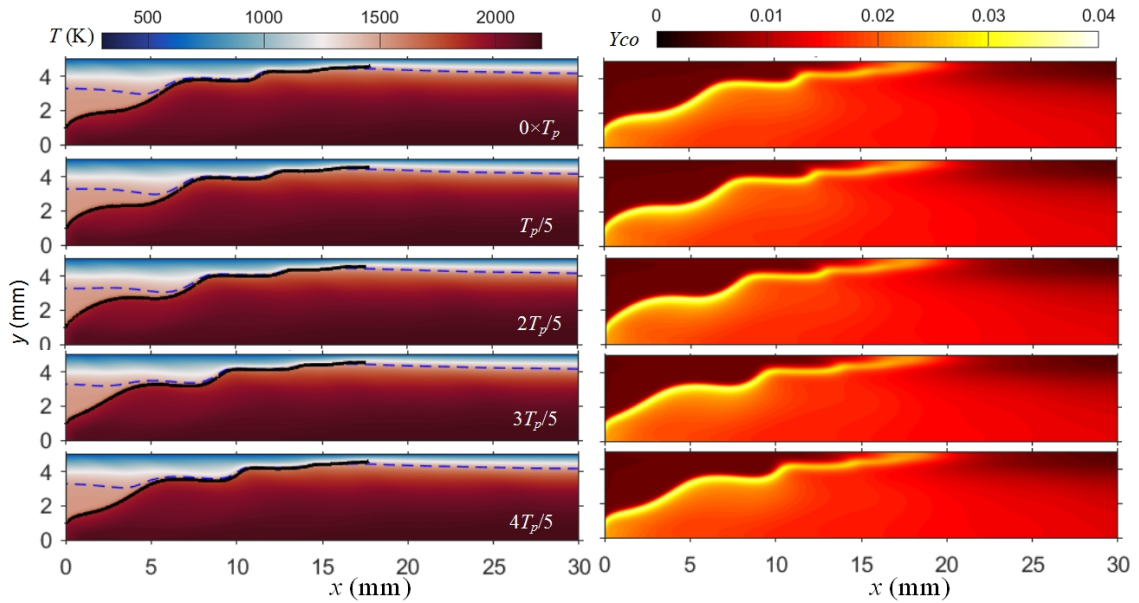


Figure 5.4: Temperature (left column) and CO mass fraction (right column) contours of forced cases at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 2$ . Solid line marks the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$  at the inlet ( $y = 3$  mm).

With reducing the forcing frequency from  $St = 2$  to 1, the flame tip location is still constant, as shown in Figure 5.5. Although the value of  $Da_f$  in the near wall region (0.045) has increased but it is still much less than 1. As a result, the near-wall CO is almost identical across all instants.

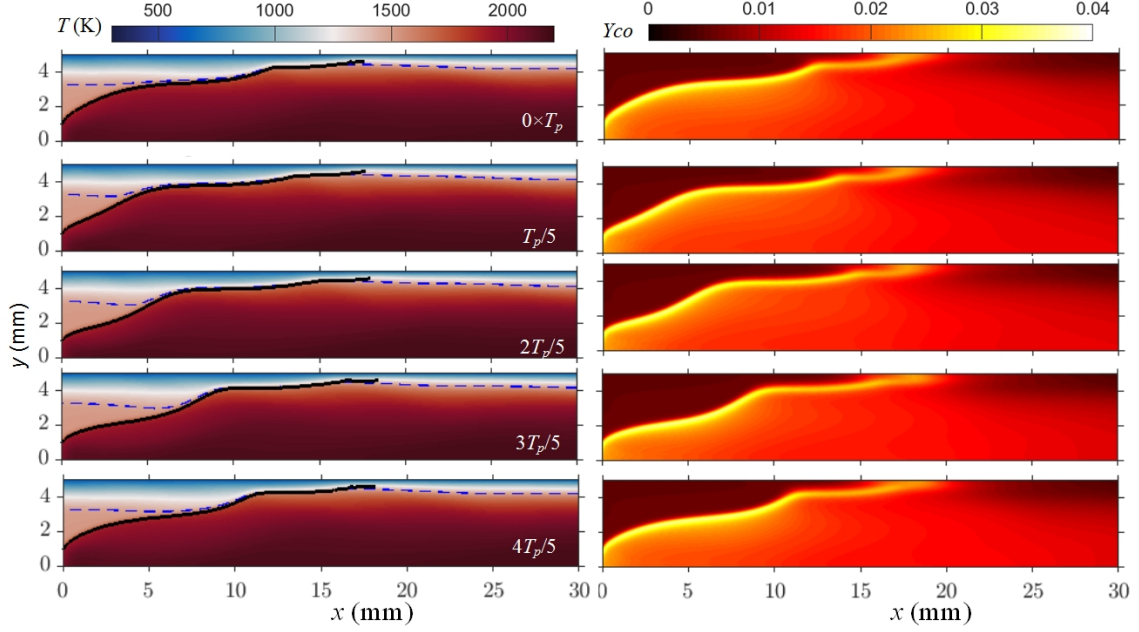


Figure 5.5: Temperature (left column) and CO mass fraction (right column) of forced cases at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 1$ . Solid line is the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$ .

For  $St = 0.25$ , the flame tip location has a considerable variation during the forcing period. The lower limit of  $Da_f$  is now approaching one ( $0.18 < Da_f < 4.8$ ) and overall, a stronger flame response is present. The movement of the flame tip has a significant impact on both near-wall and exhaust CO. At time  $= 0 \times T_p$ , a high CO tail exists after the flame tip near the wall. The formation of this long tail in the upstream motion of the flame can also be observed.



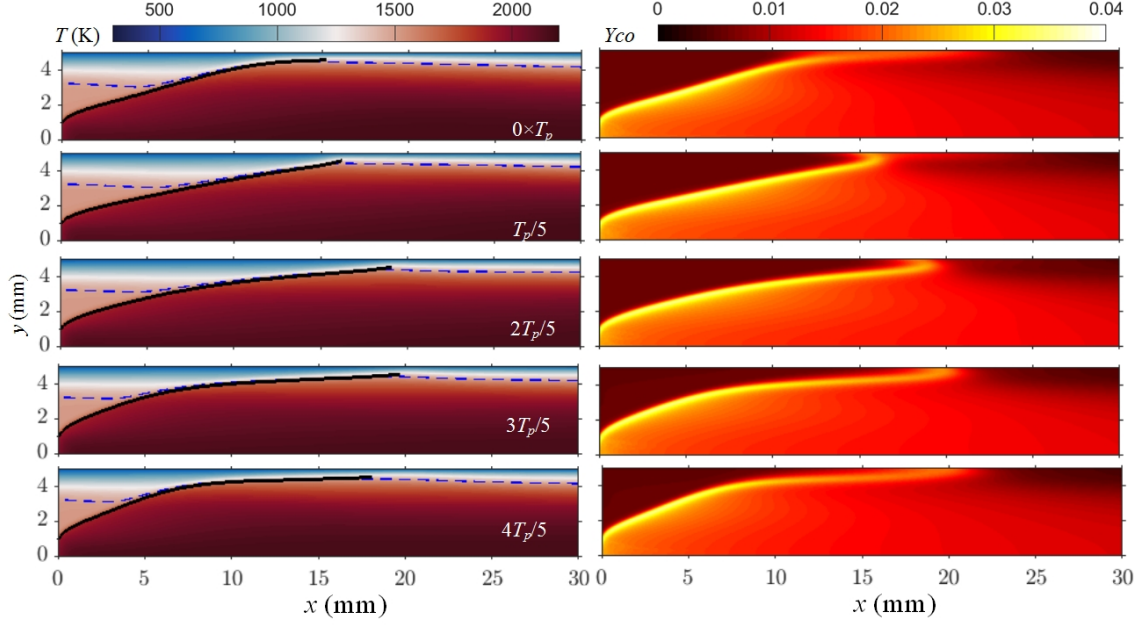


Figure 5.6: Temperature (left column) and CO mass fraction (right column) contours of forced cases at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 0.25$ . Solid line is the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$  at the inlet ( $y = 3$  mm).

Figure 5.7 shows the CO mass fraction at the wall in one cycle at different forcing frequencies. Consistent with the earlier observations, the lowest forcing frequency shows the largest variation of CO mass fraction at the wall, correlated with the large movement of the flame.

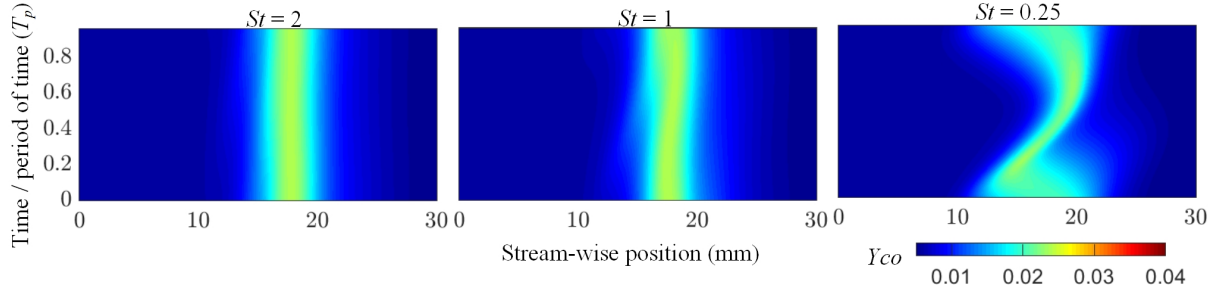


Figure 5.7: CO mass fraction at the wall over one cycle at  $St = 2, 1, 0.25$  at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K.

To examine the forcing amplitude effects, a case at  $St = 2$  was simulated with 4 times larger amplitude (100 % of the maximum inlet velocity) than the case shown in Figure 5.4. Figure 5.8 shows that the flame front was wrinkled more significantly than the case with a lower amplitude. As a result, the CO away from the wall varies more strongly. However, the CO close to the wall (within 1 mm wall distance) is

still not significantly affected. Thus, this following analysis does not include this case. This stronger forcing is also more likely to induce combustion mode switching near the thermal BL edge.

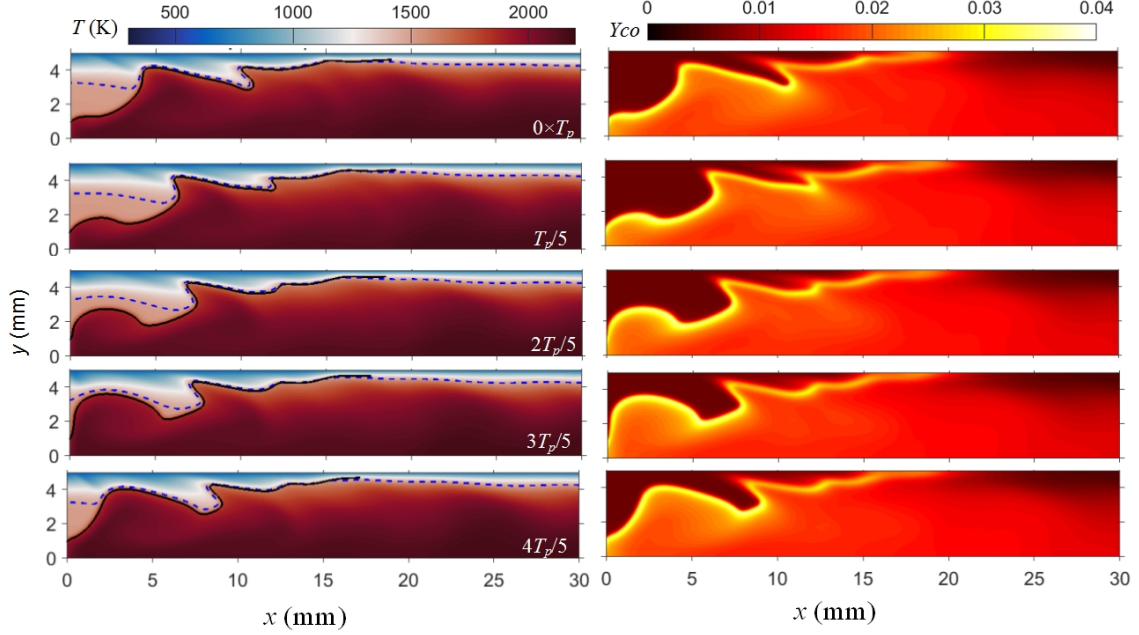


Figure 5.8: Temperature (left column) and CO mass fraction (right column) contours of forced cases at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 2$ , amplitude = 100 % of the maximum inlet velocity. Solid line marks the flame front; dashed line is the iso-line at  $0.99 \times T_{reactants}$  at the inlet ( $y = 3$  mm).

### 5.3.3 Exhaust CO Emissions

To evaluate the global CO behaviour at different dilution levels, wall temperatures and forcing frequencies, the Favre-averaged CO mass fraction and mass flux at the exit are calculated as shown in Equations 5.3.2 and 5.3.3.

$$\tilde{Y}_{CO,exh} = \frac{\sum_1^{N_y} \rho u Y_{CO} \Delta y}{\sum_1^{N_y} \rho u \Delta y} \quad (5.3.2)$$

$$\tilde{m}_{CO,exh} = \sum_1^{N_y} \rho u Y_{CO} \Delta y \quad (5.3.3)$$

Figure 5.9 shows the average CO mass fraction and mass flux for steady flames at the domain exit. The wall temperature has a strong impact on both the average

CO mass fraction and mass flux. The initial decrease of  $\tilde{Y}_{CO,exh}$  can be linked to the effects of flame length, a shorter flame provides more residence time for oxidation. However, once the temperature is above a threshold, an increase of  $\tilde{Y}_{CO,exh}$  or small changes of  $\tilde{m}_{CO,exh}$  are observed as the wall temperature increases. This might be due to the effect of temperature on equilibrium CO competing with the effect on residence time, a higher temperature for a given  $\zeta$  has a higher equilibrium CO. Now turning to the  $\zeta$  effects, one can note that a higher  $\zeta$  generally produces lower CO. This correlates with the variation of the flame length as  $\zeta$  changes for a given wall temperature.

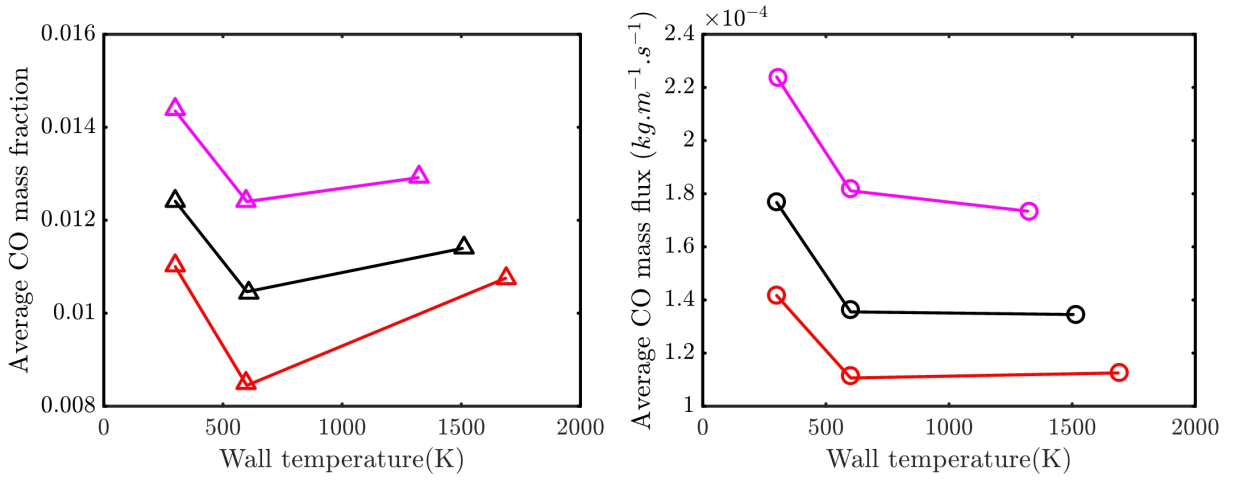


Figure 5.9: Unforced average CO mass fraction (left column) and CO mass flux (right column) at the whole exit.

Figure 5.10 shows the contribution of the near-wall CO ( $y = [3 \ 5]$  mm) at the exhaust to the total exhaust CO. The lowest wall temperature shows the highest contribution. This is expected as the tip of the flame is closer to the domain exit for this case.

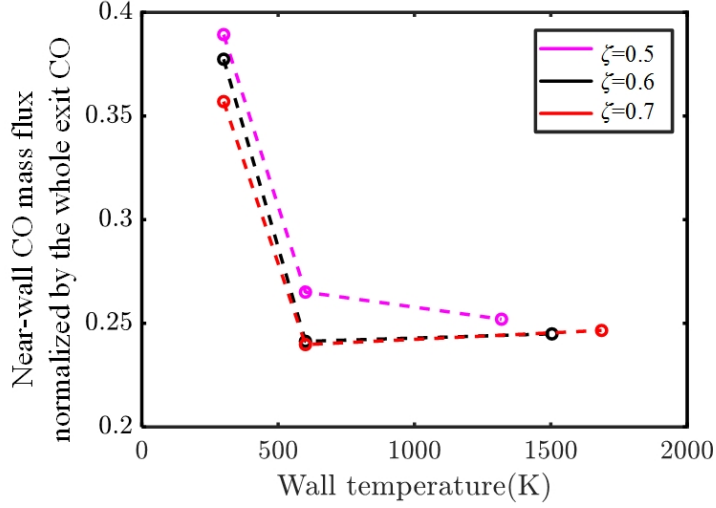


Figure 5.10: Unforced near-wall average CO mass flux within  $y = [3 \ 5]$  mm at the exit normalized by the whole exit CO.

Figure 5.11 shows the average CO mass fraction and mass flux in the forced cases. The  $\tilde{Y}_{CO,exh}$  at  $St = 0.25$  shows the largest fluctuation, consistent with the fact that the flame movement is the largest for this case. For  $St = 1$  and 2, almost identical variations for  $\tilde{Y}_{CO,exh}$  are observed. The fluctuation of  $\tilde{m}_{CO,exh}$  is similar for three  $St$  numbers. At  $St = 1$  and 2, the velocity fluctuations at the inlet are in-phase with those of the exhaust CO mass flux. However, for  $St = 0.25$ , the peak of  $\tilde{m}_{CO,exh}$  fluctuations is slightly delayed compared with that of the inlet velocity fluctuations, as the flame experiences the largest movement and therefore the residence time in the post-flame region becomes more important.

Figure 5.12 shows the temporal contribution of  $\tilde{m}_{CO,exh}$  in the near-wall region to the total CO at the entire exit. Again, the case with  $St = 0.25$  shows the biggest fluctuation. The time-averaged exhaust CO mass flux  $\tilde{m}_{CO,exh}$  over one cycle was calculated as shown in Table 5.3. The difference of mean  $\tilde{m}_{CO,exh}$  for three forced cases is less than 2%. The maximum CO mass flux is at  $St = 2$ . The mean  $\tilde{m}_{CO,exh}$  at  $St = 2$  at the entire exit and near the wall are about 2% higher than the unforced case.

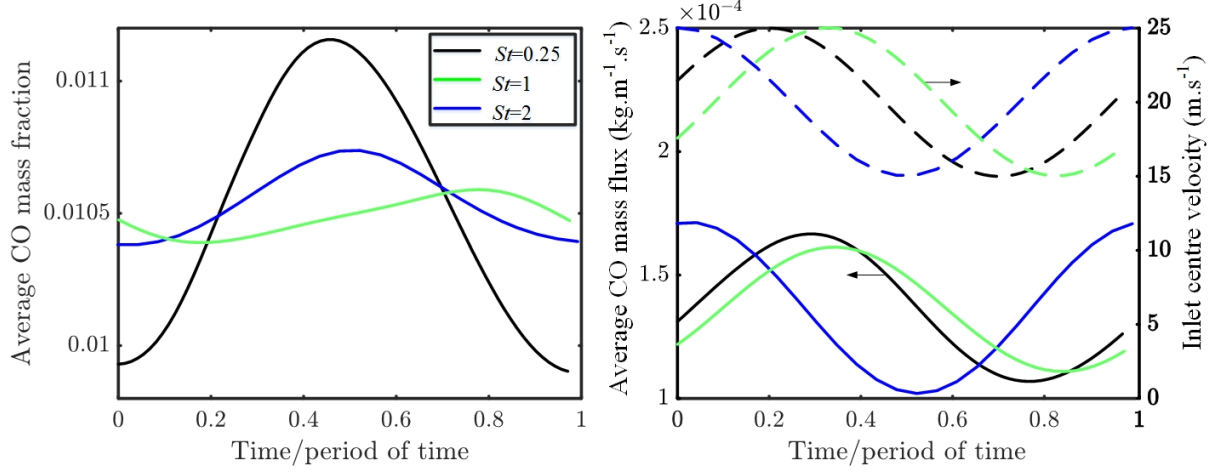


Figure 5.11: Average CO mass fraction (left column) and CO mass flux (right column) at the exit at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 0.25, 1$  and  $2$ . Solid lines are the averaged CO mass fraction (left) and mass flux (right), and dashed lines are the inlet velocity at the center.

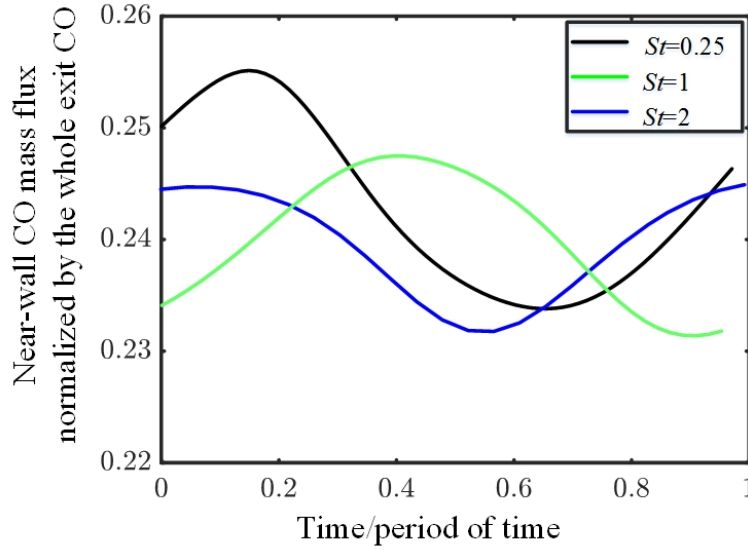


Figure 5.12: Near-wall average CO mass flux normalized by the whole exit CO at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K,  $St = 0.25, 1$  and  $2$ . Solid lines are the normalized averaged CO mass flux, and dashed lines are the inlet velocity at the center.

Table 5.3: Average  $\tilde{m}_{CO,exh}$  and its contribution to the whole exit for the forced cases over one cycle and the steady case at  $\zeta = 0.6$ ,  $T_{wall} = 600$  K.

| $St$ | $\tilde{m}_{CO,exh}$<br>( $\text{kg.m}^{-1}.\text{s}^{-1}$ ) | $\tilde{m}_{CO,exh,wall}$<br>( $\text{kg.m}^{-1}.\text{s}^{-1}$ ) | $\tilde{m}_{CO,exh,wall}/\tilde{m}_{CO,exh}$ |
|------|--------------------------------------------------------------|-------------------------------------------------------------------|----------------------------------------------|
| 0    | $1.356 \times 10^{-4}$                                       | $3.259 \times 10^{-5}$                                            | 0.240                                        |
| 0.25 | $1.358 \times 10^{-4}$                                       | $3.318 \times 10^{-5}$                                            | 0.244                                        |
| 1    | $1.365 \times 10^{-4}$                                       | $3.304 \times 10^{-5}$                                            | 0.242                                        |
| 2    | $1.384 \times 10^{-4}$                                       | $3.342 \times 10^{-5}$                                            | 0.242                                        |

### 5.3.4 Species Transport Budget for CO

To further quantify the CO behavior, the terms of the species transport budget are evaluated by using Equation 3.2.4 in Chapter 3. Figure 5.13 shows the species transport budget for CO for the near-wall region  $y = [3 \ 5]$  mm at three different wall temperatures at  $\zeta = 0.6$ . With increasing  $T_{wall}$ , all transport terms increase their peak values. The  $R$  term between the flame front and the wall at  $T_{wall} = 300$  K is positive throughout the domain, and becomes smaller downstream. This indicates the CO keeps forming near the wall, and present high CO concentration at the outlet as shown in Figure 5.3 and 5.9. With increasing wall temperature, the negative  $R$  term occupies a larger area near the wall. Unlike the  $T_{wall} = 300$  K case, the  $R$  term at  $T_{wall} = 600$  K and  $T_{reactants}$  reach zero at the outlet.

With increasing  $T_{wall}$ , the magnitude of  $D$  near the wall around the flame tip increases. The near-wall area with positive  $D$  at  $T_{wall} = 300$  K has the largest peak value among all three wall temperatures. This positive  $D$  region is the preheating zone of the flame. The peak  $C$  around the flame tip increases with increasing  $T_{wall}$ .

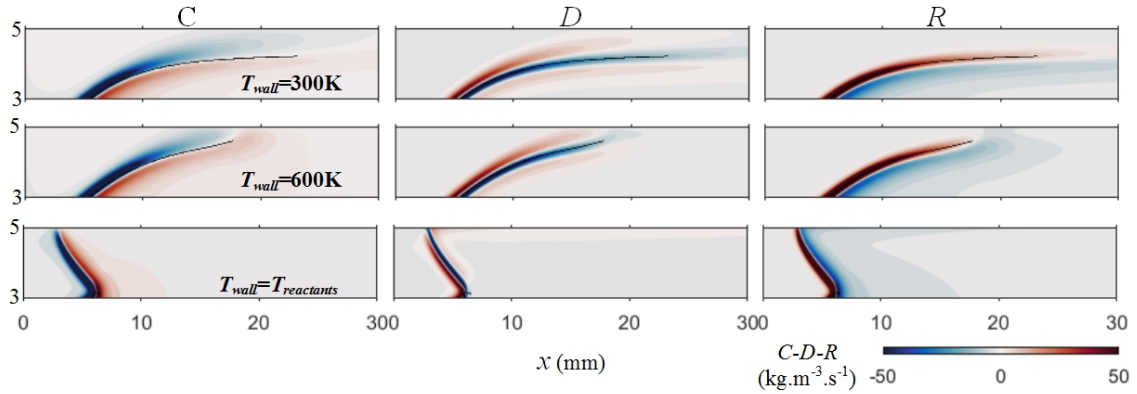


Figure 5.13: species transport budget for CO at three different wall temperatures at  $\zeta = 0.6$ ,  $St = 0.25$ . The solid black line is the marker of flame fronts. The aspect ratio is skewed with  $x : y = 3:1$  to accentuate the near-wall region.

Figure 5.14 presents the transport terms against the residence time along a streamline from  $y = 4.8$  mm at the inlet. CO transport is dominated by convection and diffusion. With increasing dilution levels, the magnitude of the transport terms and peak  $Y_{CO}$  and temperature decrease, while the total residence time and CO

oxidation time increase. The oxidation time at  $\zeta = 0.7$  is 5 times longer than  $\zeta = 0.5$  case and 1.5 times longer than  $\zeta = 0.6$  case. This oxidation time is induced by the reduction of flame length from  $\zeta = 0.5$  to 0.7. Such a flame length variation at difference dilution levels was not included in 1D HOQ in Chapter 4, as such the various CO oxidation times cannot be present in 1D HOQ configuration.

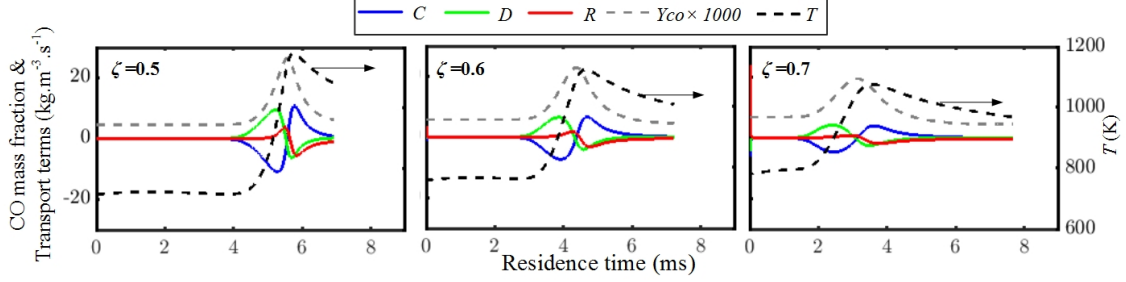


Figure 5.14:  $Y_{CO}$  and  $C-D-R$  transport budgets for CO along streamlines starting from  $y = 4.8$  mm at the inlet with varied  $\zeta$  at  $T_{wall} = 600$  K.

Figure 5.15 shows the species transport terms along a streamline from  $y = 4.8$  mm at different  $T_{wall}$ . The magnitude of the transport terms decreases with decreasing the wall temperature, resulting in a lower peak near-wall CO. With increasing  $T_{wall}$ , the total residence time and CO oxidation time increase. This is due to the more upstream flame tip (see Figure 5.3). The temperature along the streamline increases upstream, as the streamline deviates away from the wall.

The endpoint  $Y_{CO}$  decreases from 300 K ( $Y_{CO} = 17 \times 10^{-3}$ ) to 600 K ( $Y_{CO} = 4.6 \times 10^{-3}$ ) wall temperature, while increases from 600 K to  $T_{reactants}$  ( $Y_{CO} = 6.5 \times 10^{-3}$ ). The endpoint  $Y_{CO}$  at  $T_{wall} = 600$  K is slightly lower than the equilibrium CO at the inlet ( $6 \times 10^{-3}$ ).

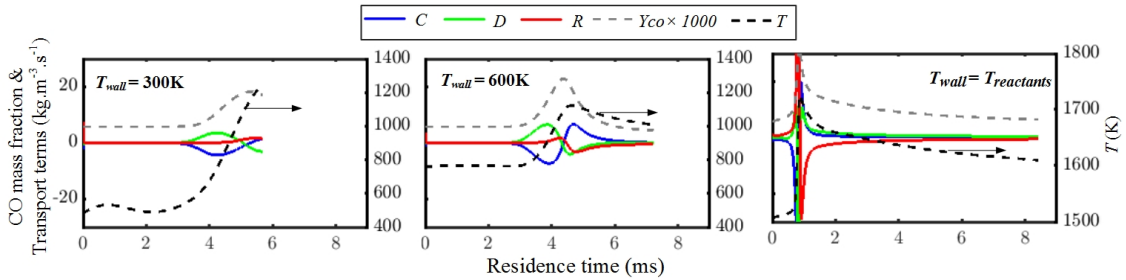


Figure 5.15:  $Y_{CO}$  and  $C-D-R$  transport budgets for CO along streamlines starting from  $y = 4.8$  mm at the inlet with varied  $T_{wall}$  at  $\zeta = 0.6$ .



### 5.3.5 Species Transport Budget for OH

As the temperature reduces in the thermal boundary layer, it may be possible to transit from autoignition stabilisation to premixed flame propagation. This can be investigated by analysing the OH species transport budget as per [60]. Transport budgets normal to the flame front are examined along two streamlines marked in red lines in the contour of Figure 5.16.

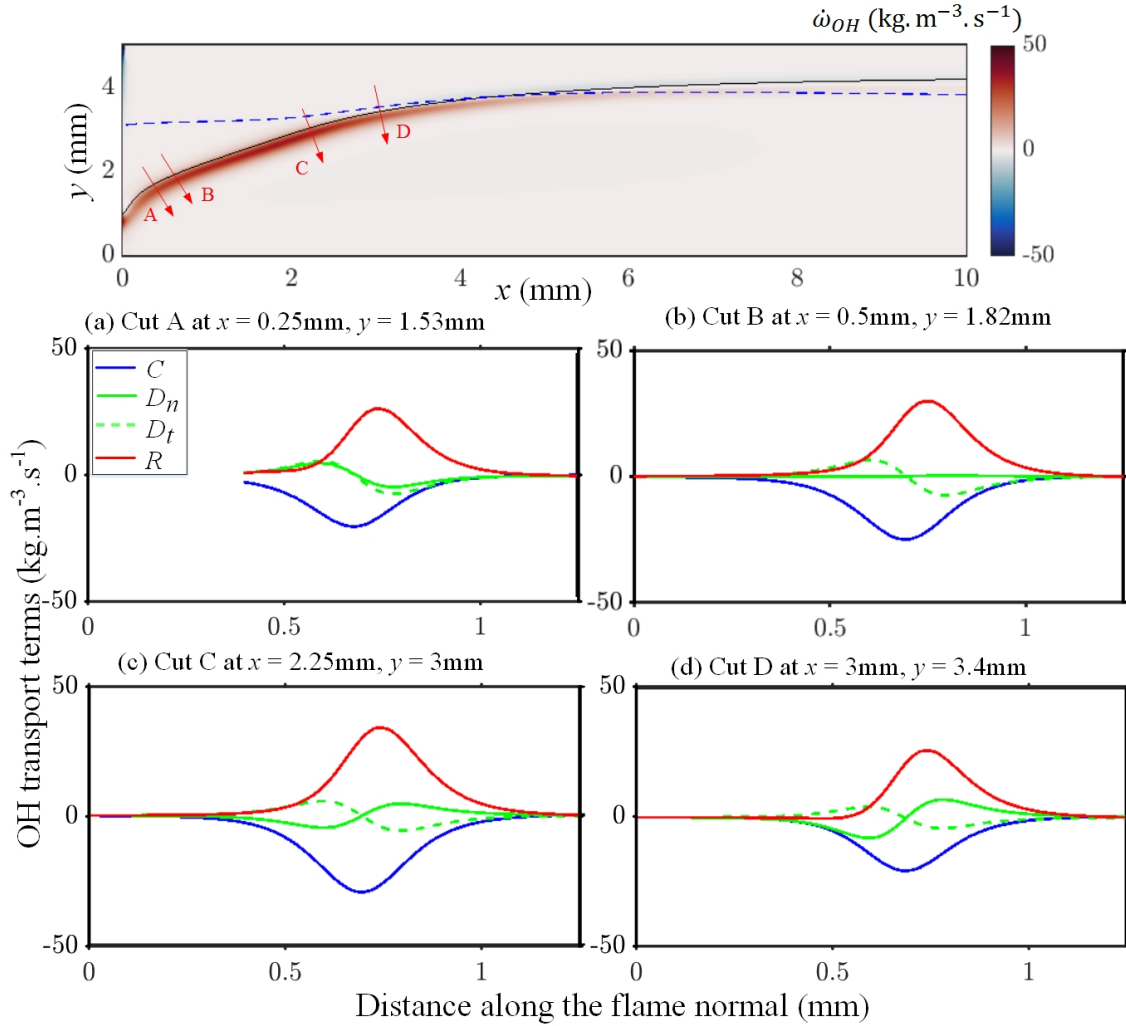


Figure 5.16: transport terms of OH species at  $\zeta = 0.7$  and  $T_{wall}=300$  K. Top contour is the  $R$  term of OH with zoom-in from  $x = 0$  to  $10$  mm. Flame front position is marked with solid black line, and the dashed blue line is the edge of the thermal boundary layer. Four normal flame cuts marked as A, B, C and D are highlighted in the contour. The corresponding  $C - D - R$  profiles are shown in the bottom four plots.  $D_n$  presents the diffusion component along the flame normal, and  $D_t$  denotes the tangential component of diffusion. The  $x$  and  $y$  locations in each title of subplots correspond to the flame front coordinates.



Cut (A) shows that diffusion is dominant at the preheating zone, representing premixed flame propagation. Cut (B) shows almost zero  $D_n$  with less than  $1 \text{ kg.m}^{-3}.\text{s}^{-1}$  magnitude, indicating autoignition. At cut (C), the combustion mode starts switching from autoignition to premixed flame propagation. Cut (D) is closer to the thermal boundary layer edge marked as a blue dashed line,  $D$  is dominant in the preheating zone, indicating premixed flame propagation.

## 5.4 Conclusions

2D fully resolved simulation with detailed chemistry was used to simulate a laminar SWQ configuration with methane/air mixture diluted by hot combustion products. An initial fully developed thermal layer is included. The effects of dilution levels, wall temperature and forcing frequency on flame dynamics, near-wall CO formation and emissions pathway were studied, and the key findings are:

1. At higher dilution levels, the peak of near-wall CO decreases (consistent with the 1D results), and the flame is shorter, making more time available for oxidation before the mixture reaches the domain exit.
2. At higher wall temperature the peak near-wall CO increases (consistent with the 1D results) but again the flame is shorter, making more time available for oxidation before the mixture reaches the domain exit.
3. The flame length is the dominant parameter affecting the exhaust CO. Due to the role of the flame length, the contribution of the near-wall CO to the exhaust CO increases as the dilution level or the wall temperature is reduced.
4. The forcing makes the exhaust CO fluctuate sinusoidally with a phase lag to the forcing frequency. The average CO mass fractions and mass flux over one cycle are close to the unforced case, although there is a slight increase in CO mass flux with forcing frequency.
5. The near-wall CO features large variations when the local Damköhler number is greater than 0.1.
6. Analysis of the CO transport budget shows the dominant role of convection

and diffusion near the wall, except during the autoignition at the wall.

# Chapter 6

## 3D Turbulent Diluted FWI

### 6.1 Introduction

This chapter presents the results of a 3D DNS featuring a turbulent diluted flame in a duct, consisting of two branches, each interacting with a wall at a given temperature. The top wall has a temperature slightly below the premixture temperature while the bottom wall temperature is much lower than the premixture temperature. This setup allows for different regimes of FWI to be studied in one configuration. The results of several 1D configurations under the same conditions as the 3D case are first discussed, providing benchmarks for further comparison. The instantaneous and time-averaged results are then analysed. CO thermochemistry is also investigated in the light of 1D results. Finally, the species transport budget of CO is used to analyse the near-wall CO transport.

### 6.2 3D and 1D Configurations

The configuration is briefly described here to highlight some of key features used to analyse a number of 1D configurations in the next section. Figure 6.1 shows the 3D domain with an iso-surface of instantaneous flame front marked by the progress variable  $c_{CH_4} = 0.94$ . The fresh reactants diluted by hot combustion products enter the domain from the left side boundary. A cylindrical hot patch was imposed at the  $y/H = 0$  and  $x/H = 1$ . This hot patch ignited the reactants, creating two flame

branches. These branches interact with the top-hot wall and the bottom-cold wall separately. The details of the computational domain and the flow parameters are shown in Table 3.6. In this configuration, some parts of the premixture will be cooled down by the cold wall before encountering the reaction front in the middle of the domain. A 1D unstrained flame with different inlet temperatures can be representative of these regions. Another feature of the 3D flame is the flame interaction with the thermal boundary layer downstream of the main reaction front. A simplified 1D configuration for these regions of the flame is an opposed-flow flames (OPPDIFF) configuration with the premixture on one side and products on the other side. Both of these configurations will be analysed in the next section.

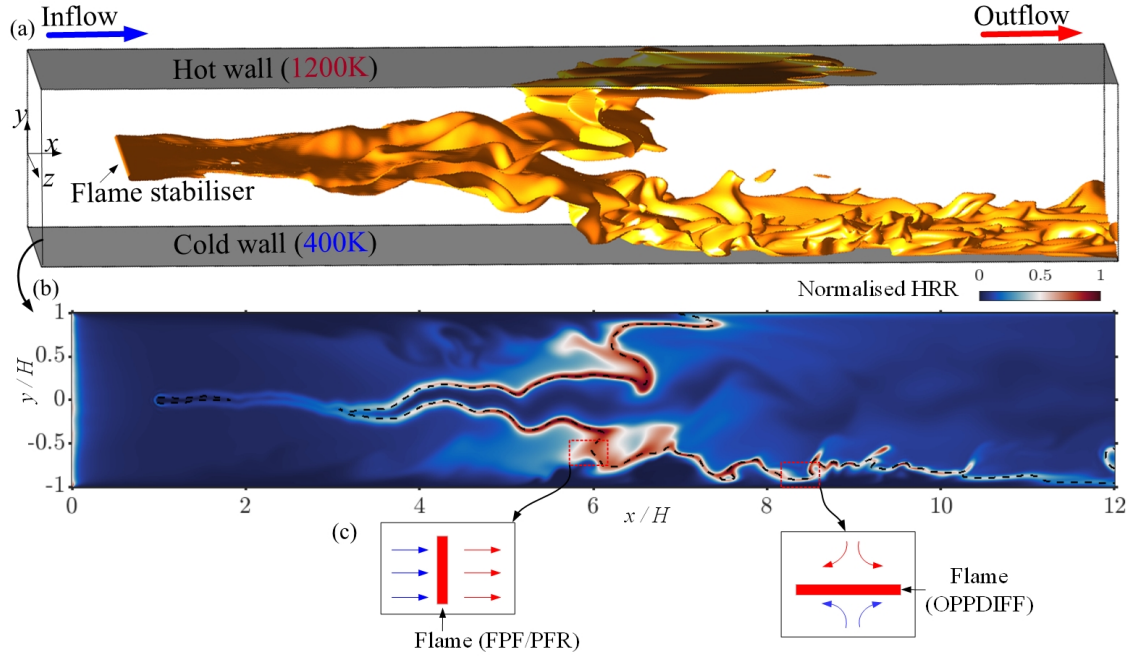


Figure 6.1: Top row: schematic of the 3D DNS domain; middle row: 2D HRR contour normalized by maximum HRR at  $z/H=3$ , and the dashed black line approximates the peak HRR positions; bottom row: 1D manifolds to present the 3D local combustion features. The flame is anchored at  $x/H = 1$  ( $H$  is half channel width, 2.5 mm),  $y/H = 0$  and throughout the  $z$  direction.

## 6.3 Results and Discussion

### 6.3.1 1D Diluted Flames

1D adiabatic, unstrained flames at different premixture temperatures ( $T_{in}$ ) were simulated with the results shown in Figure 6.2. A FPF model was used to simulate the flames with  $T_{in} = [900 \text{ } 1100]$  K. The inlet temperature of 900 K is at the flammability limit of the mixture. Once the inlet temperature is higher than 1100 K, the FPF model was unsuitable to capture the flame due to the high reactivity of the premixture. This indicates a change of combustion mode from premixed flame to autoignition for high inlet temperatures. Therefore, premixtures with  $T_{in} = [1200 \text{ } 1700]$  K were simulated with a PFR model.

Figure 6.2 shows that the peak CO mass fraction increases with increasing  $T_{in}$ . Interestingly, a jump in the peak CO mass fraction exists when  $T_{in}$  is varied from 1100 K to 1200 K. This is induced by switching from the FPF to PFR models, as the latter lacks diffusion in the direction of flow. This suggests that the central region of the 3D configuration should produce more CO compared with the near-wall region. While the peak formation rate increases by increasing  $T_{in}$ , the peak oxidation rate is relatively constant for the auto-ignitive cases. This shows that the reaction rate constants for the CO oxidation and formation have markedly different sensitivity to temperature.

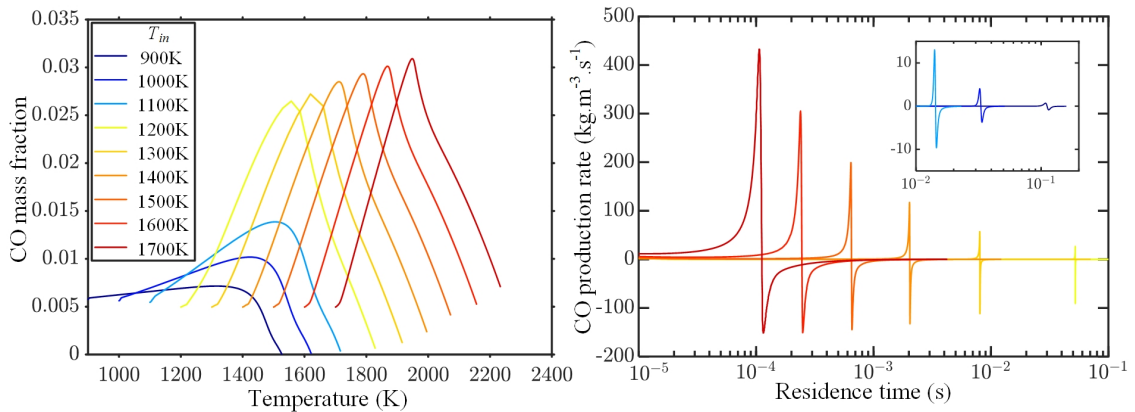


Figure 6.2: CO mass fraction versus temperature (K) (left) and the net production rate of CO (kg.m<sup>-3</sup>.s<sup>-1</sup>) versus residence time (s) (right) plots from 1D freely propagating flame solutions at inlet temperature ( $T_{in}$ ) = 900 K to 1100 K, and from plug flow reactor at  $T_{in}$  = 1200 K to 1700 K with reactants composition at  $\zeta = 0.7$ .

The second group of 1D cases were simulated using the OPPDIFF model. Figure 6.3 shows two sets of OPPDIFF solutions. One set has premixture on both sides where the temperature is 400 K at one side and 1700 K on the other side. In the second set, one side has the premixture at 400 K while the other side has combustion products at 2120 K. This configuration presents the flames supported by hot products found in the premixture of the cold wall region.

The results show that the peak temperature decreases with increasing strain rates for both configurations, and this is more obvious on the 1700 K versus 400 K configuration than the 2120 K versus 400 K. The temperature increase in the latter configuration is because the 2120 K temperature corresponds to the maximum temperature in 3D simulation. This is lower than the adiabatic temperature (2240K). In Figure 6.3(a) with 1700 K versus 400 K reactants temperature, peak CO mass fraction on the 1700 K side is almost constant with increasing strain rate from  $7000 \text{ s}^{-1}$  to  $16000 \text{ s}^{-1}$ , and then decreases after further increasing the strain rate to  $25000 \text{ s}^{-1}$ . The decrease of the peak CO mass fraction was also observed by Coriton et al. experimentally in a counter-flow burner [103]. The peak  $\dot{\omega}_{CO, formation}$  increases with strain rates from  $7000 \text{ s}^{-1}$  to  $16000 \text{ s}^{-1}$ , and decreases from  $16000 \text{ s}^{-1}$  to  $25000 \text{ s}^{-1}$ . No negative  $\dot{\omega}_{CO, oxidation}$  exists at strain rate =  $25000 \text{ s}^{-1}$ , i.e. the quenching of CO oxidation layer, as also observed by Coriton et al. and Wang et al. [104, 105].

In Figure 6.3(b), reactants on the 400 K side are able to burn, even though 400 K is under the flammability temperature limit for a freely propagating premixed flame at this  $\zeta$ . Unlike the 1700 K versus 400 K configuration, the peak CO mass fraction and  $\dot{\omega}_{CO, oxidation}$  increase with increasing strain rate monotonically in this configuration.

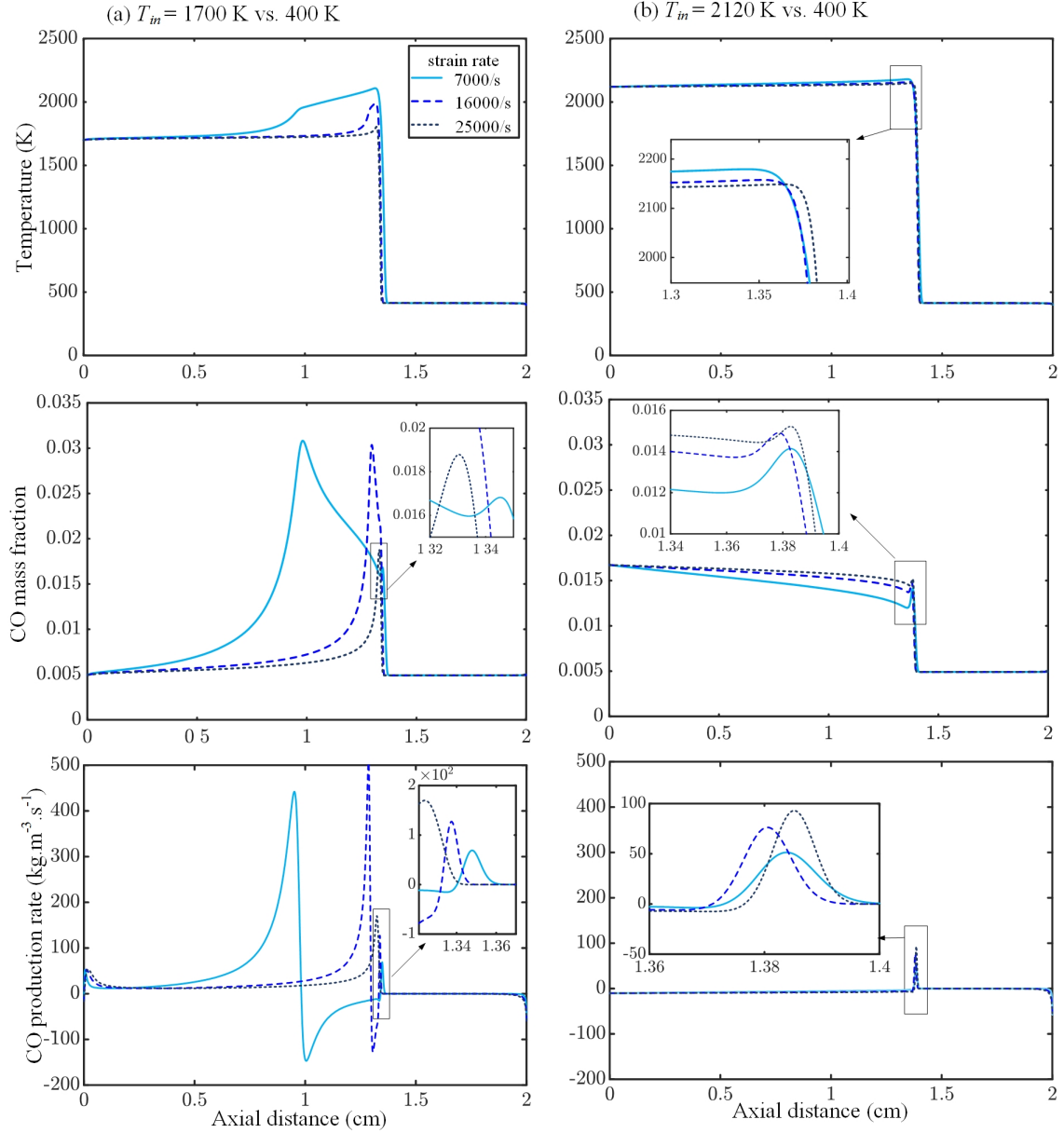


Figure 6.3: Spatial plots of temperature (K), CO mass fraction and CO net production rates from OPPDIFF solutions. (a) Left column: Inlet streams of 400 K and 1700 K with reactants composition taken from  $\zeta = 0.7$ . (b) Right column: inlet stream of 400 K reactants and 2120 K adiabatic combustion products.

## 6.3.2 3D Diluted Flames

### 6.3.2.1 Instantaneous Results

Figure 6.4 shows the instantaneous streamwise velocity, temperature, CO mass fraction and CO net production rate at the  $x - y$  plane at  $z/H = 1.2$ . The flame front is marked with a dashed iso-line at  $c_{CH_4}$  of 0.94. The white dashed lines mark the

streamwise location at  $x/H = 6, 8$  and  $10$  for further analysis. A high level of velocity and temperature fluctuations are evident near the cold wall.  $Re_\tau$  at the cold wall increases from 576 at the inlet to 810 at around  $x/H = 7$ , due to the thermal boundary layer growth.  $Re_\tau$  then reduces to 730 at the outlet, which can be caused by the preheating of the flame and further laminarisation. Both flame branches interact with the thermal boundary layer in the region downstream of  $x/H = 6$ . While the top branch enters the thermal BL and is attached to the wall at around  $x/H = 9.5$ , the bottom branch extends up to the domain exit.

A high CO region is present from  $x/H = 6$  to  $8$ . A region with high CO production rate is also present around  $x/H = 6$ . The peak CO formation rate is higher than the peak CO oxidation rate, consistent with the 1D results presented in Figure 6.2.

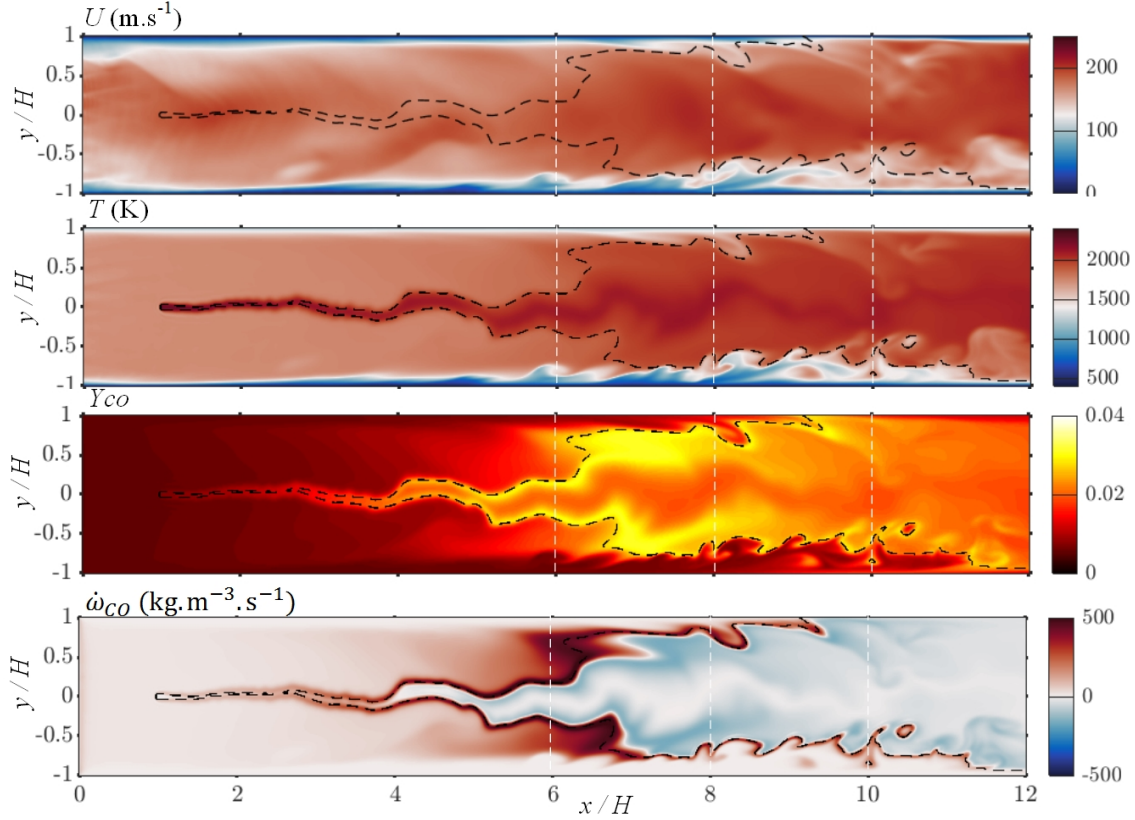


Figure 6.4: streamwise velocity ( $U$ ), temperature ( $T$ ), CO mass fraction ( $Y_{CO}$ ) and CO net production rate ( $\dot{\omega}_{CO}$ ) contours taken on an  $x - y$  plane at  $z/H = 1.2$  and time  $= 2.58 \tau_f$  (flow through time). Dashed lines mark the flame front at a contour of  $c_{CH_4} = 0.94$ . Three dashed white lines mark the positions at  $x/H = 6, 8$  and  $10$ , respectively.

The high CO region is now investigated further using the results at four sequential



instants (see Figure 6.5). Backward and forward motion of the reaction front is evident. Focusing on the hot side, it can be seen that autoignition, indicated by the spatially distributed pattern of the peak heat release rate, is occurring from  $x/H = 6.5$  to  $7.5$  in the region of  $y/H = 0.5$  to  $1$  at  $t = 2.4\tau_f$ . At a later time, autoignition is occurring in the region from  $x/H = 5.5$  to  $6.5$ . After that, the reacting region convects downstream, until upstream autoignition occurs again. This autoignition mode was indicated by the spatially distributed pattern of the peak heat release rate, occupying large areas of the channel. Whereas, in the propagating flames, the peak heat release rate is localized in thin sheets. Similar combustion modes were seen in [106]. This periodic autoignition changes the position of volumetric reaction zones where CO is formed, as shown here and also in Figure 6.4. The same mechanism is present on the cold-wall side as well.

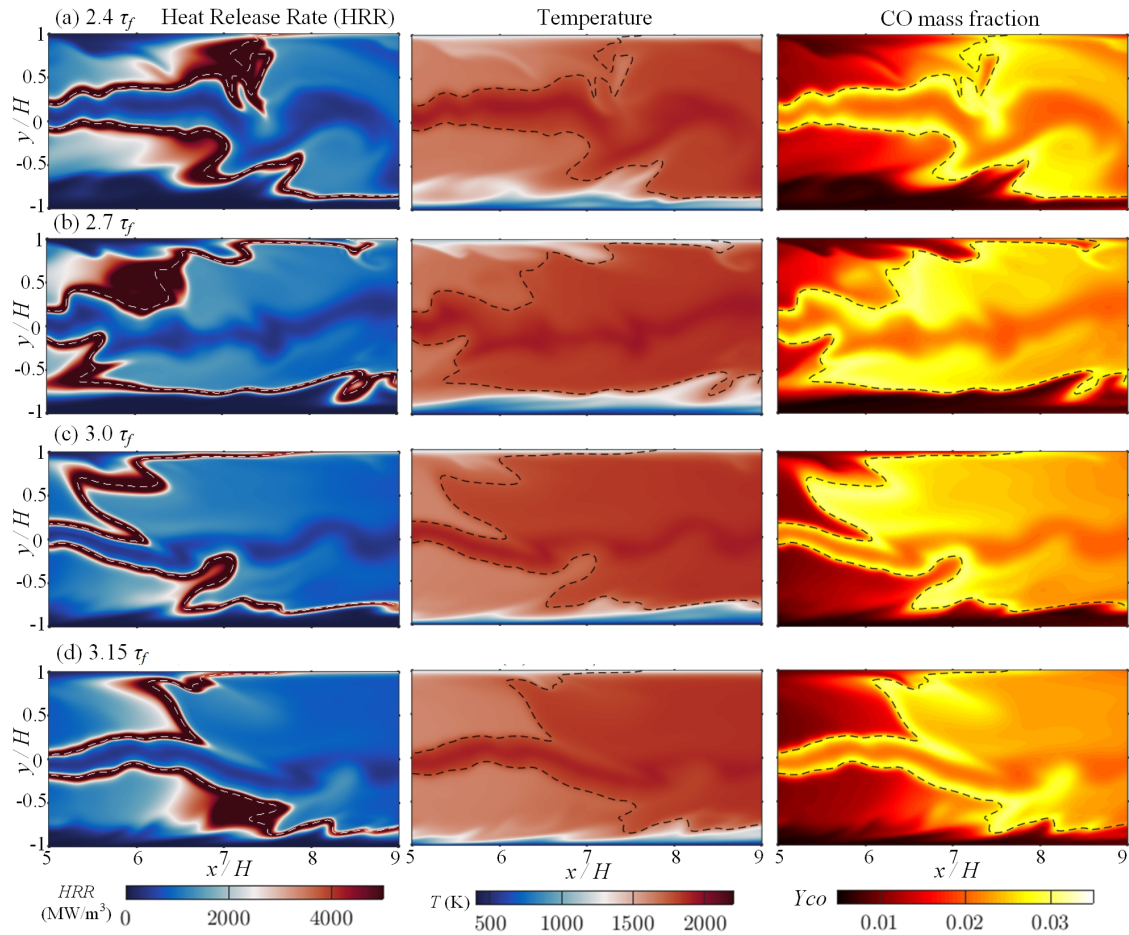


Figure 6.5: Heat Release Rate ( $\text{MW}\cdot\text{m}^{-3}$ , left column), Temperature (K, centre column), CO mass fraction (right column) contours on streamwise( $x$ )-transverse( $y$ ) planes at time =  $2.4, 2.7, 3.0$  and  $3.15 \tau_f$ . Dashed lines indicate the flame position marked with an iso-contour of  $c_{CH_4} = 0.94$ .

Figure 6.6 shows the instantaneous results on the  $y - z$  plane at  $x/H = 6, 8$  and  $10$  at the same instant with Figure 6.4. The dashed-white lines mark the  $z/H = 1.2$ , consistent with the  $z$  position of  $x - y$  contours in Figure 6.4. Large scale structures extending from  $y/H = -1$  to  $-0.5$  are frequently present at all streamwise locations. These structures have a large impact on the distribution of reaction zone and CO thermochemical state, and thus impact CO net production rate and distribution, highlighting the significance of the thermal boundary layer on the cold-wall side in terms of CO emissions. It is also interesting to note that the near-wall CO on the cold-wall side is higher than the hot-wall side at the most downstream location. Also, the high CO region identified earlier can be clearly seen at  $x/H = 8$ , demonstrating that this region is present in the entire spanwise length. Although this region features a high amount of CO at  $x/H = 6$ , CO oxidation significantly reduces this amount at  $x/H = 10$ .

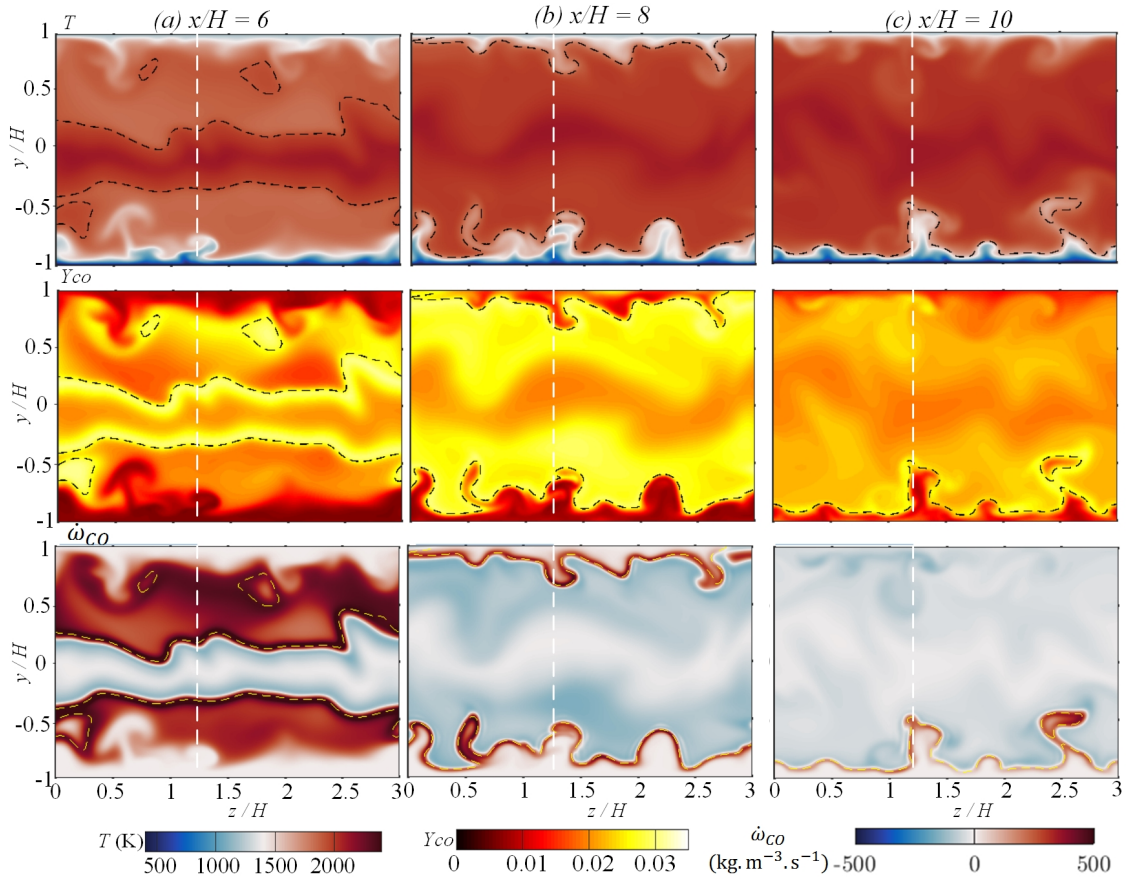


Figure 6.6: Temperature, CO mass fraction, CO production rate contours taken on  $y - z$  planes at  $x/H = 6, 8$  and  $10$  and time  $= 2.58 \tau_f$ . Dashed curves indicate the flame position marked with an iso-contour of  $c_{CH_4} = 0.94$ . White dashed lines denotes the spanwise position at  $z/H = 1.2$ .

Figure 6.7 shows the 3D flame surface on both hot- and cold-wall sides at the same instant with Figure 6.4. On the hot-wall side, streak-like flame structures seem to be the dominant feature, whereas on the cold-wall side a significant part of the flame surface is parallel to the wall. This indicates that the 1D OPPDIFF configurations are quite relevant to the cold-wall side.

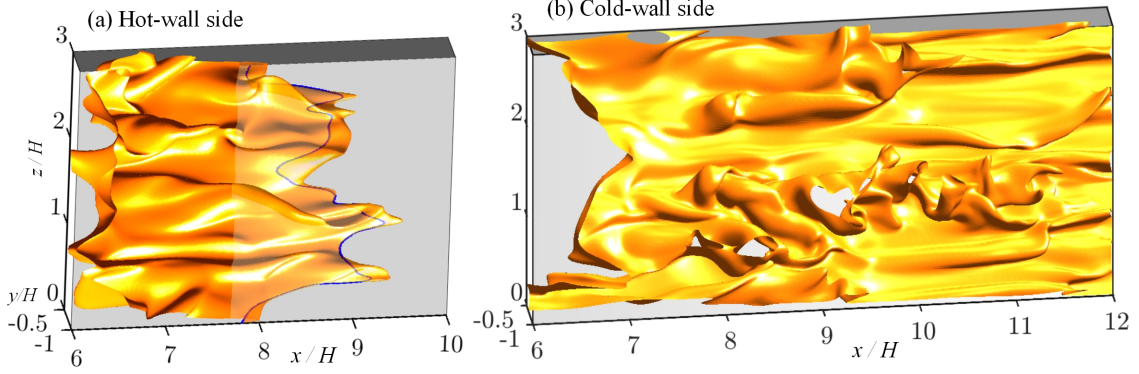


Figure 6.7: Rendered 3D surfaces of iso-contour ( $c_{CH_4} = 0.94$ ) at time  $= 2.58 \tau_f$  close to (a) the hot wall ( $0.5 < y/H < 1$ ) and (b) the cold wall ( $-1 < y/H < -0.5$ ). On the hot-wall side, both the flame data and  $z$ -coordinate were flipped to attain the same top view with the cold-wall side while maintaining the same flow direction on the paper. Blue line in the transparent region of Figure (a) is to identify wall-contact regions.

Figure 6.8 shows the CO mass fraction at the wall at the same instant with Figure 6.7. High CO mass fraction at the hot wall is mainly distributed from  $x/H = 8$  to 10, where the peak value follows the flame-wall contacting positions as marked by the blue line in Figure 6.7. High CO mass fraction at the cold wall stretches from  $x/H = 9$  to 12, and continues to increase towards the domain exit. As the flame contacts the hot wall, the peak CO mass fraction at the hot wall is about 50 % higher than peak CO at the cold wall. This CO begins to oxidise towards the domain exit on the hot-wall side. As a result, mean CO mass fraction at the exit and at the cold wall is about 30 % higher than the hot wall.

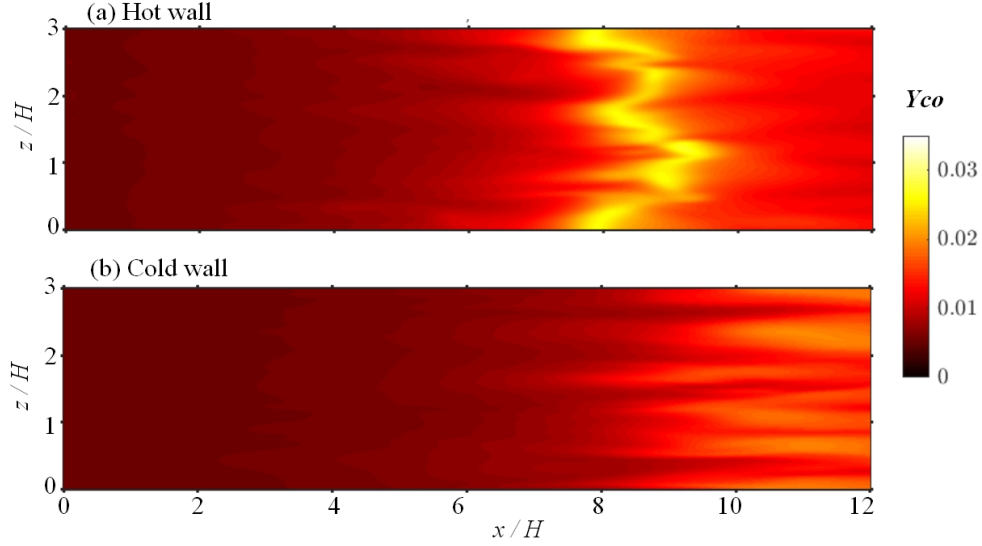


Figure 6.8: CO mass fraction contours on streamwise( $x$ )-spanwise( $z$ ) plane at the hot wall (a) and cold wall (b) taken at time =  $2.58 \tau_f$ .

### 6.3.2.2 Time, Spanwise-Averaged Results

Figure 6.9 shows the mean and RMS contours at the  $x - y$  plane. Both mean and RMS were obtained using the time and spanwise averaged data. The mean flow is accelerated after the main reaction region around  $x/H = 6$ , largely due to the decreasing density from reactants to the products. The region with high RMS values of the streamwise velocity on the cold-wall side increases in size with increasing streamwise distance. However, on the hot-wall side, the flame is attached to the wall around  $x/H = 6$ , reducing the size of this region. This is expected, as flow relaminarisation occurs downstream of the flame due to a higher viscosity in this region [24]. These results suggest that the flame has a significant impact on the near-wall turbulence on the hot-wall side; On the cold-wall side, the near-wall turbulence notably affects the flame motion.

Similar to the mean velocity, the mean temperature increases after the main reaction region at  $x/H = 6$ . Much lower RMS values of temperature are observed near the hot wall. On the cold-wall side, the region with the high RMS of temperature becomes narrower downstream of  $x/H = 8$ . This shows that the fluctuations of the flame brush occur closer to the wall with increasing streamwise distance on the cold-wall side. Comparison of this observation with the results shown in Figures 6.6

and 6.7 implies that the presence of more flat-like flame structures contributes to this observation. This phenomenon will be analysed further using the statistics of the flame surface (see Section 6.3.2.3).

Free-stream ( $y/H = -0.5$  to  $0.5$ ) mean CO mass fraction increases from  $x/H = 4$  to 8 due to autoignition events. Downstream of this region, CO oxidation reduces the mean CO mass fraction. In the RMS field, two regions with high RMS values can be distinguished: the free-stream region defined earlier and the near-wall region (from  $x/H = 6$  to 10 near the cold wall and from  $x/H = 6$  to 8 near the hot wall). Very small RMS values are observed in the free-stream region for  $x/H > 8$ , suggesting insignificant impact of velocity fluctuations on CO oxidation in this region.

Peak mean CO net production rate can be observed around  $x/H = 6$  in the free stream, with the CO formation regions extending downstream near both walls. The hot-wall side shows a complete transition to CO oxidation due to the completion of combustion, but the cold-wall side continues to display CO formation to the domain exit. It also can be seen that a high mean CO net production rate exists near the inlet, due to the quasi-equilibrium effect from the hot combustion products as the diluents. It reaches equilibrium after about  $0.2 H$  streamwise distance.

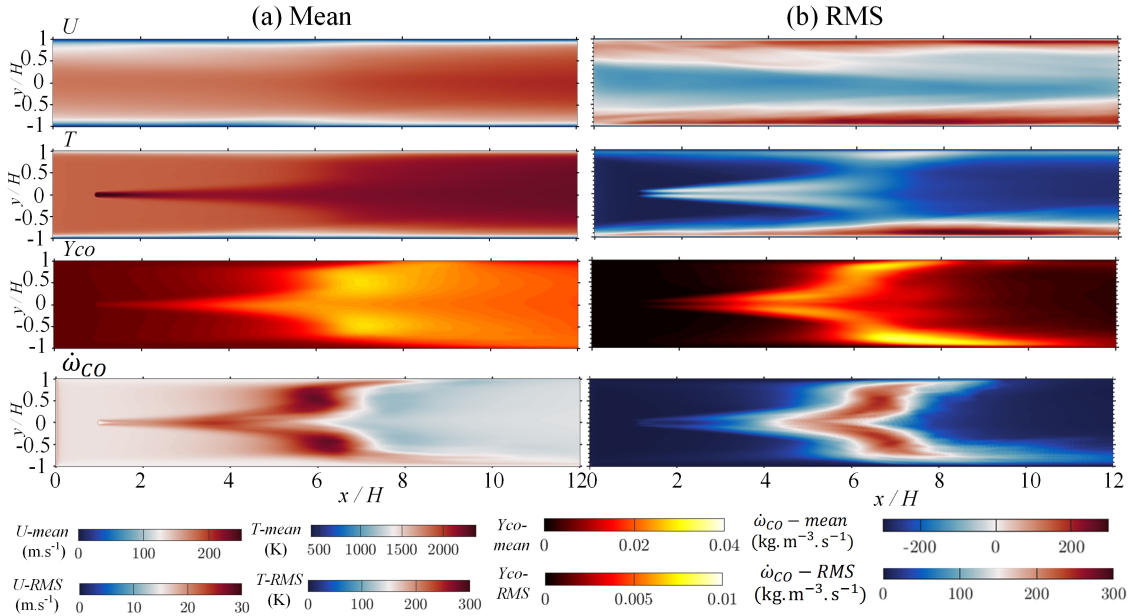


Figure 6.9: Mean and RMS  $x - y$  contours of streamwise velocity ( $U$ ), temperature ( $T$ ), CO mass fraction ( $Y_{CO}$ ) and CO net production rate ( $\dot{\omega}_{CO}$ ). Contours are spatially averaged in the  $z$ -direction and time averaged over  $2 \tau_f$ .



Figure 6.10 shows the mean and RMS of streamwise velocity, temperature, CO mass fraction and reaction rate at different streamwise locations. Interestingly, when the mean and RMS of velocity are non-dimensionalised with the bulk velocity, for  $x/H > 6$ , these quantities largely collapse. For the mean and RMS of temperature, this behaviour is observed for  $x/H > 8$  when these quantities are non-dimensionalised by the bulk temperature. This shows that the effect of combustion on velocity and temperature is mainly the increased mean temperature and velocity. While the velocity fluctuations show no noticeable difference between the hot- and cold-wall sides, the RMS of temperature near the cold wall is notably higher than the hot-wall side.

The mean CO mass fraction profiles show the increase of CO at the cold wall from  $x/H = 6$  to 12. At the hot wall, CO increases from  $x/H = 6$  to 8 and then decreases from  $x/H = 10$  to 12, once the flame attaches the wall. The difference between the free-stream CO mass fraction and that at the wall decreases with increasing streamwise location. The near-wall fluctuations of CO mass fraction is larger than those in the free-stream downstream of the main reaction front ( $x/H > 6$ ). This highlights the importance of the near-wall region in terms of the overall CO emissions.

The CO net production rate results reveal one of the mechanisms that contributes to variation of CO mass fraction. CO oxidation is strong downstream of the main reaction front in the free stream. However, at the cold wall the CO net production rate is zero (as expected). Therefore, the increase of CO mass fraction at the cold wall should be linked to other transport mechanisms. This will be discussed in Section 6.3.2.5. Consistent with the results shown for the fluctuations of CO mass fraction, the CO reaction rate also shows high RMS values near both walls compared with the free stream.

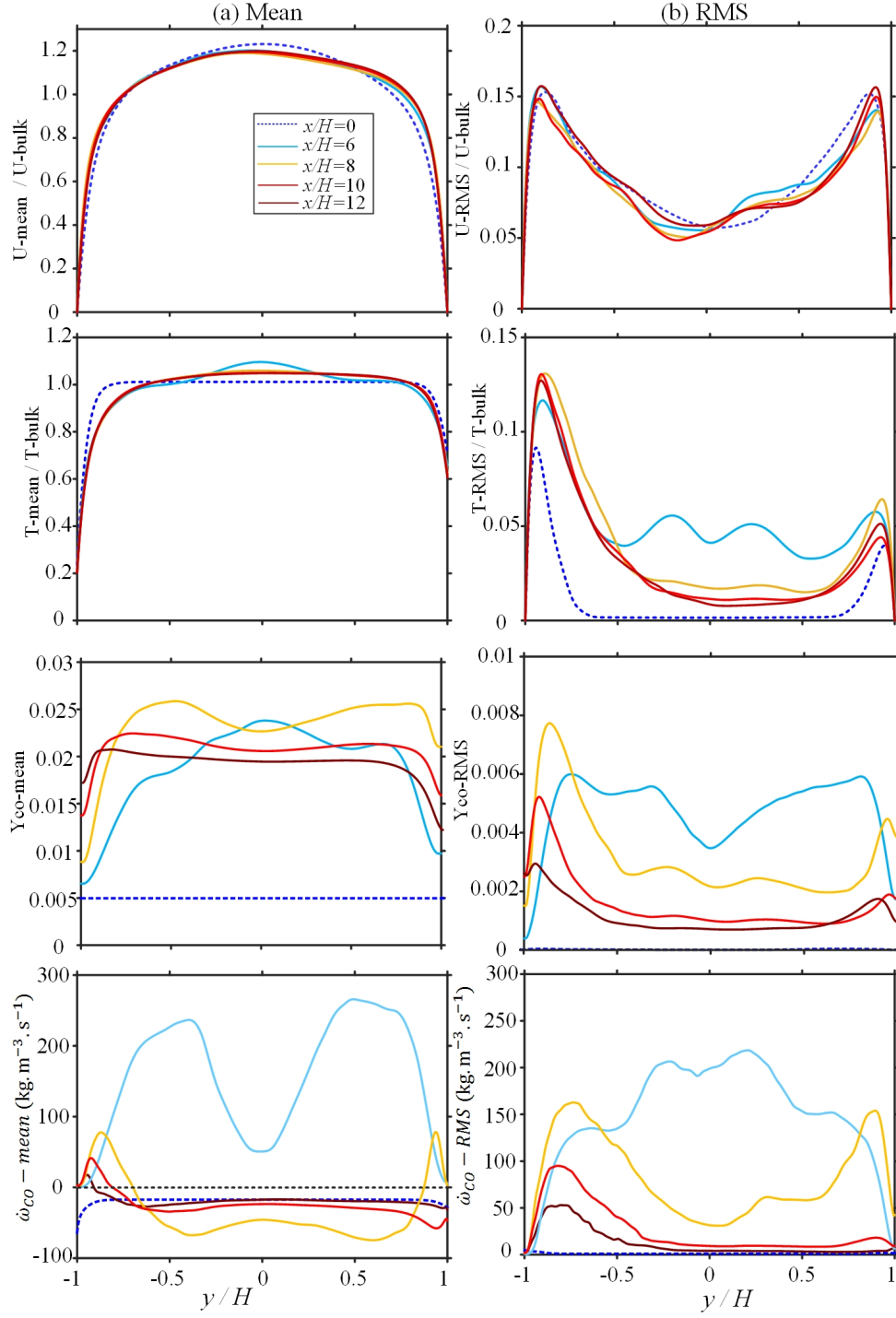


Figure 6.10: Mean and RMS profiles of streamwise velocity, temperature, CO mass fraction and CO net production rate at  $x/H = 0, 6, 8, 10, 12$ . The mean and RMS profiles of streamwise velocity and temperature are normalized by the bulk value. Black dashed line in mean CO net production rate artificially denotes the zero value for comparison.

To evaluate the exhaust CO emissions, an averaged CO mass fraction ( $\tilde{Y}_{CO,exh}$ ) and CO mass flux ( $\tilde{m}_{CO,exh}$ ) at the domain exit are calculated using Equations 6.3.1

and 6.3.2, and are reported in Table 6.1. The results show that the exit average CO mass fraction near the cold wall is 15% higher than that near the hot wall, and about 4% higher than the averaged value at the entire exit. This trend is consistent with the previous instantaneous and mean CO results as shown in Figures 6.4 and 6.10. The CO mass flux in the free-stream region ( $y/H = [-0.7, 0.7]$ ) contributes to about 75% of the total CO mass flux. The wall-affected regions contribute the remaining 25%.

$$\tilde{Y}_{CO,exh} = \frac{\sum_1^{Nt} \sum_1^{Ny} \sum_1^{Nz} \rho u Y_{CO} \Delta y \Delta z \Delta t}{\sum_1^{Nt} \sum_1^{Ny} \sum_1^{Nz} \rho u \Delta y \Delta z \Delta t} \quad (6.3.1)$$

$$\tilde{m}_{CO,exh} = \frac{\sum_1^{Nt} \sum_1^{Ny} \sum_1^{Nz} \rho u Y_{CO} \Delta y \Delta z \Delta t}{\sum_1^{Nt} \Delta t} \quad (6.3.2)$$

Table 6.1:  $\tilde{Y}_{CO,exh}$  and its relative difference to the entire exit normalized by  $\tilde{Y}_{CO,exh}$  at the entire exit,  $\tilde{m}_{CO,exh}$  and its contribution to the entire domain by normalizing with the  $\tilde{m}_{CO,exh}$  at the entire exit.

| $y/H$ bands     | Average CO mass fraction<br>(Difference to the entire exit) | Average CO mass flux ( $\text{kg.s}^{-1}$ )<br>(Contribution to the entire exit) |
|-----------------|-------------------------------------------------------------|----------------------------------------------------------------------------------|
| $[-1.0 \ 1.0]$  | 0.0193 (-)                                                  | 0.0231 (-)                                                                       |
| $[-0.7 \ 0.7]$  | 0.0194 (0.5%)                                               | 0.0175 (75%)                                                                     |
| $[0.7 \ 1.0]$   | 0.0173 (-10%)                                               | 0.0025 (11%)                                                                     |
| $[-1.0 \ -0.7]$ | 0.0200 (4.0%)                                               | 0.0032 (14%)                                                                     |

### 6.3.2.3 Flame Location and Orientation

Figure 6.11 shows the Probability Density Function (PDF) of the flame orientation at different streamwise locations. PDFs are taken at  $c_{CH_4} = 0.94$  from  $y/H = -1$  to 0 on the cold wall side and 0 to 1 on the hot wall side, with data collected at the indicated  $x/H$ , over  $2 \tau_f$  and the entire domain span ( $z$ ). The peak  $n_y$  is at 1 near the hot-wall side, while it is -1 near the cold-wall side. This difference is due to the definition of the flame normal direction pointing towards the unburned reactants. The peak  $n_x$  is zero on both sides. The preference of  $|n_y|$  towards 1 and  $n_x$  towards zero increases with increasing downstream distance. This shows that the incline of the flame is reducing with respect to the streamwise direction, as observed earlier



from the instantaneous results.

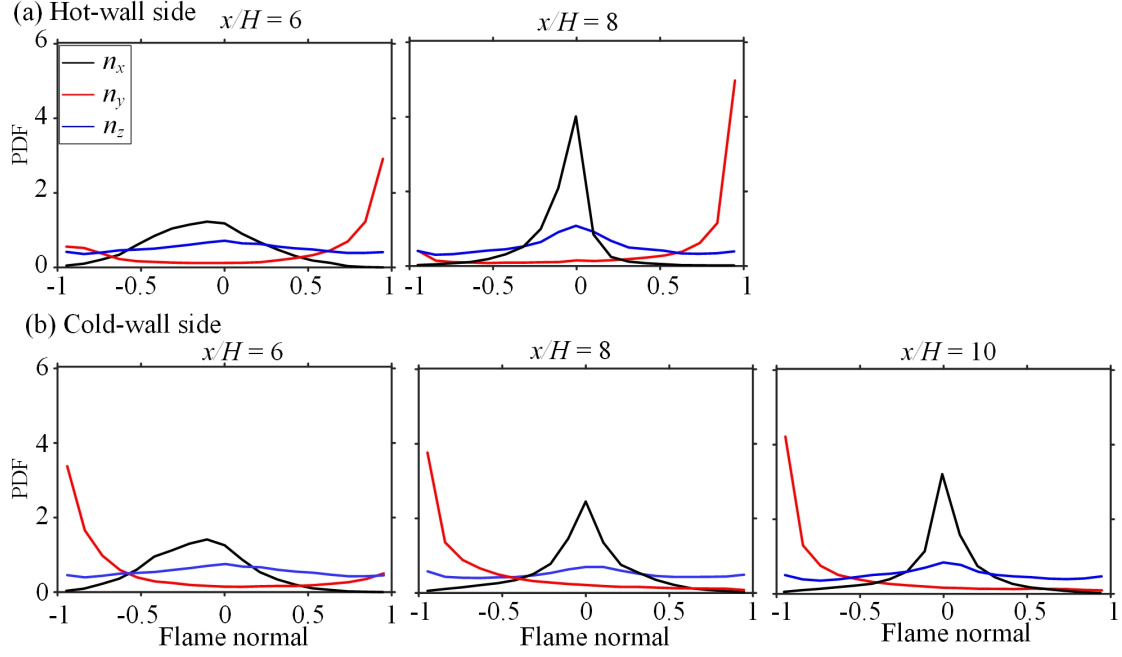


Figure 6.11: Probability density functions of flame orientation. Flame orientation is assessed at  $c_{CH_4} = 0.94$  within  $0 < y/H < 1$  on the hot-wall side (a) at  $x/H = 6, 8$  and  $-1.0 < y/H < 0$  on the cold-wall side (b) at  $x/H = 6, 8, 10$ .

Data is collected across the  $z$ -direction and over  $2 \tau_f$ .

Figure 6.12 shows the PDF of the flame  $y$ -coordinate (the flame-wall distance) at different streamwise locations. At  $x/H = 6$ , there is an almost uniform distribution in the central region. This is where the main reaction front is, and therefore this behaviour is expected. At  $x/H = 8$  and  $10$ , the PDF peak is within  $[0.1, 0.2]H$  wall distance on the cold-wall side while the peak is even closer to the wall on the hot-wall side at  $x/H = 8$ . These results can be used to define different regions and study the flame behaviour individually in these regions. Three regions are therefore defined as,

- $|y/H| = [0.9, 1]$ , where the flame is less likely to be present on the cold-wall side but highly likely on the hot-wall side at  $x/H = 8$  only,
- $|y/H| = [0.7, 0.9]$ , where the flame is dominantly present on the cold-wall side at  $x/H = 8$  and  $10$ , and
- $|y/H| = [0, 0.7]$ , where there is a strong presence of the flame at  $x/H = 6$ .

These regions will be used in the following section to investigate CO thermochemical state.

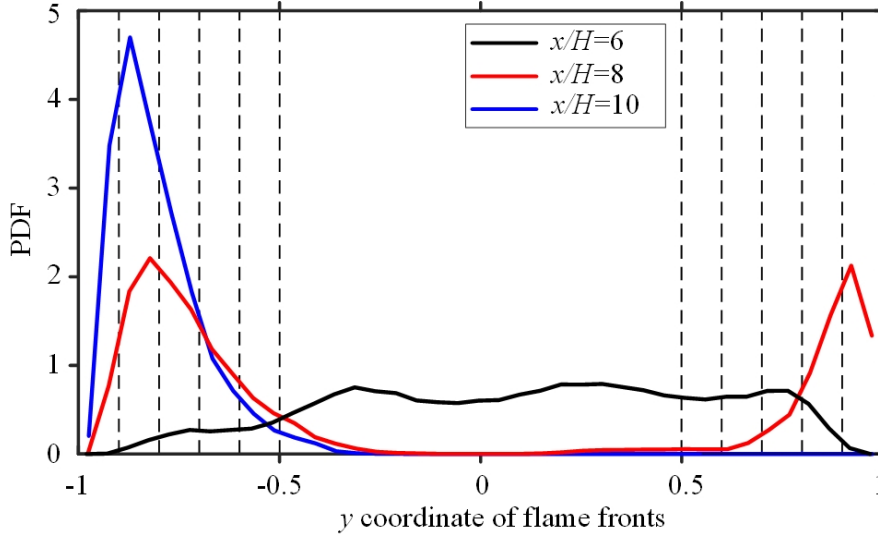


Figure 6.12: Probability density function of the  $y$ -coordinate of flame fronts at  $x/H = 6, 8$  and  $10$ . PDFs are determined at the noted  $x/H$ , across the whole domain span ( $z$ ) direction, over  $2 \tau_f$ . Dashed black lines mark the positions at  $|y/H| = [0.5:0.1:1]$ .

#### 6.3.2.4 CO Thermochemical State

To examine the wall effects on the thermochemical state of CO, the three regions defined earlier will be investigated separately. Figure 6.13 shows the scatter plots of CO mass fraction versus temperature on the hot-wall side over the defined three  $y$ -band at  $x/H = 6, 8$  and  $10$ . The points are coloured by the CO net production rate to mark the CO formation and oxidation regions. The 1D PFR solutions from Figure 6.2 are overlaid on the scatter plots. These can be used to examine whether 1D manifolds or lookup tables are suitable for modelling the 3D results.

Considering the central region, i.e.  $y/H = [0, 0.7]$ , it is noted that the oxidation branch of PFR case with the highest inlet temperature provides a boundary for the points on the RHS. All points are also occupied in the region covered by the PFR solutions. While CO formation is dominant at  $x/H = 6$ , only CO oxidation is present at  $x/H = 10$ . Considering the  $y/H = [0.7, 0.9]$  region, the points become more scattered but are still within the PFR solution. In the region of  $y/H = [0, 0.9]$ , the reactions appear to follow an ensemble of auto-igniting PFRs with varying

initial temperatures. However, in the vicinity of the wall, i.e.  $y/H = [0.9, 1]$ , there is a large region of points outside the 1D solutions and the adiabatic PFR results no longer describe the cold-gas thermochemical states around  $T = 1200$  K.

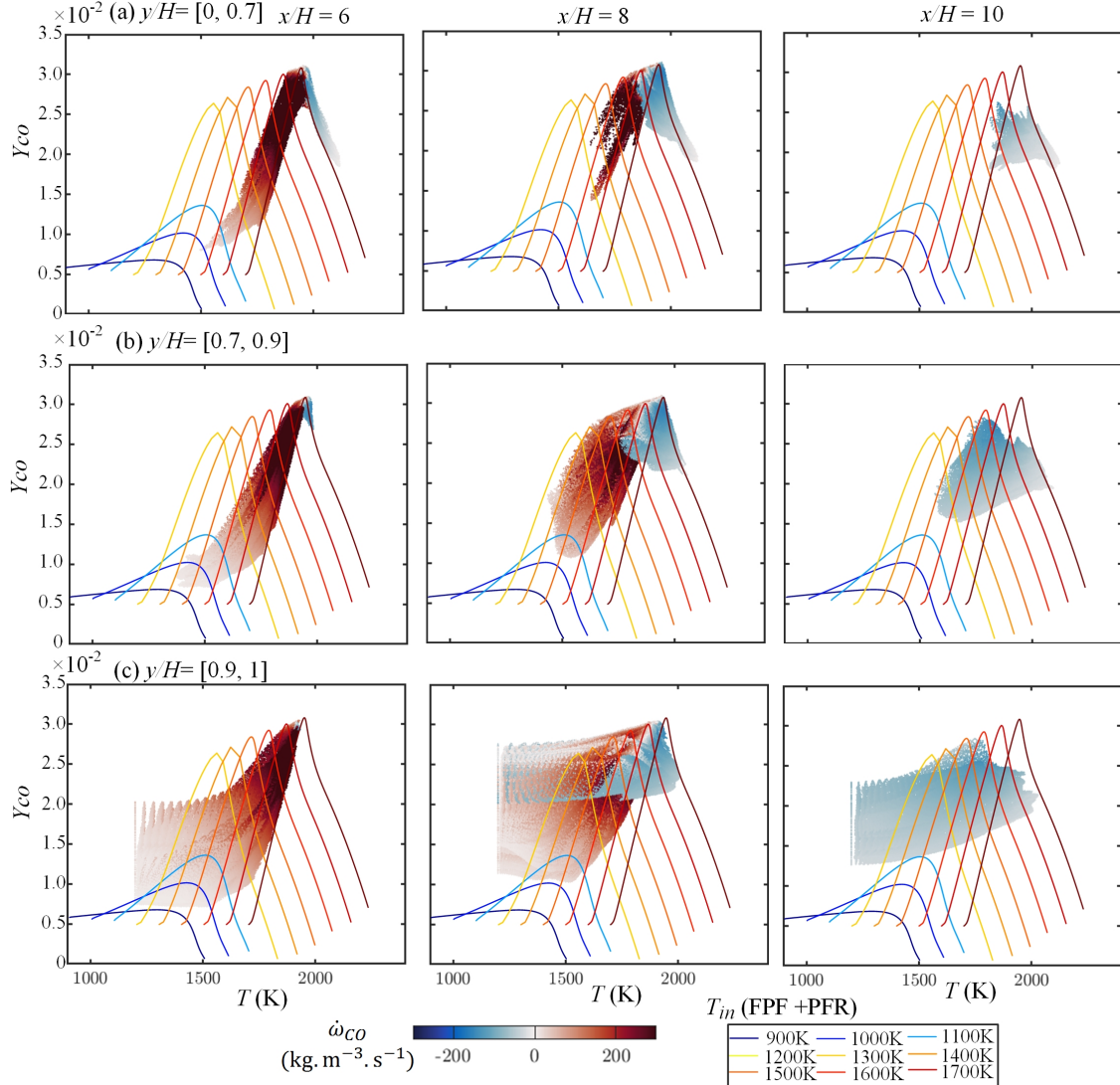


Figure 6.13: Scatter plots of CO mass fraction versus temperature at  $x/H = 6$ , 8 and 10. (a) Top row presents  $y/H = [0, 0.7]$ ; (b) Middle row presents  $y/H = [0.7, 0.9]$ ; (c) Bottom row presents  $y/H = [0.9, 1]$ . Scatter plots are overlaid with the results of 1D FPF and PFR simulations for  $\zeta = 0.7$  at the indicated reactants temperatures.

Figure 6.14 shows the scatter plots of CO mass fraction versus temperature on the cold-wall side. In the region of  $y/H = [-0.7, 0]$ , the 1D PFR and FPF solutions are shown and outside this region, the 1D OPPDIFF solutions are presented. On average, the 1D solutions can provide boundaries for the points in the central region,  $y/H = [-0.7, 0]$  and only a small portion of 3D data about 1200 K are beyond the

1D FPF solutions as can be seen at  $x/H = 8$  and 10 on the top row. In the region of  $y/H = [-0.9, -0.7]$ , a considerable number of points deviate from the unstained 1D solutions and the OPPDIFF solutions are needed to provide a complete picture. For this region, the 3D data at intermediate and low temperature regions overlap with the results of OPPDIFF solutions at varying strain rates. These manifolds appear to describe the flame sheet well. However, close to the wall ( $y/H < -0.9$ ), very high CO mass fractions ( $\approx 0.015$ ) are found, exceeding the results of the strained flames.

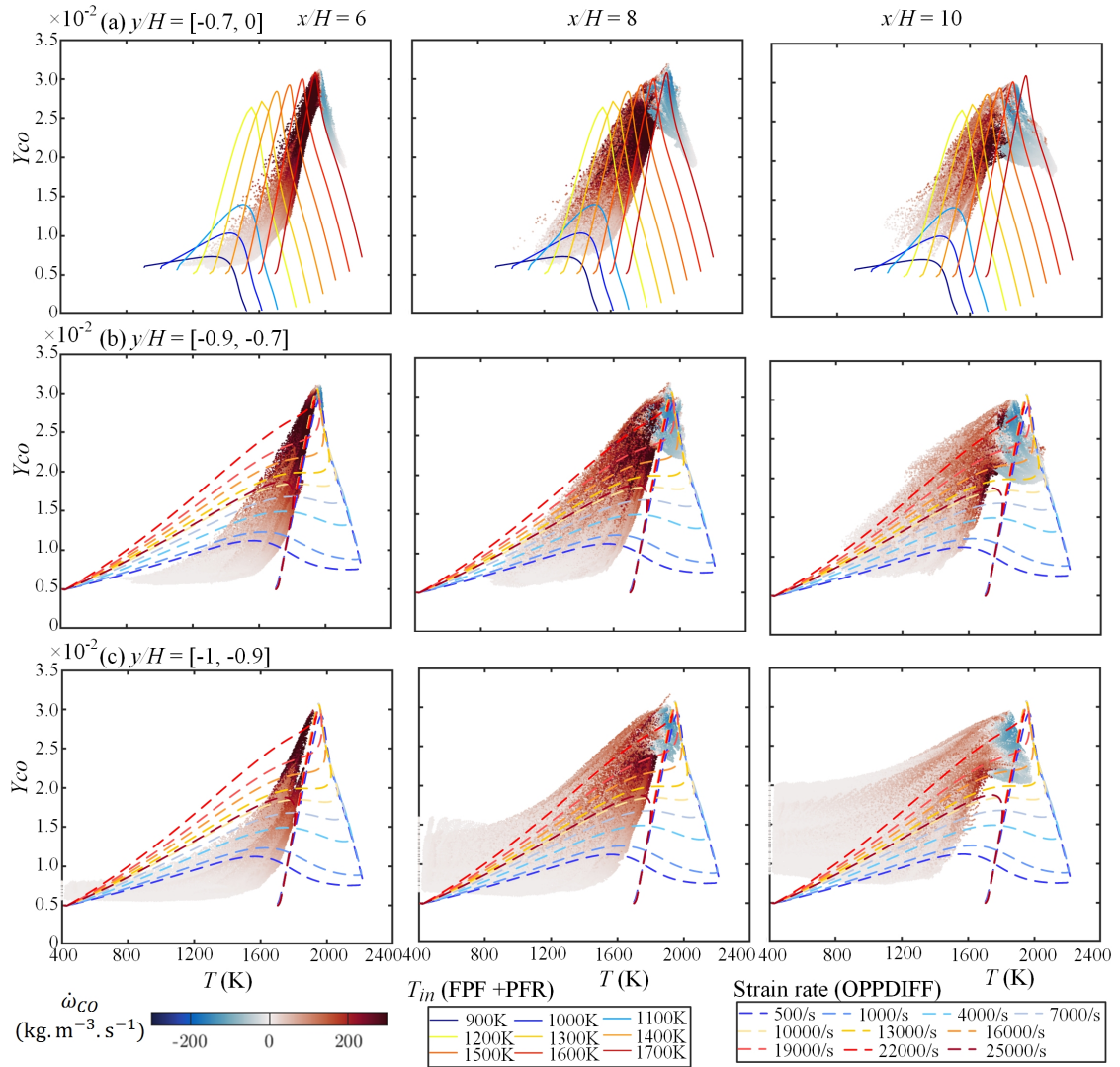


Figure 6.14: Scatter plots of CO mass fraction versus temperature at  $x/H = 6$ , 8 and 10. (a) Top row presents  $y/H = [0, 0.7]$ ; (b) Middle row presents  $y/H = [0.7, 0.9]$ ; (c) Bottom row presents  $y/H = [0.9, 1]$ . Scatter plots on the top row are overlaid with the results of 1D PFR and FPF simulations for  $\zeta = 0.7$  at the indicated reactants temperatures. Scatter plots on the middle and bottom rows are overlaid with the simulation results of a 1D OPPDIFF burner with inlet stream of 400 K and 1700 K and at the indicated strain rates.

By checking the features of these two sets of 1D solutions to understand the deviation, in addition to the features of the 1D model mentioned in Section 6.3.1, three 1D models use inlet boundary condition with imposed velocity, rather than the non-slip wall boundary condition. As such, the CO mass fraction at the inlet was constant for these three 1D models. The 1D head-on quenching manifold has a wall boundary but is constrained by the initial thermal boundary layer profile.

#### 6.3.2.5 CO Species Transport Budget

To examine the reason for the high CO mass fraction near the wall observed earlier in both instantaneous, time and spanwise-averaged results, a species transport budget of CO was analysed (see Figure 6.15). From the  $x - y$  contour in Figure 6.15(a), intermediate CO mass fractions ( $\approx 0.015$ ) can be found close to the wall from  $x/H = 9$  to 11. In this region, the reaction term,  $R$ , is almost zero, as shown in both  $x - y$  and  $y - z$  planes, leaving convection and diffusion to dominate the CO species transport. Due to the high streamwise velocity, the peak  $C$  is 3 times higher than the peak  $D$  and  $R$ , and dominates the CO transport in the main reaction zone and post-flame zone. The velocity vector is almost horizontal, although the flame can slightly bend the streamline as shown in the top-left corner contour.

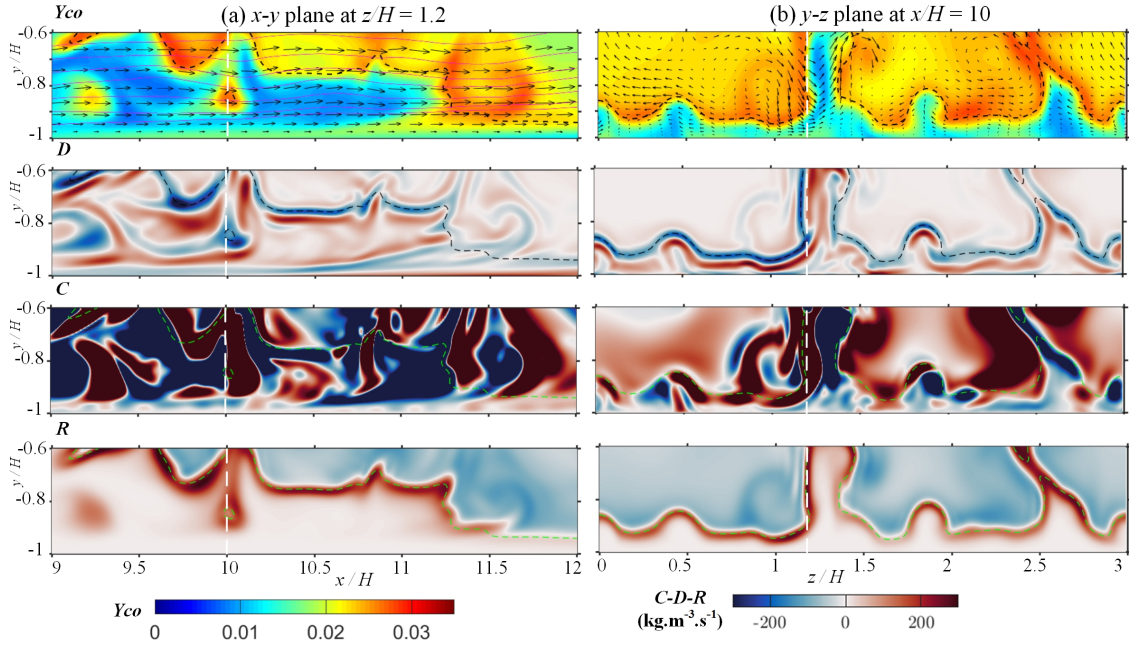


Figure 6.15: Contours of CO mass fraction (First row) and components of the species transport budget as indicated, taken at time =  $2.58 \tau_f$ . (a) Left column shows  $x - y$  plane at  $z/H = 1.2$ ; Solid lines in CO contour is the streamline. (b) Right column shows  $y - z$  plane at  $z/H = 10$ . The  $y$ -axis is magnified to accentuate the near-wall features. White dashed line indicated plot plane location. The velocity vectors in CO contours are calculated with the corresponding velocity components.

## 6.4 Conclusions

3D DNS with analytically reduced chemistry was used to simulate a turbulent flame-wall interaction for a  $\text{CH}_4/\text{air}$  mixture diluted by hot combustion products in a channel. The isothermal walls are at  $T_{\text{wall}} = 1200 \text{ K}$  and  $400 \text{ K}$  and were therefore referred to as hot and cold walls, respectively. In addition to the 3D DNS, 1D adiabatic freely propagating flame and plug flow reactor simulations were conducted under the same conditions as the 3D case at varied reactants temperatures.

The instantaneous results showed several key features: a main reaction front was present in the central region, supported by periodic bulk ignition events leading to forward and backward motion of the reaction front. A high amount of CO was produced during the bulk ignition event, as it changes the distribution of the main reaction zone, but these CO was significantly oxidised before reaching the domain exit. Near the cold wall, flame interaction with the thermal boundary layer was present up to the domain exit, thereby contributing to the exhaust CO. However, the

flame on the hot-wall side touches the wall, completing the combustion process (i.e. not quenching), and allowing CO oxidation to begin. Near-wall turbulence-flame interaction creates wrinkled and streaky flame surfaces. However, more planar-like flame structures are observed at downstream locations.

Time and spanwise-averaged results showed that the low temperature thermal boundary layer region near the wall becomes thicker before the flame touches, and then is compressed by the flame surfaces. High mean CO mass fraction locates in the free stream where the free-stream autoignition happens, while the high RMS of CO mass fraction is present closer to the wall.

The time and spanwise-averaged CO mass fraction and flux at the exit showed that the wall regions make up 25% of the total exit CO mass flux. The CO mass fraction near the cold wall was 15% higher than that on the hot-wall side.

The scatter plots of CO mass fraction versus temperature at several streamwise locations showed that the combustion processes span an ensemble of 1D flames at different initial temperatures and strain rates, except for a region within 0.1 channel half-width from the wall. Examining the species transport budget of CO showed that CO is dominantly formed due to the diffusion and convection in this region.

These results clearly demonstrate the challenges for modelling CO in the near wall region. While 1D manifolds might be suitable for modelling the changes of CO mass fraction from the centre of the domain up to a certain distance from the wall, in the vicinity of the wall other frameworks such as the species transport budget might be needed for modelling. Future works will focus on developing such models and assessing their performance using the DNS data. Furthermore, considering inhomogeneous mixing which is more relevant to practical applications is left for future work.

# Chapter 7

## Conclusions

### 7.1 Summary of Findings

Flame-Wall Interaction for methane/air flames diluted by hot combustion products was investigated. This study was conducted using Direct Numerical Simulation with one-dimensional head-on quenching, a two-dimensional laminar V-flame, and a three-dimensional turbulent V-flame in a channel. Autoignition in such combustion is inhibited by a cold-wall thermal boundary layer, either quenching the reactants, or transitioning to premixed flame propagation. Highly diluted, premixed flames can extinguish inside the thermal boundary layer, which can leave high near-wall CO. This results in disproportionate levels of CO mass flux in the near-wall regions.

The study on 1D HOQ in Chapter 4 investigated the effects on near-wall CO in FWI of several working parameters, including the dilution level, wall temperature and pressure. The CO species transport budget analysis was used to identify the dominant transport terms, and then an approximation for the near-wall CO was tested. Chapter 5 studied dilution level and wall temperature effects on near-wall CO in a 2D laminar V-flame for stationary and acoustically forced conditions. The effects of these parameters on CO was quantified by comparing the average CO mass fraction and integrated mass flux at the domain exit. The time-varying behavior of the near-wall CO oxidation was examined using a species transport budget analysis along streamlines. In Chapter 6, a diluted 3D turbulent channel flame was simulated with an analytically reduced chemical kinetic mechanism. A hot and a cold wall were



included in the domain to permit a comparison of hot and cold FWI. Autoignition and flame dynamics were presented with instantaneous and statistical results. The CO thermochemical state was examined to determine if a simplified 1D flamelet approach could be consistent for the near-wall CO modelling. Near-wall CO transport and turbulent mixing between reactants and products were examined to understand deviations in the near-wall CO thermochemical state from 1D manifolds.

The primary findings of this thesis are summarized as follows:

1. **High near-wall CO mass flux resulted from a combination of lower oxidation rates and later formation of CO, due to longer flames. This counteracted lower peak CO formation and lower equilibrium CO values found in diluted premixed flame propagation compared to autoignition of the same mixture.**

Autoignition is a necessary pre-condition in MILD combustion. In the 3D turbulent case, the autoignitive stabilisation zone moves upstream and downstream periodically, which affects the area of the interaction between the flame and thermal boundary layer. This upstream motion creates an area with high CO mass fraction in the bulk flow, which immediately begins to oxidise.

The combustion mode switches to premixed flame propagation after heat loss in the thermal boundary layer. Given the same reactant composition but lower temperature, a reduction of peak CO mass fraction can be observed in premixed flame propagation in 1D HOQ. This is related to a decrease in the CO formation rate in a cooled premixed flame compared to an autoignition of the same composition. In 1D opposed-flow flame simulations, the peak CO mass fraction in the cooled premixed flames demonstrates a greater reduction with increased strain rate than found for the autoignition of that mixture.

2. **At higher dilution level, both the CO formation and oxidation rates decrease, and the quenching distance increases.**

At higher dilution levels, the peak value of the average CO within the quenched region is smaller but oxidises more slowly. In the 2D laminar configuration, flame tips at higher dilution levels are more parallel to the wall, which enhances

the transverse diffusion of CO to the wall, and the flame length is shorter, resulting in longer CO oxidation time before reaching the exit.

**3. A lower wall temperature enhances the near-wall turbulence, inhibits MILD stabilisation, and attenuates near-wall CO oxidation.**

In the 2D laminar case, the wall temperature has a non-monotonic effect on the average CO mass fraction at the domain exit. Autoignition in MILD combustion can exist at the hot wall, completing the combustion process (i.e. not quenching), and a hot wall increases equilibrium CO and the exit-CO compared to the cold wall. At the cold wall, the flame extinguishes inside the thermal boundary layer without near-wall CO oxidation downstream, resulting in high CO at the exit. The flame is elongated at a lower wall temperature, thus reducing the CO oxidation time. In the turbulent case, the cold-wall flame is more wrinkled than the hot-wall flame and forms more localised high near-wall CO distribution.

**4. Thermal boundary layers attenuate laminar flame response to inlet forcing and laminarise the turbulent flame surface downstream.**

A low temperature region exists between the hot diluted reactants and the cold wall, similar to commonly thermal boundary layer. As the flame interacts with the thermal boundary layer, the thermal boundary layer is compressed by the flame fronts. The flame front is weakened downstream and finally quenched.

In the 2D laminar V-flame, the thermal boundary layer elongates the flame and reduces the CO oxidation time. The forced V-flames show that the thermal boundary layer attenuates the flame response by reducing the local Damköhler to be much less than 1, and also attenuates the downstream CO fluctuation. In the 3D turbulent configuration, the flame surface becomes more laminar downstream during FWI.

**5. 1D flame solutions might be sufficient for modelling CO in turbulent conditions in the free-stream region and some parts of the near-wall region, but not in the vicinity of the wall.**

In 3D, the thermochemical states of CO were examined at different stream-

wise locations. 1D flame solutions were used to interpret this data, including adiabatic, unstrained premixed flames at different reactant temperatures, and opposed flow, strained flames for various strain rates. The 3D diluted FWI data do not neatly collapse on to 1D manifolds, but span an ensemble of flames at different initial temperatures and strain rates, particularly near the wall. 1D adiabatic flames can capture the post-flame CO behaviour, while strain rate and heat loss effects need to be accounted for in the near-wall region to understand the autoignition process and the CO oxidation.

6. **In 1D HOQ, near-wall CO can be approximated with diffusion transport within certain regions, and higher dilution levels or lower pressures enlarge this region.**

In 1D HOQ, the near-wall diffusion dominates the CO transport. As a result, near-wall CO can be approximated with the integrated diffusion term only, without considering the reaction and convection. However, both diffusion and convection are important for near-wall CO transport in both 2D and 3D. Therefore, both diffusion and convection are required to approximate near-wall CO. In the 3D turbulent case, streamwise convection is much higher than diffusion, and thus it is necessary to take into account convection in modelling near-wall CO.

## 7.2 Discussion

The following aspects of this work are worth noting:

1. **Several turbulent mixing patterns exist near the wall due to coherent structures inside the thermal boundary layer, which could have a systematic impact on the CO behaviour.**

In the 3D turbulent configuration, a variety of turbulent mixing patterns are observed near the wall as shown in Figure 7.1, including reactants and products being convected towards each other (1, 2), weak mixing regions (3), and convection tangential to the flame fronts (4). When hot products are convected towards the near-wall reactants, ignition of the frozen reactants is promoted,

which increases the near-wall CO. This was also observed in the 1D opposed flow simulations in Section 6.3.1. Cooled near-wall reactants pushing towards the hot products region can push the flame front away from the wall, and leave higher amounts of near-wall UHC. These structures alter both the flame and CO characteristics, so it may be necessary to capture the statistical occurrence of these mixing patterns and quantify their separate impacts on near-wall CO for near-wall model development.

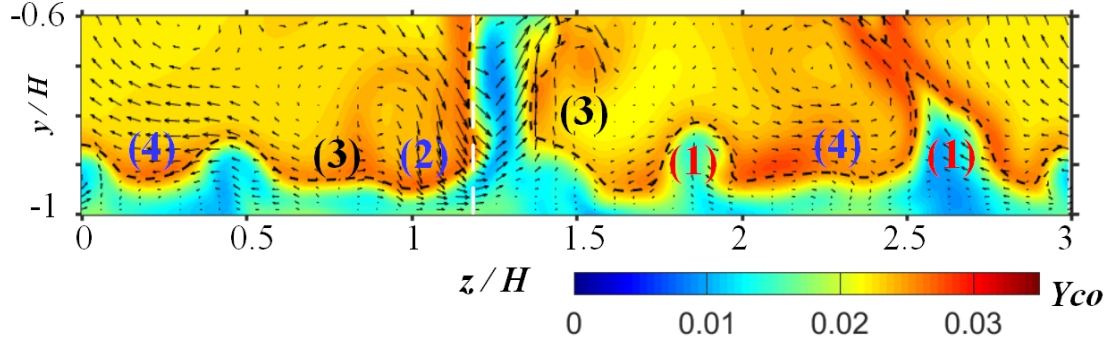


Figure 7.1: CO mass fraction ( $Y_{CO}$ ) contours taken on an  $y - z$  plane at  $x/H = 10$  and time =  $2.58 \tau_f$ . Locations (1) ~ (4) mark different mixing patterns. Dashed black lines indicate the flame fronts.

2. **Increasing  $\zeta$  leads to a shorter autoignition delay. This can lead to more upstream FWI and increase the time available for CO oxidation.**

While this work primarily focuses on the thermochemical impact of dilution on FWI, the effects of the recirculation rate on the physical location of the bulk flame stabilisation should also be considered as an important design optimisation parameter for CO minimisation. It has been demonstrated that the near-wall regions typically feature reduced CO oxidation rates, so, if FWI cannot be avoided, maximising the available residence time for CO oxidation can become an objective.

In a GT context, achieving increased  $\zeta$  comes at a penalty to combustor pressure loss due to increased recirculation required, and the increased mixture temperature may contribute to  $\text{NO}_x$  formation and increased thermal stresses on the walls. Optimising the flame-facing surface temperature of the thermal

barrier coatings may also provide a design parameter for CO minimisation.

### 3. Identifying the role of near-wall coherent structures inside the thermal boundary layers

Thermal boundary layers near cold walls increase the local turbulent intensity, which wrinkles the flame fronts. In this work, coherent structures have also been observed inside the thermal boundary layer, as shown in Figure 7.2. As both near-wall turbulence and these coherent structures can affect heat transfer and flame dynamics, quantifying their contribution to near-wall CO behaviour may be important in model development, as it is likely that near-wall modelling will not resolve these structures.

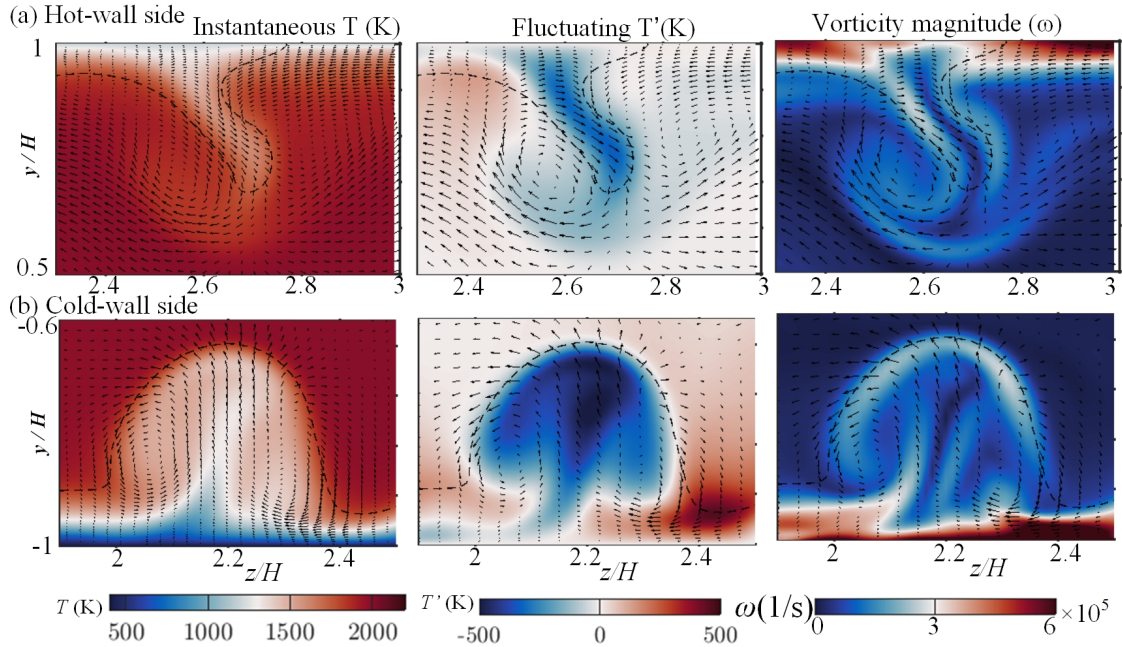


Figure 7.2: instantaneous temperature ( $T$ ), fluctuating temperature ( $T'$ ), and vorticity magnitude ( $\omega$ ) contours taken on a  $y - z$  plane near both the hot wall (top row) and cold wall (bottom row). Dashed black lines indicate the flame fronts.

Appendix A presents results of diluted FWI in HOQ for a stagnation burner. Several complementary conclusions are repeated here for completeness.

CO emissions increase with dilution levels up to  $\zeta = 0.6$  (the critical point of the transition from premixed flame propagation to autoignition), then slowly decrease beyond that point. Wall temperature does not significantly affect CO emissions. Increasing the wall temperature stabilises the low dilution level cases. The inlet ve-

locity can decrease CO emissions in premixed cases, but then for the MILD cases the CO emissions increase with the inlet velocity. CO emissions in MILD condition are less sensitive to changes in the inlet velocity than premixed flames. Higher pressure advances the autoignition, and shifts peak CO to the lower dilution levels.

## 7.3 Recommendations for Future Work

### 1. Near-wall CO modelling

- (a) It would be valuable to test existing tabulated chemistry approaches on the data generated in this work. The present results show that heat loss, stretch, 3D mixing and diffusion affect the performance of tabulated chemistry, consistent with References [46, 96]. Further testing is required to examine whether existing approaches such as FGM and REDIM can sufficiently model the CO behaviour.
- (b) As near-wall CO is generally dominated by convection and diffusion in 2D and 3D flows, it is hypothesized that a model of near-wall CO could be developed provided it has sufficient fidelity of these species transport terms. This is a non-trivial exercise where the convection models employed in RANS and LES approaches may not capture the flow feature details nor the coupled wall heat-transfer impacts on local density. Further, the molecular diffusion models are often very simplified in the bulk flow, where turbulent diffusion dominates. The data provided in this work can provide training data to explore which simplifications permit a sufficient description of the near-wall  $C$  and  $D$  for CO.

In addition, defining the spatial region of applicability for any developed model appears to be necessary, as shown in Section 4.4.3. This may require local determination of the flame-wall distance, further increasing the challenge of near-wall modelling, particularly where the flame is not resolved.

### 2. Deeper exploration of pressure effects on turbulent, diluted FWI.

High pressure combustion is the norm in the GT context. The present study

changed the pressure in 1D simulations, including the 1D HOQ and stagnation model. In 1D HOQ, the quenching distance and near-wall CO reduction rate reduce with increasing pressure. In a steady stagnation model, higher pressure advances autoignition, and shifts peak CO to lower dilution levels. Also, higher pressure results in a smaller flame thickness, and thus needs finer grid size to resolve. In 2D and 3D cases, higher pressure decreases the gas viscosity and can compress the boundary layer, and reduce the near-wall CO oxidation. The lower viscosity increases the Reynolds number and further changes the turbulence-chemistry interaction.

Therefore, pressure effects on CO formation and oxidation from diluted combustion should be systematically explored for the turbulent FWI case, particularly contrasting the hot and cold-wall effects.

### **3. NO effects on the near-wall autoignition.**

Trace NO concentrations (about 50 ~ 200 ppm) can have significant impact on low-temperature autoignition [107]. The EGR gases contain such levels of NO near the quenching position as shown in Section 4.3. Hence, the role of NO chemistry should be explored for the cold and hot-wall FWI in these conditions. However, this then requires  $\text{NO}_x$  kinetics to be included in the chemical mechanism, significantly increasing computational cost. NO effects can be systematically studied in 1D HOQ or CHEMKIN models first to find the suitable detailed chemical mechanism. Afterwards, an analytical reduced chemical mechanism can be generated with this detailed mechanism.

### **4. Exploration of CO oxidation in the cold-wall FWI after completion of fuel consumption**

Unburned gas exists inside the thermal boundary layer at the exit on the cold-wall side of the present 3D case. A longer domain could enable quantification of the final wall effect on exhaust CO. It is expected to consume more UHC inside the thermal boundary layer with a longer domain, due to the turbulent mixing and flame stretch as shown in 3D instantaneous results (see Figure 6.15) and OPPDIFF results (see Figure 6.3). However, a longer domain requires more computational cost. An intermediate wall temperature increases the CO

oxidation rate, and allows the reactants burn more completely within limited domain length could also achieve this goal.

## **5. Determine the role of surface chemical kinetics on CO oxidation**

In gas turbines, the wall temperature can reach well over 1000 K, and the surface cannot be treated as inert at such temperatures [17, 19, 20, 108]. At hot-wall conditions, the H radical adsorption retards autoignition [108]. Therefore, the surface chemical kinetics should be considered at the hot wall.

This is particularly of interest to determine under what conditions a hot wall could quench the autoignition processes. Further, downstream of the FWI, the surface reactions can alter the local OH concentrations, which is key to the CO oxidation process.

Currently, only the platinum surface mechanism has been used, in [17, 20]. Radical effects could be considered by a radical recombination surface as per [20, 108]. This allows the identification of the role of specific radical adsorption and desorption effects on autoignition and near-wall CO.

## **6. Stoichiometry, fuel types and diluents with different flame speed and autoignition limits**

Lean combustion is common in industrial gas turbines to reduce emissions. The current work is undertaken with stoichiometric methane mixtures, so globally lean combustion should be explored to determine if there are significant kinetic differences, particularly in combination with the above questions. Due to the lower flame temperature, CO<sub>2</sub> dissociation is inhibited, while the oxidation rate also reduces, similar to with a higher dilution level. However, the O<sub>2</sub> concentration increases, which can bring different CO oxidation behaviors. In addition, the flame gets thicker at a leaner condition, which can alter the turbulence-flame interaction.

Gaseous GT fuels with different autoignition and premixed combustion properties could also be explored, such as Dimethyl Ether (DME) or hydrogen-methane blends. DME features single or two-stage ignition, and has a negative temperature coefficient regime. Therefore, the autoignition behaves differ-



ently from methane. Hydrogen features high diffusivity. The present transport budget showed that the diffusion and convection dominate the near-wall CO. Therefore, CO generated from hydrogen-methane combustion may be altered by this  $H_2$  diffusivity.

In addition, the composition of the diluents in the combustion products can alter both the thermodynamics and chemistry of the dilution, as reviewed in Section 2.3.1.1. Minor radicals promote autoignition,  $CO_2$  and  $H_2O$  alters the radical pool, and may further affect the CO net production rate. These aspects deserve systematic study.

## 7. Configurations with inhomogeneous mixing

JICF and JHC configurations are common in the application of dilution with combustion products. For example, in the Ansaldo GT26, a JICF configuration exists in the mixing lance, and the FLOXCOM combustor uses JHCs to entrain the hot products to the fresh reactants.

Similar simulations as those performed here can be explored in the these two configurations, to determine if mixing and non-premixed combustion processes influence the emissions. Minamoto et al. showed that both premixed flame propagation and reaction-dominated regions exist in such in-homogeneous mixing configuration [61]. In addition, an inhomogeneous field may feature different quenching modes. Section 4.3.4 showed that a hot products near the wall promotes near-wall CO oxidation, by pushing the reaction zone away from the wall and reducing the near-wall equilibrium CO. The inhomogeneous field can create localised high CO regions or UHC pockets, and this could affect exhaust emissions.

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# Appendix A

## CO Emission of Premixed and Diluted Flames in a Stagnation Burner

In Chapter 4, 1D HOQ was used to study the transient flame-wall interaction for flames diluted by the hot combustion products. In this configuration, the reactants are initialized next to the wall without a convective flow.

In this chapter, results are included from a paper presented at the 20<sup>th</sup> Australasian Fluid Mechanics Conference in Perth, Australia (5-8 December 2016), titled “CO Emission of Premixed and Diluted Flames in a Stagnation Burner” by B. Jiang, R. Palulli, J.E. Rivera, R.L. Gordon, and M. Talei [97]. A 1D axisymmetric premixed stagnation flame was used, which is simplified from a 3D laminar solution based on the similarity in a stagnation flow [85]. This model is verified with experimental data from Bergthorson [109]. The gases next to the wall are combustion products ( $\zeta = 1$ ), and the main reaction zone was pushed towards the wall at different strain rates. It permits the study of strain rate effects on diluted flames and the corresponding impact on near-wall CO emissions. The effect of dilution level, inlet velocity, wall temperature and pressure were investigated.

## A.1 Numerical Model

The CHEMKIN PRO software package [85] was used to perform the simulations. The governing equations for the stagnation-flame reactor model were those used in the Opposed-Flow Flame Model [110]. The axisymmetric geometry consisted of a nozzle and a stagnation plane normal to the flow. The computational domain was 2 cm long. The wall was considered to be inert with a constant temperature. For the inert wall the species boundary condition on the wall satisfies a zero species flux. The simulations were run on adaptive grids to ensure adequate resolution. To calculate the exhaust composition, a cylindrical control volume which extends from the nozzle exit up to the wall was used [111]. As a result, the mass flux  $\dot{m}_{exh,\alpha}$  of a species  $\alpha$  exiting the cylinder is:

$$\dot{m}_{exh,\alpha} = \sum_{i=1}^N [2\rho_i \frac{v}{r} Y_{i,\alpha} \Delta x_i] \quad (\text{A.1.1})$$

where  $N$  is the total number of cells,  $\rho_i$  is the mixture density at the  $i$ th cell,  $Y_{i,\alpha}$  is the mass fraction of a species  $\alpha$ ,  $\Delta x_i$  is the length of the  $i$ th cell, and  $v/r$  is the scaled radial velocity by the radius  $r$ , which is a function of  $x$  alone. The mole fraction  $X_{exh,\alpha}$  of a species  $\alpha$  at the outlet is:

$$X_{exh,\alpha} = \frac{\dot{m}_{exh,\alpha}/MW_{\alpha}}{\sum_{i=1}^N [2\rho_i \frac{v}{r} \Delta x_i/MW_{mixture,i}]} \quad (\text{A.1.2})$$

where,  $MW_{\alpha}$  is the molecular weight of a species  $\alpha$  and  $MW_{mixture,i}$  is the mixture molecular weight at  $i$ th cell.

## A.2 Chemical Kinetics Model

Methane was used in this study. The gas-phase oxidation of methane was described by GRI3.0 chemical mechanism with its corresponding thermodynamic and transport databases [44]. This mechanism has been optimized at lean-to-stoichiometric fuel mixtures, over a wide range of pressures and residence times. All simulations were performed at atmospheric pressure except where noted. Mixture-averaged transport properties were used. The Soret effect was considered for all cases.



### A.3 Verification of the Numerical Model

To verify the numerical model, simulation results from Sidey et al. and Bergthorson were reproduced showing good agreements [57, 109]. The simulation results from a PFR model are shown in Figure A.1. The temperature gradient in the flame zone decreases with increasing dilution level, leading to a widening of the reaction zone, and therefore inducing a decrease of peak CO emissions and an increase of the CO before ignition.

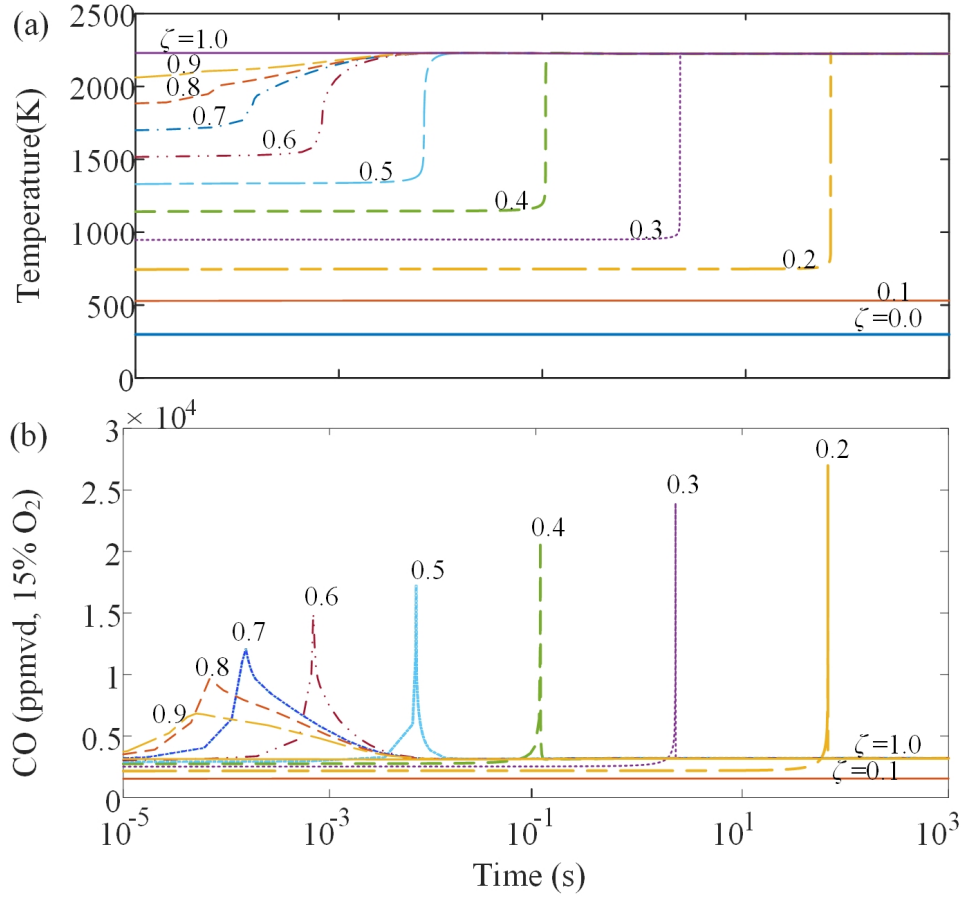


Figure A.1: Temperature (a) and CO evolution on a dry basis, corrected to 15 % $O_2$  (b) of mixtures diluted by hot products at different dilution levels (marked on the plots) in a PFR.

## A.4 Results

### A.4.1 Effects of Dilution Level

The temperature profile for different dilution levels at 300 K wall temperature is shown in Figure A.2 (a). The inlet velocity is  $10 \text{ m.s}^{-1}$  for all cases. There is no ignition for  $\zeta = 0.0, 0.1$  and  $1.0$ , as the residence time of the  $\zeta = 0.0$  and  $0.1$  cases is too short, and there is only pure hot products for the  $\zeta = 1.0$  case. For lightly diluted mixtures ( $\zeta = 0.2$  to  $0.5$ ) ignition events are characterized by a sharp jump from the preheated temperature to the adiabatic flame temperature, similar to a conventional premixed flame. At higher levels of dilution ( $\zeta = 0.6$  to  $0.9$ ), there is a gradual change in temperature. The ignition of the  $\zeta = 0.6$  case is significantly advanced compared to  $\zeta = 0.5$  case, which suggests that, between  $\zeta = 0.5$  and  $0.6$ , there is a transition to MILD combustion. In addition, for  $\zeta = 0.6$ , the inlet temperature is above 1504 K, and the oxygen mole fraction is less than 8 %, also indicating that the flame is in MILD combustion region, matching the observations of Sidey et al. [57].

The peak temperature is almost the same from  $\zeta = 0.6$  to  $0.9$  (Figure A.2 (a)). The diluents are hot combustion products at 2226 K adiabatic flame temperature. For cases with low level of dilution ( $\zeta < 0.5$ ), the post-flame reactions do not have sufficient time to reach equilibrium due to the quenching at the wall. From the CO mole fraction profile as shown in Figure A.2 (b), the peak CO mole fraction decreases with increasing dilution levels, due to the increasing post-flame zone, the main region where CO emissions are oxidised [4].

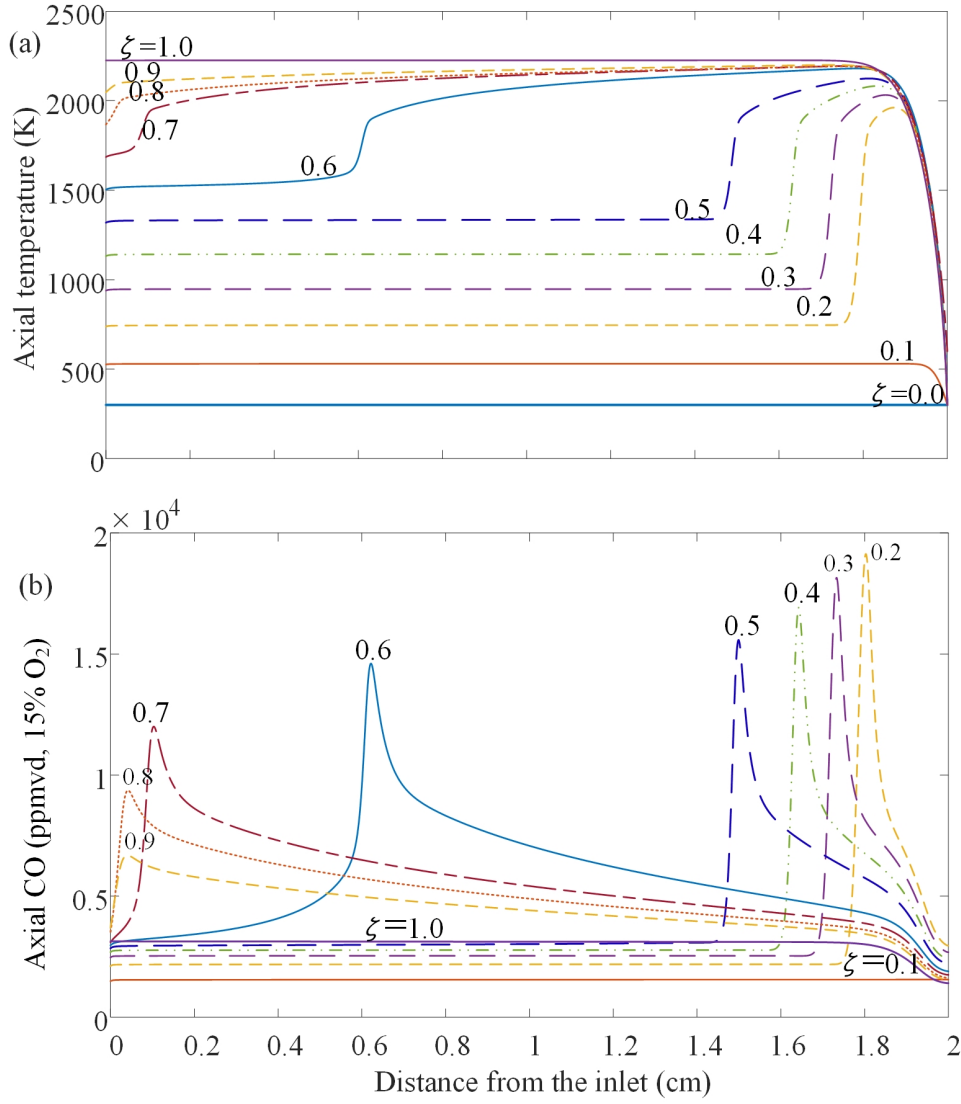


Figure A.2: Temperature (a) and CO emissions (b) on a dry basis, corrected to 15 % O<sub>2</sub> profiles from nozzle exit (0 mm) to the wall (2 mm) at different dilution levels (marked on the plots) and 300 K wall temperature, 10 m.s<sup>-1</sup> inlet velocity

Using Equation A.1.2, the exhaust CO emissions at different dilution levels are shown in Figure A.3. It shows that the CO emissions increase with the dilution level from 0.1 to 0.6. Since the ignition delay time decreases with increasing the dilution level, the residence time of the products in a high temperature regime increases with increasing the dilution level. This may promote the dissociation of CO<sub>2</sub> into CO. In addition, by increasing the dilution level, the CO<sub>2</sub> mole fraction increases and the O<sub>2</sub> mole fraction decreases, which reduces the net rate of CO oxidation. However, the trend changes direction from premixed to MILD combustion. This is because the residence time of products under high temperature for MILD cases is nearly

the same as shown in Figure A.2, but the peak CO generated in the flame front decreases with increasing the dilution level.

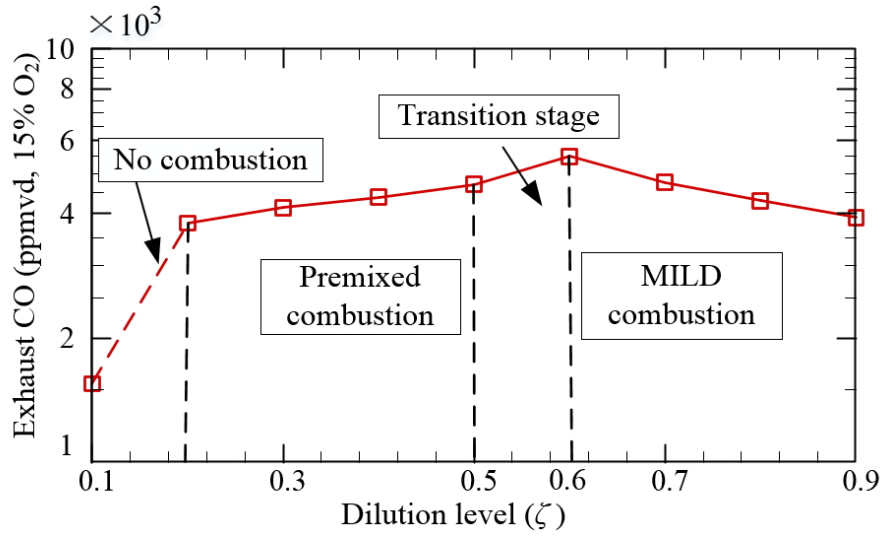


Figure A.3: Exhaust CO emissions on a dry basis, corrected to 15 % O<sub>2</sub> with different dilution levels at 300 K wall temperature, 10 m.s<sup>-1</sup> inlet velocity

#### A.4.2 Effects of Wall Temperature

The stagnation wall is inert, which means there are no surface reactions. The wall temperature ( $T_{wall}$ ) was set to 300 K, 600 K and 900 K. The dilution level was varied from 0.1 to 0.9. The exhaust CO mole fraction at different wall temperatures is shown in Figure A.4. The CO emissions increase with increasing dilution levels in the premixed cases and decrease in MILD cases, which is the same trend as shown in Figure A.4. At each dilution level, the CO mole fractions are almost identical, apart from the strain-extinguished solutions at  $\zeta = 0.1$ . At the inlet velocity of 10 m.s<sup>-1</sup>, the  $\zeta = 0.1$  case is strain-extinguished for  $T_{wall} = 300$  K and 600 K, but has an ignited solution for 900 K. This may be induced by the decrease of the near-wall temperature gradient so that the reactant can accumulate the minimum ignition energy. These results might be different if we do not assume inert wall boundary conditions. As reported by Popp and Baum [41], at a higher  $T_{wall}$ , the surface reaction and thermal diffusion can play a significant role.

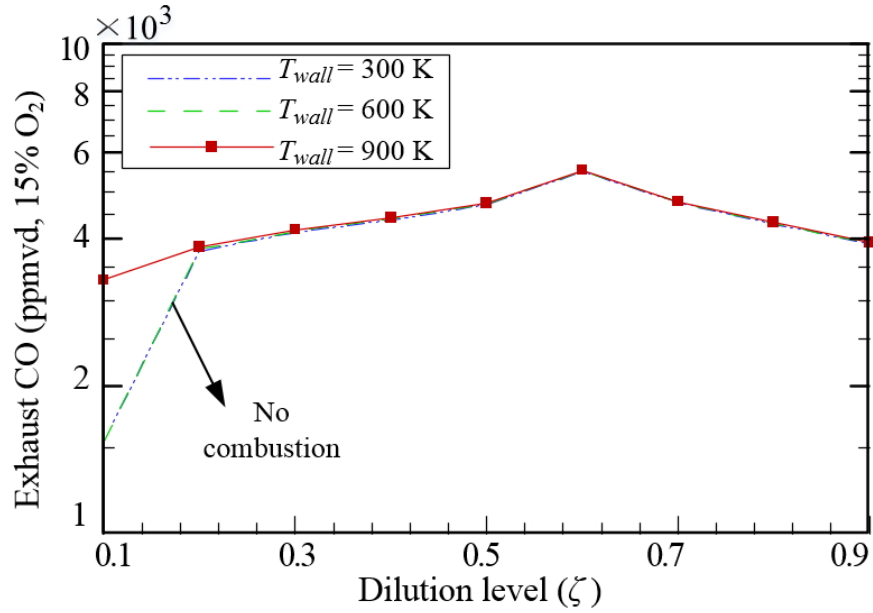


Figure A.4: Exhaust CO emissions on a dry basis, corrected to 15 % O<sub>2</sub> with different wall temperatures at 10 m.s<sup>-1</sup> inlet velocity.

#### A.4.3 Effects of Inlet Velocity or Strain Rate

To study the effect of the inlet velocity on MILD combustion and FWI, the inlet velocity was set to 10 m.s<sup>-1</sup>, 15 m.s<sup>-1</sup> and 20 m.s<sup>-1</sup> at a constant 300K wall temperature, with dilution levels from 0.1 to 0.9. The exhaust CO mole fractions with different inlet velocities at 300K wall temperature are shown in Figure A.5. It can be seen that all solutions are strain-extinguished at  $\zeta = 0.1$ . The 10 m.s<sup>-1</sup> case has an ignited solution from  $\zeta = 0.2$ , the 15 m.s<sup>-1</sup> case has an ignited solution from  $\zeta = 0.3$ , and the 20 m.s<sup>-1</sup> case has an ignited solution from  $\zeta = 0.4$ . The CO emissions decrease with increasing inlet velocity in premixed cases, but then for the MILD cases they increase with the inlet velocity. For premixed cases, increasing the inlet velocity forces the flame close to the cold wall, leading to the decrease of the peak temperature which inhibits the dissociation of CO<sub>2</sub> into CO. For MILD cases, the flame front is far away from the wall, so the peak temperature changes little at different inlet velocities. However, the width of the CO profile increases with increasing the inlet velocity, which induces the increase of CO emissions. CO emissions in MILD are less sensitive to the inlet velocity than the premixed flames

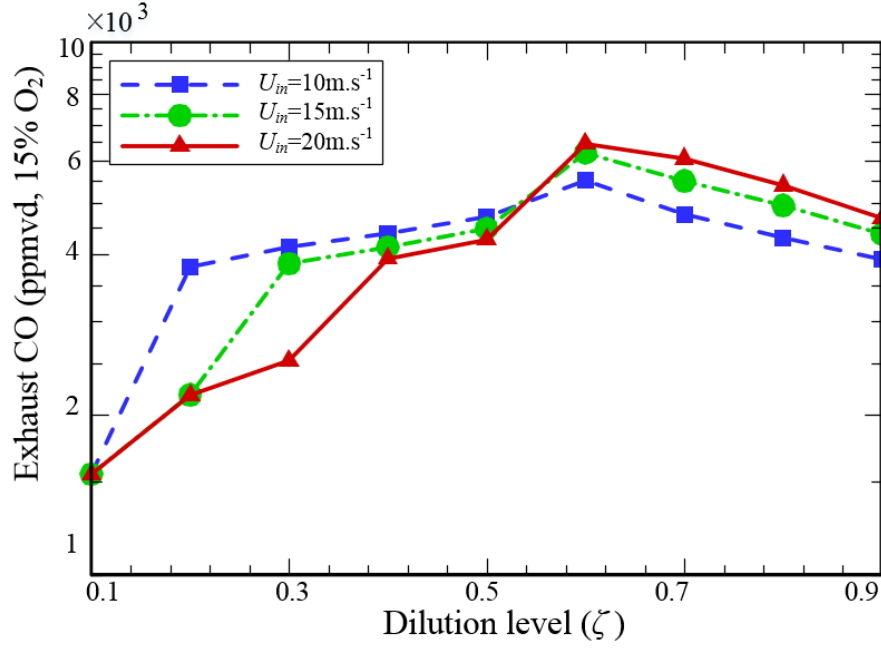


Figure A.5: Exhaust CO emissions on a dry basis, corrected to 15 %  $\text{O}_2$  with different inlet velocities at 300 K wall temperature.

#### A.4.4 Effects of Pressure

The ambient pressure was set to 1 atm, 2 atm, 4 atm, 8 atm, 16 atm and 32 atm. Figure A.6 shows that at  $\zeta = 0$ , there is no ignition except for at  $p = 32$  atm, as the minimum ignition energy decreases with the increase of the ambient pressure [112]. At the same dilution level, the CO emissions decrease with increasing pressure, likely due to the inhibition of  $\text{CO}_2$  dissociation. With increasing dilution levels at fixed pressure, the CO increases and then decreases, similar to Figure A.3. The peak CO corresponds to the transition point from premixed flame propagation to autoignition. Thus, higher pressure advances the autoignition, and shifts the peak CO to the lower dilution levels.

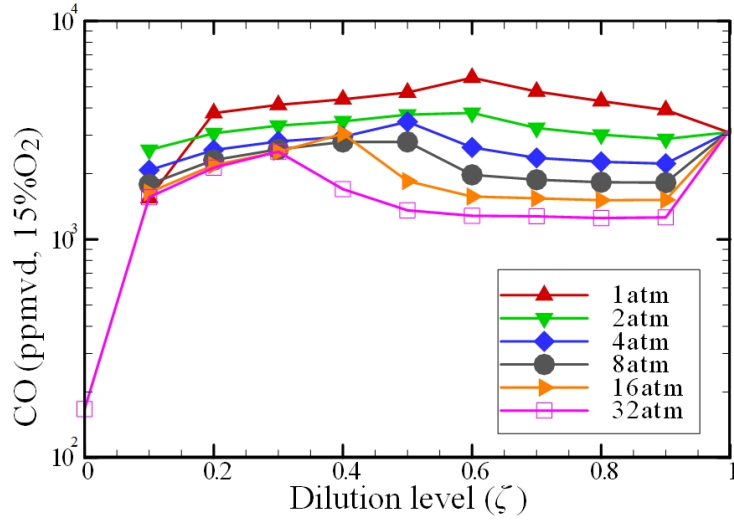


Figure A.6: Exhaust CO emissions on a dry basis, corrected to 15 %  $O_2$  with different pressure at 300 K wall temperature.

## A.5 Conclusion

The CO emissions behaviour of premixed and MILD flames have been investigated using a CHEMKIN stagnation burner geometry. The effects of the dilution level, wall temperature and inlet velocity were studied. It was observed that the CO emissions increase with dilution levels up to  $\zeta = 0.6$  (the critical point of the transition from premixed flame propagation to autoignition), then slowly decrease beyond that point. Wall temperature does not significantly affect CO emissions. Increasing the wall temperature does stabilise the low dilution level cases. The inlet velocity can decrease the CO emissions in premixed cases, but then for the MILD cases the CO emissions increase with the inlet velocity. CO emissions in MILD condition are less sensitive to the inlet velocity than the premixed flames. Higher pressure advances the autoignition, and shifts the peak CO to the lower dilution levels.